Russian Academy of Sciences Joint Institute for High Temperatures RAS Institute of Problems of Chemical Physics RAS

Kabardino-Balkarian State University



### XXVIII International Conference on

# Interaction of Intense Energy Fluxes with Matter

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### **Book of Abstracts**

Moscow & Chernogolovka & Nalchik 2013 The book consists of the abstracts of oral and poster contributions to the XXVIII International Conference on Interaction of Intense Energy Fluxes with Matter (March 1–6, 2013, Elbrus, Kabardino-Balkaria, Russia). The reports are devoted to the present-day investigations in the field of physics of high energy densities. The following questions 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 and detonation physics; equations of state and constitutive equations for matter under extreme conditions at high pressures and temperatures; low-temperature plasma physics; issues of physics and power engineering, technology projects.

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#### POWER INTERACTION WITH MATTER

#### VISCOSITY AS AN INDICATOR OF NON-IDEALITY OF STRONGLY CORRELATED SYSTEMS

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Viscosity is considered as an indicator of non-ideality of strongly correlated systems.

#### LASER FUSION—50 YEARS OF HISTORY

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This presentation is devoted to marked the exclusive direction among contemporary physical investigation, namely, laser fusion. This topic connected to 90 anniversary of academician N.G. Basov, who was the first has indicated the possibilities to ignite thermonuclear reactions by the means of laser energy. The history review of such kind of investigations is given in this presentation. It is essentially, that the contemporary problems will be resolved by means of previous studies. The key ideas are: spherical compression of thin shells, indirect (through a heat radiation) way to compress and ignite a fuel, fast ignition conception in various forms. The contemporary situation in laser fusion studies (like NIF, for example) will be discussed.

#### APPLICATION OF A LASER INTERFEROMETER AND APPLICABILITY OF AN ACOUSTIC APPROACH IN STUDYING SHOCK-WAVE SPALLATION PHENOMENA

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Method of laser interferometry is widely used in studying the spallation phenomena [1-4]. Often, when in interpreting the obtained results the formulas without substantiation of their applicability in a particular case, which is usually not considered the time response of interferometer. It can lead to incorrect interpretation of experimental data. Accordingly, this report contains the detailed analysis of the characteristics of laser interferometer to study shock wave processes in region of sub nanosecond duration. The results of measurements with laser interferometer are in base of the definitions of spall strength and strain rate the investigated material [5]. The analysis of shock wave interaction leading to spallation, essentially use the acoustic approximation. This approach was first proposed [6] for interpretation spallation phenomena in case of using explosive propellant systems to conduct research in microseconds and sub microsecond shockwave exposure durations. In this case, application of this approximation is justified in most cases. Currently, analysis of experimental data leads to the need to consider the applicability of the acoustic approximation in the case studies of mechanical properties of matter in case of using high amplitude nanosecond and sub nanosecond pressure duration. The report contains an analysis of this problem and a way of tackling them.

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#### NEW EXPERIMENTAL DATA OF SPALLATION PHENOMENA OF MATTER IN THE FIELD OF NEGATIVE PRESSURES CREATED BY MEANS OF 70 PICOSECOND LASER PULSE

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The experimental studies of spallation phenomena and dynamic mechanical strength of aluminum, alloy AMg6M, tantalum, wolfram, silicon, copper, lead and polymethylmetacrilat at the influence on them of laser pulse with duration 70 ps are presented. It was realized the strain rate up to  $4 \cdot 10^8 \text{ s}^{-1}$ . In these experiments, we used the neodymium glass laser Kamerton-T facility. The basic radiation was transformed to the second harmonic with the wavelength of 0.527 mkm and the laser pulse energy of 1.5 J. Irradiated spot on a target surface was of 0.2 to 0.8 mm in diameter. Then the maximum energy density of the laser radiation flux in the focal area was  $6 \cdot 10^{13}$  W/sm<sup>2</sup>, the ablation pressure was about 1.35 TPa. Targets had the form of plates with 50 to 220 mkm thickness. The spall phenomenon was used to obtain data on the dynamic mechanical strength of the materials under study. This phenomenon arises on the rear (free) side of a target as a result of the reflection of a compression wave caused by laser radiation. Due to the reflection, the free surface of the target is pushed into motion, which initiates the propagation of a tension wave in the opposite direction. As a result, in some plane of the target the tensile strain can exceed materials strength. This leads to the formation of the spallation layer that leaves the sample. To determine the time point of spall layer separation, the electrocontact method of measuring its velocity was employed. The results show that the dependence of spall strength of materials versus strain rate in moderate amplitudes of the shock wave impacts is in accordance with the well-known literature data. At high pressures a sharp increase of spall strength is observed, which indicates the strengthening of the material. The results of experiments confirmed the conclusion that the dynamic strength of the substance substantially depends on the amplitude and duration of the shock-wave influence on a target.

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#### SIMULATION OF FEMTOSECOND LASER ABLATION OF GOLD INTO WATER

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Laser ablation of solids in liquids is now widely used to produce colloidal nanoparticles that have found numerous applications in different areas. In experiments, the nanoparticles of different materials can be easily obtained by using laser systems with different parameters such as pulse durations, shapes, wavelengths, and fluences. In this work, we perform simulation of subpicosecond laser ablation of gold target into water. Numerical modeling of the ablation process during several nanoseconds shows that most part of the nanoparticles originates from the ablated metastable liquid layer, while only minor part is formed by condensation in overcooled gas phase. These particles will further grow/evaporate, and coagulate during much longer collision stage in the liquid colloid. The results of simulation explain the bimodal distribution of nanoparticles in solutions observed in experiment [1].

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#### THE COMPARISON OF HYDRODYNAMIC AND ATOMISTIC APPROACHES FOR MODELING OF LASER ABLATION OF METALS

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A numerical modeling of interaction of femtosecond laser pulses with metals is performed. Two methods are used: (i) a two-temperature onevelocity hydrodynamic model [1] and (ii) a combined model, which is based on the molecular-dynamics approach for ions and on the heat conduction equation solution for electrons (MD-TTM) [2]. These two models take into account electron-phonon coupling, laser energy absorption and electronic heat conductivity. The Thomas–Fermi model for electronic subsystem is used in both models, while the ionic subsystem is described by a multiphase equation of state in the first method, and by the EAM-potential in the second one. The vulnerabilities of the hydrodynamic approach are kinetic processes of spallation and phase transitions while the MD-TTM approach does not take into account the electronic pressure and ionization. Comparison of these two approaches with the experimental findings shows the domain of applicability of both methods.

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#### MELTING KINETIC EFFECTS IN METALS INDUCED BY A FEMTOSECOND LASER PULSE

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Melting of metals induced by a femtosecond laser pulse represents a non-equilibrium process specified by the following factors. First, by the time of a few picoseconds the solid and liquid phases are not reaching the equilibrium yet, that is why it is of importance to take into account the kinetics of melting [1, 2]. Second, at the initial stage of melting and medium evolution the temperature of electrons is significantly higher than that of the ions one. This difference may lead to the increasing of the crystal melting temperature [3–5], and also to more complex relations between the temperature of electrons and ions and the transport coefficients (permittivity, thermal conductivity, electron-ion exchange). We have investigated the influence of these effects on the temperature of electrons and ions of an aluminum target using the two-temperature model [6]. We used a simple kinetic model based on the evaluation of the overheated crystal lifetime and the assumption that after that time the melting process will be instantaneous. We estimated the increasing of the melting temperature by means of quasi-harmonic model and Lindeman criterion, and the equation of state for electrons and spinodal parameters of the crystals by means of numerical modeling using the density functional theory and quantum molecular dynamics method (VASP [7], quantum-espresso [8]). The equation of state for ions is semiempirical. We provided the analysis of kinetic effects of melting of an aluminum target induced by a femtosecond laser pulse for variety of intensities.

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#### SOME FEATURES OF INTENSE LASER DRIVEN SHOCK PROPAGATION IN STRUCTURED TARGET

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The investigation of matter under extreme pressure conditions is a subject of great interest in several branches of physics including studies equation of state (EOS) measurements, phase transformations, laboratory simulation of high energy density astrophysical phenomenon, inertial confinement fusion, materials science, etc. Pressures higher than few tens and even hundreds of Mbars have been generated by high-power pulsed lasers [1–3]. However, at laser high intensities collective laser absorption processes dominate generating hot electrons and hard X-rays, leading to preheat and cause difficulty in creating high target compression. From other hand the general limitations of shock-wave compression is that shock waves compress and heat the material at the same time, so pressure and temperature are not independent variables. Thereby only data on the Hugoniot curve of the material can be obtained. To obtain higher pressures with lower temperatures and as much as possible to use the impedance mismatch effect of the pressure amplification we consider constructing 3-layers structure, where a low shock impendence material sandwiched between two high shock impendence material layers. To find the optimal conditions of considered effect we have realised a number of numerical simulations (using 1D and 2D hydro-code MULTI [4]) for the sandwiched material with equation of state and opacities data from standard libraries (we have used

gold, aluminium, carbon, and plastic).

The work was partially supported by ESF (SILMI, 3964) and RFBR (11-01-00707, 12-01-96500).

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#### LASER AND WAKEFIELD DYNAMICS IN GUIDING STRUCTURES UNDER NONSYMMETRICAL COUPLING CONDITIONS, RELEVANT TO EXPERIMENTS ON ELECTRON ACCELERATION

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Use of guiding structures like capillary waveguides and plasma channels is promising tool for creation of long-length linear plasma wave behind laser pulse of moderate intensity. Such plasma wave can be used for production of high-quality accelerated electron bunches (with minimum energy and spatial spreads) in the scheme of multi-stage acceleration of electrons to high energies.

For practical implementation of such scheme the wakefield structure inside guiding system (capillary of channel) should be regular enough for achieving of high quality of accelerated electron beam. Dissymmetry of focusing of laser pulse into the guiding structure, which always takes place in real experiment, can considerably influence on the structure of wakefields behind the pulse [1, 2], and therefore should be controlled carefully.

Presented work contains analyses of the influence of dissymmetry of laser pulse focusing into guiding structures (capillary waveguides or plasma channels) on the wakefield structure and conclusions about maximum adoptable dissymmetry, under which effective electron acceleration is still possible.

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#### MONOENERGETIC ACCELERATION OF ELECTRONS INJECTED INTO A WAKE WAVE

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The trapping and acceleration of nonmonoenergetic electron bunch in a wake field wave generated by a short ( $\tau_L = 100$  fs) pulse from a Ti:Sa laser with wavelength  $\lambda_0 = 0.8 \mu m$ , a power of 78 TW, and focusing spot radius  $r_L = 68 \mu m$  in a plasma channel with a plasma density at the channel axis  $n_0 = 1.75 \cdot 10^{17} \text{ cm}^{-3}$  is studied by numerical simulation [1]. Electrons are injected into the region of the wake wave potential maximum at a velocity lower than the phase velocity of the wave. The injected electron bunch is characterized by a mean electron injection energy  $E_{inj} = 1.65mc^2$ ; the electron distribution over energy and space is assumed to be Gaussian. The bunch duration (FWHM) was 500 fs, which corresponds to standard deviation  $\sigma_{z,inj} = 51 \mu m$  in the electron distribution over the bunch length; the corresponding distribution of bunch electrons in the transverse direction is characterized by  $\sigma_{x,inj} = \sigma_{y,inj} = 50 \mu m$ . It should be noted that the length of such bunch is larger than wake wavelength  $\lambda_p = 80 \mu m$ , and the characteristic transverse radius of the bunch exceed the characteristic transverse size  $R_p = 38 \mu m$  of the wake field. Computations were performed for electron bunch with an initial relative energy spread of 0.125%, which is typical of the best available electronic photocathode rf injectors. The simulation results show that the energy spread between electrons trapped by the wake wave from a bunch varies at the acceleration stage upon an increase in the acceleration length in the same way as in the case of injection of a short non-one-dimensional bunch in which all electrons are trapped and participate in the acceleration process [2]. In this case, during trapping of electrons from a wide extended bunch by the wake field, a short bunch in which electrons are subsequently grouped in energy on a certain length of acceleration into a small region in the energy space is "cut" from the initial bunch. For the chosen parameters of the laser pulse and a bunch the absolute energy spread between electrons over optimal acceleration length  $L_{acc} = 24$  cm is minimized, and the mean energy of bunch electrons attained the value of  $E_{max} = 2.1$  GeV; the relative energy spread in this case is  $2\sigma_E/E_{max} = 0.25\%$ . Other parameters of the accelerated bunch are as follows: a characteristic length of 1  $\mu$ m, a transverse radius of 0.83  $\mu$ m, and a normalized emittance of 2.9 mm mrad.

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#### PIC MODELING OF QUASI-MONOENERGETIC ELECTRON BUNCHES GENERATION DURING THE INTERACTION OF HIGH INTENSITY FEMTOSECOND LASER RADIATION WITH NON-HOMOGENEOUS PLASMA

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This work was motivated by experiments held in IAP RAS. It was demonstrated the formation of monoenergetic bunches of accelerated electrons when femtosecond laser radiation with the intensity of  $2 \cdot 10^{17} \text{ W/cm}^2$ was focused at the end of the aluminum foil. Electrons had energy distribution with a pick in the range of 0.2 - 0.8 MeV and energy spread of less than 20%. One of the possible mechanisms of accelerated electrons with quasi-monoenergetic spectrum is a mechanism associated with the generation of the plasma wave as a result of the laser pulse self-modulation instability in underdense plasma created by a laser system prepulse coming in 10 ns before the main pulse [1]. One-dimensional PIC simulation by the code VLPL [2] of laser interaction with the plasma at a concentration of  $5 \cdot 10^{19}$  cm<sup>-3</sup> showed that in the presence of density inhomogeneities in the plasma boundary [3] and the temporary shape of the laser beam an efficient excitation of the plasma wave, capture and quasimonoenergetic acceleration of electron beams up to energies of the order 1 MeV can occur.

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#### PIC SIMULATION OF THE LASER WAKEFIELD ACCELERATION WITH WAKE-EXI AND LAPLAC MODELS WITH PARAMETERS CLOSE TO REAL EXPERIMENT

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The numerical simulation of finite charge electron bunch acceleration was made in plasma channel after external injection to the high nonlinear plasma wave generated by powerful relativistically intensive laser pulse with using of different models LAPLAC (LAser PLasma ACceleration) and WAKE-EXI (WAKE + EXternal Injection). Comparison of obtained results was made for the same initial parameters as for the results obtained previous authors.

#### TERAHERTZ RADIATION GENERATION AT FEMTOSECOND LASER PULSE INTERACTION WITH OVERDENSE PLASMA

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One of the main reasons for terahertz (THz) radiation generation is the change in the nonlinear polarization of plasma during the action of a femtosecond laser pulse. The characteristic frequency of generated THz radiation is  $\omega \sim 1/\tau$ , where  $\tau$  is the laser pulse duration. The features of THz radiation generation considerably depend on the relation between the carrier frequency of the laser pulse  $\omega_0$  and the plasma frequency  $\omega_n$ . In overdense plasma  $\omega_0 < \omega_p$  and the field of laser pulse is localized in a skin layer. If electron thermal velocity  $v_T$  satisfy the inequality  $v_T/\omega_0 < c/\omega_p$ , where c is the speed of light, then for the field with laser pulse frequency the high-frequency skin effect takes place. In contrary for generated THz field it is easy to realize the conditions of anomalous skin effect, when  $v_T/\omega > c/\omega_n$ . This communication is devoted to the consideration of THz field generation in an overdense hot plasma under conditions of the anomalous skin effect, when there is a high-frequency skin effect for the carrier frequency of a femtosecond laser pulse. We found the nonequilibrium correction to the initial Maxwellian distribution function, which is created by the ponderomotive force of the laser pulse in the plasma skin layer, and

calculated the density of low-frequency electric current. We construct the general solution of inhomogeneous equation for the low-frequency field in plasma and found the field of THz radiation in a vacuum. The spectrum of THz radiation is calculated. It is shown that the emission spectrum has a broad line near the frequency  $\omega \sim 1/\tau$ . It was established that for a given total energy and laser pulse duration, the total energy of THz radiation is stronger the sharper laser radiation focusing. This tendency found under the conditions when the focal spot size of the laser pulse is not too small, and one can not take into account diffraction effects. We find a pattern of low-frequency radiation as a function of the degree of laser pulse focusing and show that the smaller the size of the focal spot, the more radiation propagates along the plasma surface. With temperature increasing, the skin depth in the low-frequency anomalous skin effect conditions increases. Consequently part of the energy of the laser pulse, which is converted into terahertz radiation is reduced, that leads to a corresponding decreases in the radiation pattern and in the spectral composition of radiation. However, for typical experimental conditions these decreases are relatively small.

#### THEORETICAL AND EXPERIMENTAL STUDIES OF RADIATIVE AND GAS DYNAMIC PROPERTIES OF SUBSTANCES AT INTENSE INTERACTION OF ENERGY FLUXES WITH MATTER

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Mathematical modelling of radiative and gas-dynamic processes in plasma is carried out for experiments, where both intense laser and heavy ion beams are used. The brief review of theoretical models, which are used for the radiative opacity calculations, is given. 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 is used for temperature diagnostics of CHO plasma target in combined laser–heavy ion beam experiments [2]. Finally, joint radiative and gas-dynamic calculations are performed for comparison with experiment, where hohlraum radiation transmits through the CHO plasma target, and the theoretical spectrum of transmitted radiation is compared with experiment.

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# GENERATION OF $K_\alpha$ X-RAYS IN FOILS BY RELATIVISTIC LASER-PRODUCED HOT ELECTRONS AT PHELIX

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The goal of the experiments carried out at GSI with high intensity laser system PHELIX is the investigation of mechanisms leading to effective production of photons with energies above 20 keV. These photon energies are required for monochromatic backlighting of high Z targets, such as Al, Pb, heated by heavy ion beams.

During the interaction of a high intensity laser beam with a solid, collective absorption mechanisms transfer part of the laser energy into hot electrons, which are accelerated to multi-keV energies and penetrate into the cold solid behind the surface plasma, where they generate characteristic X-rays via K-shell ionization.

The  $K_{\alpha}$  photon yield from Ag foil in given direction into a unit of solid angle per laser pulse energy  $N_k$  was measured experimentally, and also determined according to the model [1], which takes into account dependencies of the conversion efficiency of laser energy into hot electrons  $\eta(I_L)$ and hot electron temperature  $T_h(I_L)$  on the laser pulse intensity  $I_L(r, t)$ , spatial and time dependent, and self-absorption of  $K_{\alpha}$  X-rays in a foil of arbitrary thickness d. In case of Gaussian laser pulse we get

$$N_{k} = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} \sqrt{v} \, dv \frac{\eta(v)e^{-v}}{T_{h}^{2}(v)} \int_{E_{k}}^{E_{0}} dE_{0} \exp\left[-\frac{E_{0}}{T_{h}(v)}\right] \frac{dN_{em}(E_{0})}{d\Omega},$$

where  $dN_{em}(E_0)$  is the number of photons per steradian emitted by an electron, normally incident with initial energy  $E_0$  into the foil from the front side [1].

Calculations of the  $K_{\alpha}$  photon yield  $N_k$  were carried out for the experimentally realised parameters: silver foils of thicknesses 10, 100  $\mu$ m and 3 mm in the range of intensities  $I_0 = 5 \times 10^{17} - 3.5 \times 10^{19} \text{ W/cm}^2$ , at the given observation angle of 45°, and reveal a good agreement with measured in the experiment dependencies on the laser intensity.

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#### ATOMIC DATABASE SPECTR-W<sup>3</sup>: CURRENT STATUS AND PERSPECTIVES

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The Spectr-W<sup>3</sup> information-reference system was developed in 2001– 2010 and realized as an online Web resource based on the factual atomic database Spectr-W<sup>3</sup> (http://spectr-w3.snz.ru). The information accumulated in the Spectr- $W^3$  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- $W^3$  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-W<sup>3</sup> atomic database is still the largest factual database in the world, containing the information on spectral properties of multicharged ions.

In 2010 the new stage in the development of the Spectr- $W^3$  atomic database was started. The purpose of this stage is the creation of a qualitatively updated version of the Spectr-W<sup>3</sup> atomic-data information-reference resource on the Web to provide free access to an essentially extended Spectr-W<sup>3</sup> atomic database. Spectr-W<sup>3</sup> and its local version Spectr-CD have been essentially updated by: 1) the inclusion of new experimental and theoretical information on the multicharged-ion spectra both published in literature and obtained in the participating organizations (JIHT RAS and RFNC-VNIITF); 2) introduction of the new data type on the autoionization-transition rates; 3) inclusion of the results of systematic calculations and high-resolution measurements obtained in the participating organizations as well as presented by the other authors; 4) selection and inclusion of the most important experimental and theoretical data published after 2010; 5) software and equipment of the Spectr- $W^3$  website have been upgraded; 6) functionality and informative content of the Spectr-W<sup>3</sup> Web-pages have been extended.

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#### STRONG FIELD EFFECTS IN ORIENTED CRYSTALS AT HIGH ENERGIES

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The recent studies of different collaborations focus their attention on fields of super powerful lasers. For example, the attainability of Schwinger's limit with extreme power lasers is discussed in [1]. High intensity colliding laser pulses can create abundant electron-positron pair plasma which can scatter the incoming electromagnetic waves [2].

We consider electromagnetic strong field effects like hard energy photon emission by electrons (positrons) and pair creation by high energy gamma quanta in oriented crystals at the projectile energy region from 100 GeV up to few TeV. At such energies the Schwinger's field parameter exceeds unity, so the observation of strong field effects becomes possible [3–5].

The properties of channeling radiation spectra for above hundred GeV electrons have been studied with account of multiple scattering and radiation cooling [6]. It has been shown, that the shape of a spectrum does not depend neither on energy of electrons, nor on the atomic number of a target when the energy of electrons exceeds  $\sim 1$  TeV. The consideration is

based on the uniform field approximation (UFA). Simple phenomenological expressions are given which describe the radiation spectrum with good degree of accuracy. It has been shown, that the radiation length in the high energy limit does not depend on the energy of incident electrons.

The pair creation is considered within the frame of trial trajectory method [7, 8]. We demonstrate that pair production cross-section can have an appreciable value under conditions at which the ordinary approaches like UFA provide vanishing result.

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#### THE INTERACTION OF HIGH-POWER LASER EMISSION WITH MULTICOMPONENT POLYCRYSTALLINE ROCKS

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The interaction of laser emission with multicomponent polycrystalline rocks at  $q \sim 10^{10}-10^{13}$  W/cm<sup>2</sup> is poorly understood, although it is of particular interest for modeling hypervelocity meteorite impact [1], studying of matter at extremely high pressures as well as for various technological applications. Such a research requires complex theoretical models and time-consuming numerical calculations. Therefore it is important to investigate the possibility of application of the analytical estimates obtained in the works on laser thermonuclear synthesis to the study of the interaction of intense laser pulses with a target of polycrystalline multicomponent rocks, with thermophysical and optical properties that are radically different from the properties of metals and dielectrics. The experiments were performed on the "Saturn", which is a powerful multi-stage laser system. The parameters of the emission output are as follows: width 30 ns., energy up to 50 J, power density at the target from  $10^{10}$  to  $5 \cdot 10^{13}$  W/cm<sup>2</sup>.

The dependence of the crater parameters on the intensity of irradiation of andesite targets was investigated. In all experiments the crater diameter was substantially greater than the diameter of the focal spot. It indicates the presence of a failure mechanism other than simple melting and vaporization of the target material. The test firing at AL targets and comparing the experimental data with the theoretical model of transformation of laser energy into energy of shock wave by ablation process on the target surface in hydrodynamic regime of the interaction [2] allow us to suggest the nature of the interaction.

A series of experiments with thin targets was conducted to study the mechanism of energy transfer to the back surface. The plasma temperature which did not exceed 200 eV was measured by X-ray methods. The products of expansion of the plasma torch were investigated on the substrates of chemically purified silicon. The speeds of cosmic dust particles were estimated in the simulated experiments.

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#### AB-INITIO CALCULATIONS OF THE THERMAL CONDUCTIVITY METALS WITH HOT ELECTRONS

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The interaction of ultra-short laser with metal result in the twotemperature (2T) state in which the temperature of the electronic subsystem  $(T_e)$  by orders of magnitude greater than the ion temperature. Description of 2T state is important for understanding the mechanisms of laser ablation, since at this stage number of relevant phenomenon occurs: transfer of laser energy to the ions, creation of warm layer which determine the future dynamics of the system. The numerical simulation of laser ablation requires the kinetic coefficients of the metal with hot electrons. However, phenomenological dependencies are mostly used with contains adjustable parameters determined from the asymptotic behavior at low and high  $T_e$ . Ab-initio methods don't have such deficiencies, because there are no adjustable cofficient. This paper presents a ab-initio calculation of the thermal conductivity of the metal with hot electrons, calculated from the Kubo-Greenwood formula. The calculation is performed for liquid aluminum in the range of Te from 0 to 6 eV. The dependence of thermal conductivity is in a good agreement with calculations from kinetic equation [1].

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#### KINETIC COEFFICIENTS OF METALS ABLATED BY THE ACTION OF FEMTOSECOND LASER PULSES

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Dynamics of ablation of metals under the action of ultrashort laser pulses essentially depends upon their transport properties such as electron thermal conductivity and energy exchange between electrons and ions [1, 2]. At the early stage of a laser pulse and a metal target interaction the metal state can be characterized by electron and ion temperatures, which differ to a great extent from one another, and by the minor change of a target volume. Electron kinetic characteristics of a metal define the depth of the surface layer of a metal target heated by the laser pulse. This heated layer is produced by the electron heat propagation and heat transmission from electrons to ions resulting in the equalization of electron and ion temperatures. Because of its high temperature, target surface layer has a high pressure giving rise to the onset of ablation. We have calculated electron heat conductivity coefficient and electron-phonon coupling factor, governing the electron-ion energy relaxation. Among metals used as the targets, when laser ablation is investigated, we consider metals with different electron energy bands: simple metals with only s- and p- electrons excited under the action of laser irradiation and also rare and transition metals with laser-excited d-electrons [3].

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#### DEPENDENCY ANALYSIS RADIATION RESISTANCE OF SODIUM CHLORIDE ON THE ULTRASHORT LASER PULSE DURATION

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Radiation resistance is numerically characterized breakdown threshold: a flux density of optical radiation, from which the volume or on the surface of irreversible changes in the anomalous absorption of the light flux. For beam breakdown of transparent solids by short laser pulses is a certain threshold of radiation damage dependence on pulse duration. Experiments have shown as a rule, with decreasing pulse duration radiation resistance increases. Study of the nature of this dependence, helps to understand the mechanisms and patterns of laser breakdown.

The paper was asked to review the nature of radiation resistance of sodium chloride in the femtosecond laser pulse duration range. Used some of the experimental data [1–3]. A number of possible mechanisms for the destruction of an optically transparent solids by laser pulses.

The irradiation of solids by laser pulses of high energy can lead to the removal of material from the surface of the material. This phenomenon, known as laser ablation, is the main mechanism of destruction of ionic crystals in the femtosecond range. Ablation is widely used in various applications for example for microfabrication of surfaces, and pulsed laser deposition (PLD, pulsed laser deposition) thin films and coating.

One of the characteristics of ablation using high-power pulses of laser radiation is the formation of different kinds of particles (clusters, droplets or solid fragments). Ability to predict and control the ejection of particles and the composition of the cloud of ablation products is important for optimization of process parameters in many practical applications.

Because ablation is characterized by certain laws, this fact can be used to analyze the dependence of radiation resistance of the pulse duration in the femtosecond range.

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#### ON THE THERMAL CHARACTERISTICS OF IONIC CRYSTALS AT ACTION OF FEMTOSECOND LASER PULSES

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High-intensity laser radiation can lead to radiation breakdown of transparent solids, and the appearance in the irradiated medium intense heat flow, for the consideration of which is necessary to use the concept of nonequilibrium thermodynamics. Problem description of the thermodynamic properties of materials under extreme conditions associated with the occurrence of high temperature and pressure is of significant interest to the physics of high energy densities. This comes out, for example, to identify previously unexplored regions of the phase diagram.

Analysis of thermal processes occurring during irradiation of matter ultrashort laser pulses is carried out using high-temperature phase diagrams. Similarly, consider, for example, the effects of femtosecond laser pulses on aluminum and gold [1]. In the literature data on the critical parameters of a number of metals and some of the compounds [2, 3], however, information on the critical parameters of sodium chloride in need of some clarification.

In experiments conducted by us previously investigated the effects of femtosecond laser pulses at a series of ionic crystals [4]. Determination of the critical characteristics will be built on the basis of the collected data the phase diagram of sodium chloride in a wide temperature range. In the thermodynamic description of the most important and little-studied area of classical theoretical methods, to date, are ineffective. In this regard, of particular interest are the semiempirical equations of state for the calculation of the thermal characteristics of ionic crystals when subjected to a dielectric medium of femtosecond laser pulses.

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#### THE CHEMICAL ACTION OF FOCUSED LASER RADIATION ON THE OXIDATION-REDUCTION REACTIONS IN LIQUID PHASE

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Scanning a dielectric surface with a focused laser beam in a special solution gives rise to a local oxidation-reduction reaction in the solution; as a result, metallic structures appear on the surface of the substrate. Especially great interest is the deposition of copper due to its high specific electrical conductivity [1].

This question has been examined in [2, 3]. Our group showed that the condition for high-conductivity copper structures to appear is the formation of closely-packed nanodisperse copper particles generated by surface crystallization in the focus of the laser beam. A major shortcoming of the compositions proposed in [2, 3] is the low rate of the deposition process not exceeding 0.0025 mm/s. The aim of this work was to study the possibility to increase the rate of the laser-induced deposition process by changing the composition of a copper plating solution.

In order to improve rate of the deposition process we proposed solutions based on copper formate (II) for use in the process laser copper plating. We took alcohols with one and two hydroxyl groups, methanol, ethanol and ethylene glycol, as reductants and 7% aqueous solution of copper formate (II) as a source of copper for the deposition. Obtained nanostructured metal tracks (and separate copper nanoparticles) have been investigated by electron, laser and optical microscopy, EDX and powder XRD analysis, and by impedance spectroscopy.

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Man'shina A.A., Povolotskiy A.V. et al. // Glass Phys. and Chem. 2007. V.3. No.33.
#### SIMULATION OF LASER-INDUCED PHASE TRANSFORMATIONS IN HETEROSTRUCTURES WITH SiGe LAYER

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Thin layers of polycrystalline silicon-germanium alloys have attracted much attention due to their wide application in different electronic devices such as thin film transistors, photodiode, infrared detectors, solar cells and others. The new methods of growth of Si based heterostructures are developed. However there is the problem of the changes of properties of grown layers. One of the methods of modification and improvement of properties of grown samples is laser treatment. This work is devoted to the study of the laser-induced processes in SiGe heterostructures at the laser irradiation by numerical simulation methods.

The objects of the investigations were three–layered heterostructures  $Ge_xSi_{1-x}/pc-Si/c-Si$  and  $Ge_xSi_{1-x}/SiO_2/c-Si$  with different layer thicknesses and Ge content. We considered the laser irradiation of heterostructures by single pulses of a ruby laser in wide range of energy densities. The simulation was carried out on the base of the numerical solution of Stefan problem in one–dimensional approximation. The temperature and phase state dependences of thermal and optical parameters were taken into account.

The dependences of the peak temperature at the surface and at the layer interfaces and melting depth on irradiation energy densities were obtained. The melt times for each layer were calculated in different regimes of laser irradiation. It is shown that the scenario of phase transformations depends on irradiation energy density. The peculiarities of temperature changes are analyzed. In particular, two plateaus are observed in the time dependence of the surface temperature at the solidification stage. The first plateau corresponds to crystallization of molten Si and the second one—to crystallization of  $\text{Ge}_x \text{Si}_{1-x}$  layer. The plateau durations depend on the type of multilayer structure. The temperature dynamics essentially depends on irradiation energy density and the thickness of heat-insulating layer (pc–Si or SiO<sub>2</sub>). The reasonable agreement between calculated and available experimental data is obtained.

#### REFLECTIVITY DYNAMICS OF PbTe IRRADIATED BY NANOSECOND LASER PULSES

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The method of optical probing with time-resolved reflectivity measurements is widely used in the study of laser-induced phase transitions in semiconductors. The method is based on the registration of the changes in reflectivity under transformation from solid to liquid phase. In this work time-resolved reflectivity measurements were carried out at the laser irradiation of heterostructures with PbTe thin films.

The samples were prepared by deposition of PbTe from a steam phase on glass substrates. The film thickness was about 5  $\mu$ m. The study with electron microscopy showed that films have nanogranulated structure.

The samples were irradiated by single Gauss pulses of a ruby laser ( $\lambda$ =694 nm, FWHM=80 ns). The energy densities varied in the range from 110 to 350 mJ/cm<sup>2</sup>. The laser optical scheme ensured the high homogeneity of irradiation in cross-section. The *in situ* monitoring of the ruby laser-induced processes in the samples was realized by using a nonspiking pulsed Nd:Glass laser as a probing radiation source. The probing beam consisted of two harmonics with  $\lambda_1$ =1064 nm and  $\lambda_2$ =532 nm.

It is found that the dynamics of reflectivity differs from the same observed in other semiconductors in which the increase in reflectivity is observed under transitions solid-liquid phase. The laser-induced melting of PbTe films leads to the decrease of reflectivity. The lessening in reflectivity reaches about 30% at  $\lambda_1$  and 50% at  $\lambda_2$ . The peculiarities in reflectivity dynamics of PbTe can be explained by an unusual dependence of band gap on temperature. In defference with other semiconductors the band gap increases with temperature rise. We can also suppose that the phase transition semiconductor-semiconductor takes place under melting of PbTe.

# MOMENT METHOD IN ABLATION THERMAL MODEL Mkrtychev O.V.,\* Shemanin V.G.

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The laser ablation mechanism has been described in the thermal model frame [1–3]. The one-dimensional equation of the heat conductivity such as  $\frac{\partial H}{\partial t} = v \frac{\partial H}{\partial z} + \frac{\partial}{\partial z} \left(\kappa \frac{\partial T}{\partial z}\right) - \frac{\partial I}{\partial z}$  were considered in these works. The given difficult nonlinear differential equations in partial derivatives was treated in the present work by the moments method [1]. It allows to reduce this problem to the solving of the ordinary differential equations system

$$\begin{split} T_s &= f_1(T_s, l, h, v), \\ \dot{l_s} &= f_2(T_s, l, h, v), \\ \dot{h_s} &= f_3(T_s, l, h, v), \\ \dot{v_s} &= f_4(T_s, l, h, v), \end{split}$$

where  $T_s$ —surface temperature,  $l_s$ —characteristic thermal length (distance on which the temperature in the solid sample decreases in 2.7 times),  $h_s$ —the crater depth,  $v_s$ —the surface moving velocity. Such an approach has allowed to fulfill the computer simulation of the thermal field distribution at the laser ablation. Temperature dependence of the material characteristics accounting essentially complicates the analysis, and the moments method allows to take into account easily as the optical and thermo physical properties temperature dependences of the studied materials as the effects connected with the plasma plume and phase boundaries. These dependences of coefficients on the temperature or the time looked like:  $c = c_0 - c_1 \cdot e^{\frac{c_2 - T}{c_3}}$ —for the thermal capacity,  $\kappa = \kappa_1 \cdot \left(\frac{T}{\kappa_2}\right)^{\kappa_3}$ —for the heat conductivity coefficient and  $I_s = I_0 \cdot A \cdot e^{\frac{-t \cdot h \cdot a_g}{t_1}}$ —for the incident radiation intensity.

Computing experiments have been fulfilled for the parameters values simulating PMMA and glasses surfaces laser ablation. Numerical experiment results were well agreed with the experimental data in [1].

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#### LASER-INDUCED EVAPORATION OF IRON NANOPARTICLES OBSERVED BY LASER LIGHT EXTINCTION AND LASER-INDUCED INCANDESCENCE

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The nanoparticle vaporization is frequently used in various applications such as fuels combustion and high temperature nanopowder synthesis. The vaporization possibly occurs when condensed particles interact with a pulse laser radiation in optical diagnostics. This study is devoted to the investigation of iron nanoparticles vaporization process using nanosecond Nd:YAG laser pulse. The iron nanoparticles were synthesized by pulse Kr-F excimer laser photolysis of Fe(CO)<sub>5</sub> at room temperature (details of experiments are given in [1]).

The drop of particle volume fraction due to vaporization after the Nd:YAG laser pulse was observed by laser light extinction at wavelength of 633 nm. The advantage of present experiment is the coaxial adjustment of the heating laser beam and the diagnostic one. The peak particle temperature during laser heating was measured using two-color pyrometry at the wavelength of 488 and 760 nm. The particle size was evaluated by time-resolved laser induced incandescence (LII) technique to be in the range of 5–9 nm in a diameter, depending on the experimental conditions.

The main experimental result is that the evaporated part of the volume fraction of iron nanoparticles depend on the laser fluence, pressure and kind of a bath gas. The evaporation decreases with an increase of bath gas pressure; the most intensive evaporation of nanoparticles was observed in mixtures diluted by 0.1 mbar Ar even at low laser fluences. The maximum temperature of laser heated iron particles was independent of laser fluence and its value was found to be in the range of 2100–2600 K, that is below than the boiling temperature of iron (around 3100 K). This fact could correspond to the size dependence of equation of state of iron nanoparticles.

This work has been supported by the Russian Foundation for Basic Research (grant No. 12–0831034 for young scientists) and by the Ministry of education and science of Russian Federation (project N 8754).

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#### SEARCH OF RATIONAL PARAMETERS OF THIN-WALLED DESIGNS AT JOINT THERMAL AND MECHANICAL ACTION OF INTENSIVE FLUXES OF ENERGY

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Hulls of modern aircraft (AC) represent thin-walled multilayered composite shells which are very defenceless to intensive energy fluxes of the various physical nature [1]. The additional requirement to hulls is providing with them the set level of shielding of radiations and the particles fluxes passing in a design. Design of AC hulls having protection is very difficult task as security of absorption of energy fluxes for this shielding strengthens thermal and mechanical action on hull. Besides, introduction of protective layers in a design significantly increases the hull weight and search of rational parameters for design is necessary.

As a rule, such search is carried out separately for protective layers and other part of the hull. Unreasonable place of such separate approach is the task of critical impulses of pressure and critical temperatures of heating for carrier layers at thermal and mechanical actions of energy fluxes as it has aprioristic and expert character.

In this work design optimization is offered to be performed as a whole. Consequences of thermal and mechanical actions of energy fluxes on the protected hull are predicted [2] in the course of search of rational parameters and the question of a task of critical values doesn't arise.

The general recommendations about rational parameters of the standard AC hulls are developed as a result of systematic calculations. It is shown that the account of fillers geometry for modern covering is essentially important in problems of search of rational parameters of protected AC hulls.

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#### CRITERIA OF APPLICABILITY OF INDEPENDENT RESEARCH OF THERMAL AND MECHANICAL ACTIONS OF IONIZING RADIATION ON THIN-WALLED CONSTRUCTIONS

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The problem about possibility of independent consideration of thermal and mechanical actions of the ionizing radiation (IR) has great practical interest when forecasting consequences of IR action for the thin-walled multilayered constructions protected by the heterogeneous covering (HC). This problem is reduced to the solution of two tasks. The first task is research of need of the accounting of heat exchange having between the HC components when forming thermomechanical IR action in sheeting. The second task is an assessment of influence of temperature dependence of materials properties at calculation of parameters of reaction of a heated thin-walled multilayered construction on mechanical IR action.

The set of the dimensionless variables determining parameters of loading taking into account heat exchange is received for a task of formation of mechanical IR action. Intervals of change of dimensionless parameters at which heat exchange during formation of mechanical action can be neglected are defined as a result of systematic calculations. The mathematical model of an elementary heat-conducting cell was used in these calculations. In particular, it is shown that the accounting of heat exchange is necessary at the average amount of inclusions less 2.5–4 mkm. This result is right for characteristic times of IR impulse in case of metal discrete fillers (tungsten, nickel) and the polymeric binding.

The formulation of criteria of need of taking note of temperature dependence of materials properties at determination of parameters of construction reaction is carried out on the basis of results of the analysis [1] using the dimensions theory. Intervals of change of the specified dimensionless thickness at which is admissible to neglect thermal action (heating) at calculation of parameters of reaction of a multilayered design are defined. Dimensionless dependences [1] for the maximum deformations are used for this purpose.

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## ACTION OF HIGH-SPEED MACROPARTICLES FLUXES ON FLAT MULTILAYERED BARRIERS

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New technologies of hardening of details surfaces, and also problem of meteoric protection of spacecrafts demand forecasting of consequences of action of high-speed fluxes of macroparticles on multilayered barriers. It is quite clear that the role of numerical modeling in such researches is essential as it allows determining rational parameters of an influencing particles flux of or of protective barrier layers.

In this work researches of high-speed macroparticles action on a barrier are conducted by a method of finite-size particle in cell [1]. Influence of thermal processes on characteristics of macroparticles impact consequences (crater sizes and depth of particle penetration into a barrier) is studied. It is shown that this influence is essential at the micron sizes of particles. The assessment of interference of wave processes is carried out for a case of joint action of macroparticles on a barrier. It is received that interference is essential at distances between macroparticles less their characteristic size.

Results of calculations of characteristics of consequences are represented in the form of sedate dependences having uncertain coefficients. These coefficients are defined by a method of the smallest squares, using settlement data obtained by means of a method [1]. In particular, it is received that the relation of depth to diameter of a crater practically doesn't depend on the a macroparticle impact speed and changes within 0.5...0.6.

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#### INSTABILITY AND FRAGMENTATION OF ABLATED LAYER AT HIGH-CURRENT ELECTRON BEAM IRRADIATION OF METALS

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Action of a high-current electron beam on metal leads to rapid heating, melting and expansion of substance in a zone of the beam energy absorption [1]. Fast expansion of the melted substance generates negative pressure and provokes cavitation in it. Nucleation, growth and consolidation of micro-bubbles results in fracture of liquid metal with formation of a set of little drops. This problem attracts attention as an example of fracture in a liquid state, as well as a method of production of superdispersed powders of metals.

Our previous numerical investigation [2] was based on a one-velocity multiphase medium mechanics with phase transition, which was described through kinetics equation of the bubbles generation and growth. It reveals that at the action of a nanosecond electron beam with parameters close to SINUS-7 [1], a cavitation zone is formed near the irradiated surface as a result of the fast expansion of the melted metal. A number of droplets with diameters of several hundreds of nanometers are formed inside this zone. But between the cavitation zone and the metal surface there is a foremost flat layer of continuous metal without any bubbles. This layer is most close to the free surface; therefore, negative pressure in it is not enough for cavitation. This situation is similar to the ultra-short laser irradiation [3, 4], where such foremost layer is also observed.

The foremost layer is unstable due to its accelerated motion and due the action of surface tension. Instability results in its fragmentation. Dynamics and fragmentation of this layer substantially influence on the resulting size distribution of the produced metal particles. The present study is devoted to analysis of such instabilities and to determination of characteristic size of the resulting fragments.

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#### MULTISCALE MODELING OF DEFECTS ACCUMULATION IN NUCLEAR MATERIALS UNDER IRRADIATION

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The evolution of nuclear material properties under irradiation by fission products is a multi-scale phenomenon. Traditional theoretical approaches deal mostly with the meso-scale description within kinetic rate theory of radiation defects. However, such models include an extended set of microscopic parameters, characterizing the crystal defect structure, thermo-physical and thermo-chemical properties of the irradiated material. The present report describes a progress in the evaluation the microscopic parameters for U–Mo and UO<sub>2</sub> nuclear fuels.

Current computational facilities restrict the system size available for nuclear fuels study within ab initio approaches to a few hundreds of atoms. However substantially larger systems are required for the consideration of the key processes governing the accumulation of defects under irradiation (such as production, diffusion and interactions of radiation defects). That is the reason the basic method involved in our calculations is the classical molecular dynamics (MD) with the interionic potentials, correctly reproducing formation energies of basic defects, and verified against up-to-date ab initio studies (along with the thermal expansion and elastic constants available from experiments). In particular, embedded atom method potentials are created for U–Mo alloys with Xe inclusions by adjusting the interatomic potential functions to optimally reproduce per-atom forces (together with total energies and stresses) computed at the ab initio level for a fine-tuned set of reference structures.

Diffusion coefficients of basic radiation-induced defects, rate constants of recombination and clustering, the sink strength of surfaces for interstitials and vacancies are evaluated for the meso-scale description of nucleation and growth of dislocation loops, voids and Xe bubbles. The kinetics of the processes has been studied by tracking the change of defects concentrations with time in the system during the non-equilibrium MD simulation. The number of defects formed by the stopping of fission products with the energy ~100 MeV is calculated from the combination of: a) the energy distribution of the primary knocked-on atoms from the Monte-Carlo modeling in the TRIM code, and b) the number and type of defects pro-

duced in collision cascades of the primary knocked-on atoms with different energies from the MD simulations.

## ATOMISTIC SIMULATION OF DEFECTS FORMATION IN NUCLEAR FUELS DUE TO HEAVY ION IRRADIATION

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At moving of the swift heavy ion (e.g. Xe ion—the typical fission fragment), the defect formation takes place in nuclear materials. There is a large interest in understanding of the mechanisms of defect formation. In this work, the atomistic simulation of defect formation due to the swift heavy ion irradiation is performed for various nuclear materials  $(U, U-Mo, UO_2)$ . The two-temperature atomistic model with explicit account of electron pressure and electron thermal conductivity is used. This two-temperature model describes ionic subsystem by means of molecular dynamics while the electron subsystem is considered in the continuum approach. The various mechanisms of defects formation are examined. The comparison to the experimental data is performed.

#### ATOMISTIC SIMULATION OF DEFECTS DIFFUSION IN URANIFEROUS NUCLEAR FUELS

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The diffusivities of point defects are important parameters in kinetic models for description of the evolution of point defects to voids and clusters, the irradiated fuel behavior and fission products release. However there is a large uncertainty in the experimental estimations of the corresponding values. Basic properties of self-interstitials and vacancies in metals usually are not measured directly, but inferred from the experiments with the irradiated materials. The present work describes an attempt to evaluate the diffusivities of point defects in several uranium-based nuclear fuel materials (pure  $\gamma$ -U, U-Mo alloy, and uranium dioxide UO<sub>2</sub>) using molecular dynamics (MD) simulations with the appropriate interatomic potentials [1–4]. Diffusion coefficients of vacancies and self-interstitial atoms were obtained for each of the materials studied as a function of temperature. The corresponding point defects formation energies were evaluated and compared to the existing density-functional theory calculations and experimental data. The results allow to consider the features of the defect diffusion in gamma-U, U-Mo and  $UO_2$ , and predict predominant point defect type in each case.

The proposed MD models also reproduce experimentally observed phenomena related to the diffusion processes, e.g. the diffusivity calculated for U-10Mo alloy appears to be lower then the one calculated for pure  $\gamma$ -U, and atomic mobilities of U in U-10Mo are significantly larger than those of Mo. Both facts agree with the recent experimental study [5].

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## INNER STRUCTURE INFLUENCE ON PECULIARITIES OF EVOLUTION OF ATOMIC CASCADES IN Fe CRYSTALLITES

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The molecular dynamic simulation of the development of the atomic cascade displacements in Fe crystallites was carried out. The interatomic interaction was calculated in the approximation of the Finnis-Sincliar method. The energy parameters of point defects, structure of interfaces and elastic moduli were good described by used potentials what was important for study of atomic cascade evolution in simulated materials. The cascades were generated by primary-knocked atoms with its energy varied from 1 to 10 keV. The inner structure of iron crystallite was taken into account in the calculations. The peculiarities of interaction of atomic cascades with point defect complexes and symmetrical tilt grain boundaries were studied. It was discovered that the presence of structural defects strained cascade energy dissipation and led to point defect cluster formation with sizes which were larger than in the case with crystallites having ideal structure.

The work was performed with financial support of RFBR grant No. 12–03–00488–a.

#### ULTRA-HIGH VACUUM EXPERIMENTAL SETUP FOR CREATION AND DIAGNOSTICS OF SURFACE NANOSTRUCTURES BY SCANNING PROBE MICROSCOPY

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Recently different kinds of nanostructures and nanomaterials become more and more interest for applications in high energy density physics experiments. In particular, in experiments with powerful laser pulses special nanometer foil and nanocluster structures are actively used as targets which have shown the efficiency for generation in plasma of intensive streams of ions, electrons, gamma and x-ray quanta. At the same time development of special thin-film detectors of ionizing radiation and multilayered or gradient materials for optical components is a very perspective direction. Methods for surface nanomodifications by influence of coherent radiation with intensity near an ablation threshold intensively expand.

Progress in these fields demands development of the corresponding high-precision tools for creation and diagnostics of surface nanostructures. Thus, one of the most powerful methods of a surface research is the scanning probe microscopy.

We present our original experimental setup designed around scanning probe unit for manipulations in ultra-high vacuum  $(10^{-11} \text{mbar})$  (UHV) and very low temperature (down to 280 mK) with presence of magnetic fields (up to 7 Teslas). The main unit of the setup is AFM/STM unit especially designed for using in UHV systems in in-situ experiments where high spatial resolution (up to atomic and subatomic) is required. Scanning unit of our STM is equipped by lateral sample positioning system and tip landing system. Sample positioning system consists of three pairs of inertial piezo-drivers, positioned in the vertexes of a regular triangle and sapphire sample holder in between them. The sample holder is equipped by eight contacts which are used either for fixation of a standard "Omicron Nanotechnology" sample holder or as independent electric contacts for different goals like a sample heating.

Setup possibilities allow to use it in researches and development of new generation nanoelectronics based on high-temperature superconductors.

# THE METHOD OF PULSED GAMMA RADIATION GENERATION OF NUCLEUS SHORT-LIVED ISOMERS Petrovskiy V.P.,\* Ovchinnikov A.V., Romashevskiy S.A., Chefonov O.V.

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The attempts to create gamma radiation sources due to short-lived  $(<10^{-6} \text{ s})$  nucleus isomeric states excitation by various mechanisms directly in a femtosecond laser pulse induced plasma have been undertaken in the following papers [1–6]. But the absence of selectivity between nuclear transition emission and hot laser plasma emission, which in turn is the bright source of high energy electrons and ionizing radiation in a wide spectral range, is the lack of the present technology.

On the basis of suggested technique there is a new approach both to isomeric state excitation of the  ${}^{57}$ Fe isotope at the energy of 14.4 keV and the lifetime of 98 ns, and to radiation detection by isotope relaxation [6]. The main idea of the given approach is using of two space-divided targets. The laser plasma created under the action of high power femtosecond laser pulses on the first Me-target is the source of electrons with the energy of more than the second target isomeric level energy (more 14.4 keV for <sup>57</sup>Fe) and x-ray emission in the energy range of 14.4 keV. Then these electrons and x-ray emission are directed to the <sup>57</sup>Fe isotope containing second target, where the first isomeric level excitation with energy of 14.4 keV takes place. Radiation detection of <sup>57</sup>Fe nuclei is realized with a time delay that is slightly less than the life time of the <sup>57</sup>Fe isotope excited state. Due to such experimental conditions the reliability of interpretation of the findings as a nuclear radiation is greater as compared with the following studies [1-5]. However, the development of a method that enables to decrease dramatically a noise level of laser plasma is still required for efficient implementation of the given approach.

X-ray spectra created in 1 kHz femtosecond laser pulse interaction with

solid targets is presented for laser intensities up to  $10^{17}$  W/cm<sup>2</sup>. For given spectra the estimate of the energy conversion efficiency from laser light to x-ray photons is performed and presented.

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#### THE DEVELOPMENT OF MOBILE TESTING FACILITY BASED ON VOLTAGE IMPULSE GENERATOR FOR TASKS SOLUTION RELATED TO LIGHTNING PROTECTION

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There are tasks now of experimental studies of lightning its impact on the grounding devices and as a consequence the development of methods of protection against lightning. One way of solving these problems is the measurement of earth resistance together with pent therein electrodes of lightning protection facilities with currents close to the current of a lightning strike. Therefore there is creating a mobile complex on the basis of impulse voltage generator (GIN) to measure the resistance of the soil in the range of 10–50 Ohm at a discharge current of 17–40 kA and total pulse energy up to 4 MJ. The Generator is made by the scheme Arkadieva–Marx. Because of the wide range of solids differing in conducting properties there is a need for creating a mobile system which consists of 4 s which dimension and weight allows transporting them on truck and conducting on-site installation. This work examines the design of the mobile complex and the results of development of GIN nodes.

# APPLICATION OF SYNCHROTRON RADIATION TO STUDY GaN/AIN MULTIPLE QUANTUM WELLS

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Spectroscopic and diffraction methods using synchrotron radiation beam at the VEPP3 storage ring of the Budker Institute of Nuclear Physics (Novosibirsk) have been used to study electronic and spatial structure of GaN/AlN multiple quantum wells (MQW). MQW are promising materials for novel optical applications. They serve as base materials for light emitting devices operating in ultraviolet spectral region, and high-speed infrared intersubband optical modulators and photodetectors. Hexagonal GaN/AlN MQW with 400 nm thick AlN buffer layer were grown by ammonia MBE on (0001) oriented sapphire substrates. GaN well and AlN barrier thicknesses were varied from 1.0 to 4.0 monolayers, whereas the number of period ranges from 20 to 260. It is well known that the optical properties of nitride QWs are strongly affected by arrangement of heterointerfaces. EXAFS (Extended X-ray Absorption Fine Structure) above the GaK edge [1], SAXRD (Small Angle X-Ray Diffraction) have been used to study the local structure of heterointerfaces in GaN/AlN MQWs grown by ammonia molecular beam epitaxy. Thickness of AlN and GaN layers in MQWs were evaluated using HRTEM (High-Resolution Transmission Electron Microscopy), X-ray diffraction and Raman- spectroscopy. Two sets of MQWs structures with the number of period about of 20 and more than 100 were studied. The Ga-Ga interatomic distance in MQWs is lower than that in the bulk GaN due to elastic compression of GaN layers in MQWs. This effect is less pronounced in thick structures because of almost full relaxation of GaN layers. The Ga-Al interatomic distance in thick MQWs is too long (about 0.1 Angstrom longer than typical values for AlGaN alloys). The effect may be due to generation of vacancies at the interfaces. Number of Ga cations in second coordination shell of Ga atoms is lower than one predicted for abrupt heterointerfaces that evidences in intermixing of heterointerfaces. An intermixing degree depends on total thickness of MQWs.

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## RESONANT RAYLEIGH SCATTERING AS A PROBE OF SPIN POLARIZATION IN 2DES

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The resonant Rayleigh scattering (RRS) in two-dimensional electron system (2DES) in a wide range of magnetic fields has been studied. A new differential technique for obtaining high quality RRS spectra is developed. Oscillations of the RRS scattering efficiency correlating with the electron filling factor are observed and explained in terms of redistribution of electron spins within two spin subbands of the zero Landau level. The attention is focused on the RRS and the photoluminescence (PL) involving electron-hole states in the zero Landau Levels (0–0). A scattering process is possible for electron-hole pairs localized in space on a length much shorter than the light wavelength. It is proportional to the number of localized states multiplied by the squared matrix element for the corresponding RRS transition. The peak energies for the RRS and the PL lines corresponding to the (0-0) optical transitions nearly coincide, the major difference appearing in the efficiencies of two events. The integral PL intensity does not show any marked changes with the magnetic field, but an oscillating behavior for the RRS efficiency is observed. The latter correlates with the electron filling factor. The variation in the RRS efficiency is to be divided into two major parts, a monotonic growth due to arising new empty states in the zero Landau level and a vet unexplained oscillating part. To understand the origin of the oscillating part, a few samples with different electron densities were studied. In the stydied magnetic field range both spin components of the (0-0) optical transition are well resolved. The reduction of RRS intensity relative to its value at the filling factor 1 is accompanied by developing an extra RRS line at a lower energy. The latter is associated with the optical transition involving electrons in the lowest spin state. This line appears both at the filling factor less than 1 and at the filling factor exceeding 1. Since at the filling factor larger than 1 both spin states in the zero Landau level are occupied, the only reason for the extra RRS line is a redistribution of electrons between two spin states. From the relative integral intensities of two RRS lines one can extract the spin polarization. The RRS can thus serve as an optical noninvasive technique to probe the electron spin polarization. This is extremely important since the measurement of absorption or transmission demands generally a severe modification of 2DES.

#### RESEARCH AND DEVELOPMENT OF ELECTROCHEMICAL DOUBLE LAYER CAPACITORS

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In development of electrochemical double layer capacitors are engaged many scientific laboratories and commercial firms. These works are very urgent because of the great demand for supercapacitors in different spheres of technics such as hybrid transport, traditional and alternative power engineering.

Carbon materials are widely used as electrode materials for supercapacitors. The reason of it is a number of unique properties of carbon such as high corrosion resistance, sufficient electronic conductivity, high temperature stability, possibility of the specific surface and porous structure regulation during the synthesis process. Besides, the variety of carbon materials allows to choose electrode materials rather flexible.

The purpose of our work was to create the pulse supercapacitor cells with high specific energy.

Porous structure research of various carbon materials was carried out, the technology of electrodes producing was developed and electrochemical characteristics of the investigated supercapacitors were studied.

The porous structure of carbon materials for supercapacitors with sulfuric acid as electrolyte, was investigated by the original adsorption method-Limited Evaporation technique. 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 included measurement of charge and discharge curves in galvanostatic and potentiostatic modes, definition of the resistance, specific characteristics of the supercapacitor (capacity, energy and power).

Due to the opportunity to influence activated carbon structure during synthesis we obtained carbon with micropore volume only  $0.5 \text{ cm}^3/\text{g}$  but with rather high capacity around 300 F/g. So the pulse supercapacitor cell with the specific energy 3.9 Wh/kg was made. This characteristic is calculated per the weight of the unpackaged cell. Components of the

unpackaged cell are current collector-thermoexpanded graphite, two electrodes, a separator, electrolyte.

#### COMBINED UV LASER–DC ELECTRIC DISCHARGE THRESHOLDS INVESTIGATION IN RARIFIED AIR

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Gas laser breakdown thresholds are known to be strictly dependent on radiation wavelength. UV quantashould significantly increase multiphoton ionization probability. DC electric field presence decreases this probability since electrons are constantly removed from laser beam waist.

For combined laser (266 nm, 12 ns)—electric impact regimes two strongly different effect patterns are observed. For Paschen curve right branch optical and electrical components threshold are close to pure mode ones. For Paschen curve left branch ( $p \leq 60$  Pa, optical breakdown thresholds are much bigger than in previous case) significant threshold decrease: 1 order of magnitude for electrical ( $\sim 2 \cdot 10^5$  down to  $\sim 2 \cdot 10^4$  V/cm) and more than 3 orders for optical ( $\sim 10^{12}$  down to  $\sim 5 \cdot 10^8$  W/cm<sup>2</sup>) component is observed. No such influence was observed in our experiments with 532 nm laser radiation.

For the first time significant effect of combined UV laser and DC electric impact for rarified air breakdown thresholds decrease is demonstrated. This phenomenon may be quite useful in a wide range of gas discharge devices.

# PECULIARITIES OF COMBINED LASER–DC ELECTRIC DISCHARGE IGNITION IN NOBLE GASES MIXTURES

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Penning effect for ionization energy decrease is well-known for binary gas mixtures. Theoretically, this also should lead to electric breakdown voltage reduction, but in fact it resulted in optical (532 nm, 18 ns) breakdown threshold decrease (3 times) and DC electric breakdown voltage increase (1.5 to 3 times) in  $10^2-10^5$  Pa pressure range.

Triple gas mixtures, to the best of our knowledge, are almost not investigated. Being Penning additives, both Ar and Kr 1% (mol.) itself decreased Ne optical breakdown threshold in our experiments (Kr was more effective).

For the first time we demonstrated negative interference of two Penning dopants added at once which led to mixture optical, electric and combined breakdown thresholds equality with the main gas. This phenomenon is important since demonstrates Penning multi-dopant ionization energy reduction impossibility.

# HIGH-CALORIFIC GAS FROM BIOMASS Lavrenov V.A.,\* Kosov V.F. JIHT RAS, Moscow, Russia \*v.a.lavrenov@gmail.com

The problem of waste processing is very important at the moment. Wood and agricultural waste can be used as a cheap source of renewable energy. Gas obtained by thermal conversion of biomass can used in gas-engine power plants. The main difficulties of existing technologies of biomass thermal conversion into fuel gas are complex and expensive system of gas purification, the necessary of liquid products processing and low calorific value of the gas. This causes necessity of development the technology that enables highly efficient conversion of biomass into high calorific gas.

At the Joint Institute for High Temperatures has been designed and tested the pilot plant capacity of 5 kg of biomass per hour based on the two-stage thermal conversion of biomass. The first stage is pyrolysis of biomass into solid, liquid and gaseous products. During the second stage the pyrolysis products are blown through the porous carbon at the temperature of about 1000°C, where there is their conversion into hydrogen and carbon monoxide. The main advantage of the technology is a high degree of energy conversion of biomass. In existing technologies based on pyrolysis this value does not exceed 0.18, in the technology developed in JIHT it is 0.78. The quantity of syngas is about 1.4 Nm<sup>3</sup> per kg of processed biomass and its calorific value is about 3000 kcal/Nm<sup>3</sup>. The absence of the liquid fraction in the final products is also an advantage of the proposed scheme.

The high-efficient methods for the biomass conversion into gas may be a basis for the creation of distributed power generation based on local renewable resources.

#### THERMOTECHNICAL CHARACTERISTICS OF GRANULATED FUEL MADE OF CHICKEN LITTER RESEARCHING AND WAYS OF IT UPGRADING

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By-product volume in industrial breeding shifts required manure volume. For this reason chicken litter utilization as a fuel is developing.

In JIHT we research granulated chicken litter with a view to define possibility of its using as a solid fuel. Differential scanning calorimetric method allows to define combustion heat of initial raw material. Received value is two times less than combustion heat of wood and comparable to slate coal combustion heat. Average ash-content value (specified by mass of unburnt rest) is 16% and this value is big enough. For reference ash-content of fen peat is about 10%. Experiments were carried out on thermoanalyzer SDT Q600 with initial raw material and torrefied granulated chicken litter (230, 250 and 270°C).

Torrefaction (low-temperature pyrolysis) was carried out for the purpose of upgrading fuel quality (increasing of combustion value and decreasing of hygroscopicity). This method is the heating in oxygen-free (nitrogen) environment with  $10^{\circ}$ C/min heating rate up to temperatures of 230, 250 and 270°C with following holding in isothermal conditions. Holding time was selected equal to 40 minutes.

Hygroscopicity definition researching for torrefied and non-torrefied samples was also carried out.

Based on received data it is possible to make following conclusion: Direct combustion of granulated chicken litter is inefficient because of low value of combustion heat however combustion heat of torrefied granulated chicken litter is compatible to peat and about 10-12/5 MJ/kg. As the result granulated chicken litter can be recommended for using as a solid fuel.

#### SHOCK WAVES. DETONATION. COMBUSTION

# TIME-DEPENDENT PROCESSES IN SHOCK WAVES Kanel G.I.

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The latest results of investigations into high-rate inelastic deformation, fracture and detonation phenomena under shock-wave loading of condensed matter are reviewed with emphasis on unsolved problems. The subjects of measurements and analysis are the wave structure as well as wave evolution and interactions. The structural transformations, elasticplastic transition, physical and chemical transformations are accompanied by changes in material compressibility and, as a consequence, manifest themselves in the structure of the compression and rarefaction waves. All these phenomena are time-dependent and cause specific peculiarities in evolution of shock waves. In particular, shock wave in elastic-plastic media splits into elastic precursor wave and plastic shock wave. Measurements of decay of the elastic precursor wave give us information about the initial plastic strain rate as a function of the stress and measurements of the rise time of plastic shock wave give addition data on later stages of highrate compression. The temporal resolution of such measurements in some cases may be now as high as  $\sim 1$  picosecond that allows an approaching of ultimate values of shear and tensile strength of solids.

The shape of elastic precursor wave may be different and depend not only on material but also on the test temperature and the wave propagation distance. Investigations in picosecond time range are associated with strong non-linearity of the elastic-plastic response. Establishing of quantitative criteria of the precursor wave evolutions, including its part in the picosecond time range, would allow getting of additional important information about mechanisms and kinetics of high-rate deformation of solids. Further development of analysis of wave interactions at spalling would provide new capabilities to get additional information about the high-rate fracture kinetics. The structure of detonation wave may differ significantly from that suggested by the detonation theory that presents natural challenge for analysis. Shock compression of hard brittle materials may be accompanied by formation of subsonic failure waves but any theory of the phenomenon does not exist yet.

#### STUDY OF EXTREME STATES OF CONDENSED EXPLOSIVES AND DETONATION PRODUCTS USING SYNCHROTRON RADIATION

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An overview of the work carried out in the Siberian Center for Synchrotron Research in recent years is presented. The study was carried out on the 4 directions: (i) the front structure, tomography of density, pressure and velocity behind the detonation front propagating through a cylindrical sample of powerful explosives (measuring the transmitted radiation); (ii) obtaining experimental data on the condensation of carbon nanoparticles by detecting small-angle X-ray scattering (SAXS measurements); (iii) obtaining experimental data on shock compression of continuous media (aerogel, TATB); (iv) getting information about the parameters of the structure and defects in samples of explosives (synchrotron-radiation microtomography and diffractometry).

Explosives were investigated with the initial density of 0.6 (a mixture of PETN and soda) to 2.0 g/cm<sup>3</sup> (CL-20). But the emphasis was on the study of mixtures based on TATB. Measurements of dynamic diffraction signals in explosion experiments allow us to obtain the distribution of condensed nanoparticles size. Similar experiments with the strikers at 1 km/s obtained at APS (USA) in 2012.

## THE INFLUENCE OF THE ADMIXTURE OF THE FULLERENE C<sub>60</sub> ON STRENGTH PROPERTIES OF ALUMINUM AND COPPER UNDER SHOCK-WAVE LOADING

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It is well known, that the mechanical properties of commercial and constructional materials depend on their internal structure, which, in turn, depends on the technologies or methods of them production and processing. In this work, the Hugoniot elastic limit and dynamic (spall) strength measurements of pressed aluminum and copper samples with admixture of

the fullerene  $C_{60}$  under shock-wave loading were carried out. The undoped aluminum and copper samples and samples, pressed from the mixture of Al or Cu powder and fullerene  $C_{60}$ , were investigated. The undoped samples were pressed under peak pressure 5 GPa, the samples with fullerene  $C_{60}$ were pressed under pressure 10 kbar and 5 kbar for aluminum and copper samples, respectively, under the temperature of 280°C. For all samples, the density, sound speeds and hardness were measured. The density for Al- $C_{60}$ and Cu– $C_{60}$  samples was equal 2.6 g/cm<sup>3</sup> and 7.8 g/cm<sup>3</sup>, the sound velocity was equal of 5.4 km/c and 3.5 km/c, correspondingly. The measurements of the microhardness of aluminum samples with fullerene  $C_{60}$  have shown its increasing with a factor 3–4. The admixture of the fullerene to the samples also leaded to increase their Vickerses hardness three times in aluminum samples and 1.3 times in cupper samples. Shock-wave loading of sample of 2 mm in thickness was created with a plane aluminum impactor of 0.4 mm in thickness accelerated by explosive facilities up to velocity of 0.66 km/s. The measurements of strength properties were based on the recording and following analysis of the free surface velocity history, obtained with VISAR laser-Doppler velocimeter. In the experiments, it was found, that the admixture of 5 wt% and 2 wt% fullerene in the samples leads to the increase Hugoniot elastic limit 10 times for aluminum samples. This agrees with high growth their microhardness. The measured values of Hugoniot elastic limit from the free surface velocity profiles were equal of 1.3 GPa for aluminum samples and 1.5 GPa for cupper samples. As it was expected, the spall strength of the samples with fullerene decreased about tree times in comparison with undoped samples. Probably, the decrease of the strength related with influence of solid fullerene particles on the process of dynamic fracture under high strain rates: fullerene conglomerates are as a concentrators of tension stresses in material, where the damages of material are generated and lead to its macro fracture.

#### SHOCK-INDUCED PHASE TRANSITIONS, SPALL STRENGTH AND DYNAMIC ELASTIC LIMIT OF TETRAGONAL ZIRCONIA

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Specimens of the ceramics based on zirconia partially stabilized by yttria of the 97 mol. % ZrO<sub>2</sub> + 3 mol. % Y<sub>2</sub>O<sub>3</sub> composition were prepared. The densities of the specimens were 5.79 and 6.01 g/cc. The ceramics mainly have the tetragonal structure (93–98 wt. % of t-ZrO<sub>2</sub>). The mechanical action on the ceramic initiates the transformation of the tetragonal phase into the monoclinic one: at the abrasive cutting-off or at the hammer shock fracture, the content of the monoclinic phase increases. The same trend was observed in the specimens, recovered after stepwise shock compression up to 36, 52 and 99 GPa. It was found that shock compression do not initiates tetragonal-monoclinic phase transition directly, and this transition is caused by the destruction. In addition, we did not observe any trace of the phase change which was reported by Mashimo [1] at pressures 30–35 GPa. The ceramics were subjected to the action of low temperatures. There were no significant changes in the specimens recovered after storage in liquid nitrogen and helium. Recording of the profiles of the free surface velocity of the specimens during single-stage shock compression allowed us to determine the dynamic elastic limit  $\sigma_{\text{HEL}}$ , as well as spall strength of the material  $\sigma_{\rm sp}$  versus maximal shock pressure  $P_{\rm max}$ . The experimental details are described elsewhere [2]. As for the high-density ceramic,  $\sigma_{\rm HEL} \sim 15.1 \,{\rm GPa}, \sigma_{\rm sp} \sim 1.3 \,{\rm GPa}$  at  $P_{\rm max} \sim 7.9 \,{\rm GPa}, \sigma_{\rm sp} \sim 0.8 \,{\rm GPa}$ at  $P_{\rm max} \sim 13.7$  GPa,  $\sigma_{\rm sp} \sim 1.1$  GPa at  $P_{\rm max} \sim 20.9$  GPa. As for the lowdensity ceramic,  $\sigma_{\rm HEL} \sim 9.2$  GPa,  $\sigma_{\rm sp} \sim 1.1$  GPa at  $P_{\rm max} \sim 8.1$  GPa,  $\sigma_{\rm sp}\sim 0.6$  GPa at  $P_{\rm max}\sim 14.2$  GPa,  $\sigma_{\rm sp}\sim 0.8$  GPa at  $P_{\rm max}\sim 20.6$  GPa.

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#### SHOCK COMPRESSION OF CARBON NANOTUBES UP TO 100 GPa

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Recent experiments in a diamond anvil cell (DAC) [1], [2] demonstrate high structural stability of double walled carbon nanotubes (DWNTs) exposed to a static pressure of 35 GPa. Here we report on the study of DWNTs after application of stepwise shock compression in a recovery assembly. In the different shock wave experiments the pressure was ramped to a certain level (14, 19, 26, 36, 52 and 98 GPa) with a new CNT sample but always from the same source batch. Peak shock pressures in the specimens were achieved by several reverberations of waves between the walls of the recovery ampoules. The recovered samples were characterized by Raman, XPS and HRTEM revealing outer wall disruption along with unzipping and shortening of the CNTs. Structural damage of the CNTs increases with the shock pressure. Simultaneously, the Raman data exhibit a steep increase of D/G-band intensity ratio.

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# EXPERIMENTAL INVESTIGATION OF COMPRESSION WAVES IN CERIUM AT PRESSURES UP TO 6 GPa Zubareva A.N.,\* Kolesnikov S.A., Utkin A.V. IPCP RAS, Chernogolovka, Russia \*zan@ficp.ac.ru

Cerium (Ce) has a number of unusual thermodynamic properties as compared to other metals. Their presence leads to the formation of a complex pattern on the Ce phase diagram in the region of relatively low pressures [1], [2] and to appearance of multi-wave structures during fast dynamic loading of Ce. In particular, it is shown theoretically in [2] that the anomalous behavior of  $\gamma$ -phase cerium compressibility up to the pressure of  $\gamma$ - $\alpha$  transition (~0.8 GPa at room temperature) leads to the impossibility of a shock front formation at that pressures. It means that compression of Ce must be isentropic in that region. With further increase of pressure the appearance of a two-wave structure consisting of the head-on wave of isentropic compression and the following shock wave was expected.

In this study the experiments on one-dimensional dynamic loading of 2 and 4 mm thick,  $\emptyset$ 30 Ce samples with 0.4–2.0 mm thick metal flyer plates that were accelerated with various types of plane wave explosively driven generators were conducted. In those experiments dynamic compression pressures of 0.5 to 6 GPa were reached. Profiles of free surface velocity of loaded Ce samples were obtained with VISAR laser velocimeter.

At the loading pressure of about 0.5 GPa the isentropic compression wave which was blurred in time was registered. It was caused by the anomalous compressibility of  $\gamma$ -phase of Ce. At the increase of loading pressures to values higher than 0.8 GPa that corresponded to  $\gamma$ - $\alpha$ transition the predicted [2] two-wave configuration was observed which consisted of the similar wave of isentropic compression and the following shock jump. Moreover, at the profiles obtained for experiments with thin (0.4 mm) aluminum flyer plates the shock rarefaction wave was clearly registered in Ce samples, the appearance of which was also expected due to the anomalous compressibility of  $\gamma$ -phase.

In several samples spall phenomena were also registered. The analysis of corresponding wave profiles shows a strong dependence of the spall strength of Ce on the strain rate. At its increase by an order of magnitude  $(3 \cdot 10^4 \text{ to } 3 \cdot 10^5 \text{ s}^{-1})$  the spall strength rises from 0.4 to 0.6 GPa.

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## ELASTIC-PLASTIC PHENOMENA IN SHOCK WAVES CAUSED BY SHORT LASER PULSES. COMPARISON OF HYDRODYNAMIC AND MOLECULAR DYNAMICS SIMULATION

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A comparison of the hydrodynamic calculations of shock waves in the target, caused by short laser pulses, using a standard equation of state and with the additional consideration of elastic shear stresses in the solid was studied.

In contrast to the liquid in which the pressure is isotropic, in the solid stress depends on the direction and there is an additional stress associated with shear deformations. In the approximation of isotropic continuum under uniaxial compression along the x-axis in the linear approximation, this additional stress can be taken in the form  $S_{xx} = (4/3) G \partial (x-x_0) / \partial x_0$ , where G—shear modulus,  $x_0 = x(t = 0)$  in unperturbed media. This additional elastic shear stress results in an effective increase in the rigidity of the substance, which leads, in particular, to increase the speed of sound.

We have included the allowance for the contribution of the elastic shear stress in the scheme of two-temperature thermo-hydrodynamic calculations.

The calculations are compared with similar calculations without elastic shear and the results of molecular dynamics simulations and experiments reported at Elbrus-2010. This comparison shows the fundamental importance of the elastic shear stresses.

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# CRITICALITY OF DAMAGE–FAILURE TRANSITIONS UNDER DYNAMIC AND SHOCK WAVE LOADING

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Statistical theory of evolution of typical mesoscopic defects (microcracks, microshears) revealed specific type of criticality—the structural– scaling transitions and allowed the development of phenomenology of damage-failure transition based on the definition of non-equilibrium free energy of solid with defects. The key results of statistically based phenomenology are the establishment of characteristic multiscale collective modes of defects responsible for damage-failure transition in glasses and ceramics. These modes have the self-similar nature of the solitary wave and blow-up dissipative structure, and provide the multiscale mechanisms of damage-failure transition under dynamic crack propagation, power scaling laws of fragmentation statistics and spall failure. Dynamic and shock wave experiments coupled in-situ with VISAR particle velocity, fracture luminescence and the following structural (SWFM and AFM surface morphology) study of recovered samples in terms of scaling invariance supported the linkage of the evolution of these modes with material responses in large range of load intensity (dynamic crack propagation, fragmentation statistics, spall failure) allowed the interpretation of the following effects: - Nonlinear crack dynamics and the transition from the steady-state to the branching regime of crack propagation in PMMA. The existence of two critical velocities, three characteristic regimes of crack dynamics as the precursors of fragmentation;

-In-situ power law temporal statistics of fracture induced luminescence and fragmentation statistics of recovered fused quartz samples under dynamic and shock wave loading;

–Nonlinear asymptotic laws of damage kinetics under spall failure in shocked materials, the interpretation of dynamic branch phenomena supported by the SWFM and AFM spatial scaling laws of defects statistics in spall area of recovered samples.

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#### SPALL FRACTURE OF VERY COARSE GRAIN VANADIUM

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Coarse grain vanadium specimens were investigated under plate impact loading conditions. Specimens were 100 mm in diameter and thickness was 5–15 mm. Grain size was 10–15 mm which is close to the thickness of the specimen. Free surface velocity was measured by VISAR. Area where free surface velocity was measured was 0.2 mm diameter in order to investigate single grain. Plastic front have a several changes of slope which can be related to the interaction between plastic waves in adjacent grains. Consecutive microphotographs of structure in longitudinal section of saved samples were obtained by high-resolution SEM and optical microscopy. Damage of material close to the spall surface was found in form of microcracks.The formation of these microcracks has essentially crystallogeometrical nature. Investigation of the spall surface shows that brittle fracture is dominant. Quantitative analysis of obtained data allowed us to reveal regularities of defect ensemble evolution and compare it with theoretical predictions.

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#### NUMERICAL SIMULATION OF SHOCK WAVE LOADING OF METALS AND CERAMIC

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Hard ceramics as an alternative to metals used in conditions associated with intense impact loading, and thus exhibit plastic properties. Because of the high cost of complex ceramics becomes a relevant forecasting result of impacts by numerical simulation. In present investigation theoretical research and numerical simulation of shock wave loading of metals and ceramics was carried out. The high strain rate response of ductile and quasibrittle materials (strain and damage localization) is linked to a specific type of criticality (structural-scaling transitions) in microshear and microcracks ensembles [1–3]. The constitutive model developed in [4] and considering the influence of defects kinetics on relaxation processes in metals and ceramics are analyzed on the basis of results of the statistic-thermodynamic description of collective behavior of defects. The additional macroscopic variables characterizing evolution of structure are the tensor of density of defects (the deformation induced by defects) and dimensionless parameter of a structural scaling, representing the relation of scales of dislocation structures (their size and distance between them), involved in process of a structural relaxation. Numerical simulation of shock wave loading for ceramic (silicon carbide) allowed us to obtain a satisfactory agreement with experimental data.

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#### NUMERICAL SIMULATION OF THE PLASTIC FLOW LOCALIZATION AT THE HIGH STRAIN RATE SIMPLE SHEAR AND UNIAXIAL COMPRESSION

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Localization of plastic flow often takes place at dynamic deformation and it influence on the resulting strength of the material. From classical viewpoint it is connected with thermal softening, which leads to a combined increase of temperature and deformation—formation of the adiabatic shear bands [1]. But this scenario is inapplicable in the case of thermal strengthening of material against shear, which is experimentally observed [2] at least in pure metals at high strain rates. The plastic relaxation rate is restricted by the number of dislocations and by their velocity [3]; at the high strain rate it leads to a strain softening, which can be another reason for the localization of plastic flow in dynamical conditions.

We numerically investigate an influence of initial perturbations of temperature or dislocation density and of the stress concentrators on the localization of plastic flow. A high-rate simple shear of micro-sample was simulated as well as a shock compression of the perturbed sample. Twodimensional case was considered with use of the continuum mechanics and the dislocation plasticity model [3, 4]. Perturbations of the temperature or dislocation density lead to restricted localization of plastic deformation, but they can not initiate instability of the plastic flow as a self-sustained and increasing process. Nonuniformity of acting stresses is the main factor of the localization of the plastic deformation. Therefore, the process of localization must substantially depend on the loading conditions and on the internal structure of the material (on the presence of inhomogeneities, pores, inclusions and of the other stress concentrators).

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## ABNORMAL HALL–PETCH RELATION IN ULTRAFINE-GRAINED COPPER AND ALUMINUM AT EXTREMELY HIGH STRAIN RATES

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Materials with ultrafine-grained structure as well as nanocrystalline materials were widely investigated both theoretically and experimentally for the last twenty years. This goes in parallel with the development of experimental technic and molecular dynamics simulation methods, which are useful for simulation of the extremely high rate deformation with the strain rates above  $10^6 \text{ s}^{-1}$ . Such high strain rate creates an unique deformation condition with some additional effects which are not typical for a quasi static deformation. For investigation of the internal defect structure influence on the macroscopic strength and ductility one can take some microscopic mechanisms proposed by theoretical investigations and molecular dynamics simulations and to include it in the modeling in the framework of continuum mechanics. Simulation results could be verified by comparison with experimental data for the shock wave propagation [4] and Taylor rod experiments. This way, supplemented by the procedure of

averaging over the substance volume, allows us to monitor the change of defect structure and its influence on the strength parameters of different metals. In the frame of the proposed in [1, 2] plasticity model we have two competing mechanisms of plasticity. Model for plasticity caused by the dislocation slipping proposed in [3]. Model for describing grain boundary sliding proposed in [2]. Simulation results demonstrate that at strain rate above  $10^6 \text{ s}^{-1}$  the ultrafine-grained metals have the maximum dynamical yield strength and it is the most persistent to spall fracture initiation because energy dissipation is maximal. Abnormal and inverse Hall-Patch relations in the ultrafine grained copper were demonstrated by numerical simulations; dislocation starvation effect is related for its explanation.

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#### SIMULATION OF MULTI-MATERIAL HYDRODYNAMIC FLOWS USING ADAPTIVE MESHES

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In this work, we consider the hydrodynamic model of a multi-material media, combined with a procedure for constructing of the block-structured adaptive meshes that is implemented in the package Chombo. Adaptive meshes can efficiently redistribute computing resources and substantially save a machine memory to solve multi-dimensional problems. The described approach is implemented in a computer program GORGONA to simulate a variety of problems of the physics of high energy densities. The effectiveness of adaptive mesh refinement approach has been studied in massive parallel calculations.

#### NUMERICAL MODELING OF THE PROCESS OF PENETRATION OF LONG PROJECTILES INTO TARGET TAKING INTO ACCOUNT RADIAL OSCILLATIONS

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The results of computational experiments of process penetration of long projectiles into layered targets are presented. As projectiles we used the the steel cylinders with ogive, conical and flat head parts of same mass and diameter. Object of study was impact of projectile on a three layered target with an additional reinforce layer, located in different parts of the obstacles. In the 2D axial formulation process perforation by projectiles of various targets was investigated. Model behavior of medium corresponds to the modern physical notions of deformation and destruction of homogeneous and heterogeneous media under shock wave and explosive loads. It is elastic plastic, porous model of medium that takes into account fracture under shock wave loading. The model includes the concept of joint formation of spall and sheared destructions. Equation of State is selected in the form of Walsh. As the tool of research used the numerical method of finite elements, which is complemented by the mechanisms of splitting nodes and destruction of finite elements. The originality of technique is a new way of allocating surfaces breaking the continuity of material that does not impose serious restrictions on the modern dynamic contact problems of mechanics of deformable solids. This method is already more than 15 years in the Department of Mechanics of Deformable Solids in the Research Institute of Applied Mathematics and Mechanics at Tomsk State University. Updated method has a new mechanism of splitting nodes, applies to both volume and forces criteria of destruction of materials. This innovation allows to get picture closest to real destruction under shock wave loading. Series of computational experiments on shock loading of barriers by projectiles were performed. Calculations were carried out for the axial symmetrical statement. The initial impact velocity was equal to 700 m per sec. The process of perforation was studied for the normal impact. Computations were carried out by using the SKIFF Siberia supercomputer. Results are presented in the form of configurations target and projectile, graphs and tables.

#### 3D-CODE FOR CALCULATION OF STRESS WAVES IN THE SHELL WITH VISCO-ELASTIC FILLER HAVING THE INTERNAL CHANNEL

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The action of pressure impulse upon thin-wall cylindrical shell with filler that has inner canal of arbitrary form is considered. The model of linear viscoelastic media is used for polymeric deformation description. The equations of nonstatic filler motion are written in cylindrical coordinates. The shell motion is considered within the framework of the Kirgof-Lava model for thin-wall elastic shells.

The displacement and radial stress equalities are given on the boundary between filler and shell. The circumference displacement discontinuity is possible, because free slip of shell in relation to filler is expected. At the borders of filler-shell system the conditions of rigid wall are used. The inner boundary (the canal surface) is taken to be free from stress.

It's proposed that the pressure impulse distribution at the surface of given construction and canal surface has the same symmetry plane, that passes along cylindrical shell axis. In numerical calculations it makes possible to consider just half of calculating area.

The solution of equations that describes the united nonstatic shell and filler deformation is complicated by the fact that boundary conditions are formulated at curvilinear canal surfaces. That's why it's convenient to make spatial variables converting that image calculation area into unit cube. Written in new variables the equations can be calculated with finitedifference method by implicit scheme. The scheme is built by spatial variables separation method. As well as after the exchange of variables in equations the mixed derivations are appeared the multycyclical scheme of separation is used.

At every cycle the solution of algebraic equations system that were obtained after linearization of initial equations in finite-differences form by Newton method is made by matrix running with the main element choice by column that is theoretically correct for any defined system of equations (in comparison to the usual running the practical "diagonal prevalence" criterion isn't required).

The results of pressure pulse action upon composite material shell with filler that has a canal in the form of six-beam star were provided by elaborated code. The possibility of damage appearance during compression wave reflection from canal surface because of expanding forces concentration between the beams is shown.

# THERMAL EFFECTS IN A GAS WITH CONDENSED PARTICLES AT SHOCK WAVE CONDITIONS Obruchkova L.R.,\* Baldina E.G., Efremov V.P.

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Two-phase media (gas and condensed particles) is generated by severe accidents and volcanic eruptions conditions. Guarantee of supersonic aircraft flight safety in these conditions requires carrying-out of an analysis of micro environmental perturbations associated with the particles. Body streamlined by gas produces both the pressure and thermal disturbance on the flow. It is known [1] that Stokes formula can be applied to describe the force impact of the body into the flow at low Reynolds numbers. The aim of this study is to investigate the thermal influence of the body on shockwave gas flow around single particle. Shock wave simulation is realized by means of the two-dimensional hydrodynamic code. The shock wave was initiated by instant removal of the diaphragm, which divided areas of high and atmospheric pressure. A particle was placed at such a distance from the diaphragm when distribution of all flow parameters was time independent. In other words, current observation time exceeded velocity and thermal relaxation times. The ideal gas equation was chosen as equation of state. The heat transfer between the tube and the flow and between the flow and particle was not taken into account. Flow temperature in front of the particle increases because of flow stopping with pressure increasing. This effect is obtained numerically by varying the value of higher pressure (ahead of the diaphragm) and the diameter of the particles. The present study is directed to estimate and analyze the thermal effects in a gas with condensed particles at shock wave conditions.

<sup>1.</sup> Prandtl 's Essentials of Fluid Mechanics. New York: Springer, 2004

#### DEVELOPMENT OF TWO-STAGE ELECTRO-THERMAL WAY TO ACCELERATE SOLID BODIES

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The paper describes some results of experiments with the aim of development of two-stage electro-thermal way to accelerate solid bodies. Indepth information for this way was represented in [1]. Current research is directed to increase accelerated bodies' mass and to design spark switchboard having higher value of efficiency. Velocities in 2.0 and 3.1 km/sec were achieved for bodies with mass of 280 and 106 mg accordingly. Velocity was calculated empirically by crater's parameters in semi-infinite target. Accelerated bodies and targets were made from AMG-6 aluminium alloy. Two switchboard constructions were designed, created and tested. However both of them were destructed when capacitance loop was discharged at 12.5 and 19.5 kV of charging voltage accordingly. Earlier results [1] showed good efficiency of acceleration in 10% with using non-permanent switchboard. The prototypes of reusable switchboard had efficiency 2.9% for first construction and 1.4% for second one. Efficiency decreasing was explained by the poor mechanical resistance of switchboards and their premature destruction. Switchboard's construction is planned to be improved in the near future.

The researches were conducted with using of hot plasma generator under financial support of Ministry of Education and Science of Russian Federation within the bounds of government contract No. 14.518.11.7005 and President's Grant MK–1091.2013.10.

Spitsin D.D. Zikova T.S. Yanevskiy V.D. Vorobiev A.A. Experimental research of micrometeorites impact on spacecrafts in laboratory environment. Physics of Extreme States of Matter—2011. Chernogolovka. P. 59–61.
## GENERATION AND PROPAGATION OF SHOCK WAVES IN UNDER MECHANICAL PULSED LOADING

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Response of dusty plasma clusters on mechanical pulsed loading on the base of the molecular dynamics method was investigated. Simulated dusty plasma systems had cylindrical shape. Yukawa potential was used to describe interparticle interaction. Dust particles were confined by parabolic electrostatic potential in two directions and by rigid walls in third one. Shock waves were generated in the simulated system by high rate shift of the rigid wall.

Calculations showed that above mentioned loading led to generation of compression and tensile waves. Amplitude of the compression wave decreased with time. At the same time the amplitude of the tensile wave that came after a compression one increased. It was revealed that the propagation of the shock wave did not break the shell structure

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## REFLECTION SHOCK WAVE ATTENUATION DEPENDS ON POSITION OF DESTRUCTIBLE OBSTACLE

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Construction of devices for weaken of the explosion effect is a prospective issue, especially for purposes of protecting people from terrorist attacks and industrial explosions. Most damage of explosion is caused by reflection shock wave.

There are several approaches to the creation of the method, which reduces the intensity of the shock wave. Those methods based on usage of easily destructive materials with a different material properties. In several issues suggested to use granular materials [1] and walls of wet sand [2] as barriers to isolate potentially dangerous substances. The using of material without large fragments can significantly reduce the intensity of the incident shock wave [3]. In the event of an explosion in a confined space it is important to study the weakening of the shock wave reflected from the wall, as it has a greater intensity. But attenuation of the reflected shock wave is depends not only on material properties but also on boundary conditions.

In this paper the shock wave reflection from obstacle made of easily destructible material was investigated. The technique of studying of shock wave attenuation after reflection from easily destructible obstacle was developed. The attenuation of reflection shock wave is depends on thickness of the obstacle and also depends on distance from obstacle to the wall. Different mechanism of shock wave reflection depends on sizes and boundary condition was obtained.

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## SHOCK COMPRESSIBILITY OF LOW SENSITIVE HE OF VARIOUS INITIAL POROSITY

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Shock compressibility of HE is conventionally studied by optical lever method in experiments with wedge samples, or with the help of electromagnetic gauges of wave and mass velocity. In this work, parameters of shock wave in low sensitive HE were registered simultaneously by piezo resistive and radio interferometric methods. Loading of HE with various initial porosity was performed with the help of explosion shock wave generator. Piezo resistive gauges registered pressure of shock wave, which enters the charge out of HE under study. Detailed tracking the trajectory of shock wave (with an error of several percents) permits to determine the initial velocity of shock wave, which enters the HE under study, and together with the data on pressure measured by piezo resistive method to determine points on Hugoniot of unreactive HE with various initial porosity. Comparison of the data on shock compressibility obtained in this work with the data obtained by optical lever method showed good agreement. Along with this, method of getting Hugoniot realized in this work has several advantages in comparison with optical lever method. Having high informativity, optical lever method can not be used for investigating shockwave compressibility of porous (heterogeneous) materials. It is related to the fact that while analyzing the results, one uses a condition of mass velocity doubling, when shock wave arrives at the free surface of HE sample under study, which violated for porous media. The method proposed in this work has no such limitations and can not be sued for investigating shock compressibility of high explosives with various initial porosity.

#### SHOCK-TO-DETONATION TRANSITION IN POROUS LOW-SENSITIVITY HIGH EXPLOSIVES

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Usually information about shock wave transition into detonation (SDT) under initiation of HE is obtained with the help of experiments with wedge HE samples, or by registration of evolution of wave pressure profiles or mass velocity. In this work, transition of shock wave transition into detonation was registered simultaneously with the help of piezo resistive and radio interferometric techniques. Piezo resistive gauges registered parameters of shock wave entering the charge out of HE under study and parameters of shock/detonation wave coming from it. Radio interferometer registered x t diagram of the process of shock wave (SW) propagation and its transition into detonation wave (DW). Precise processing of trajectories of shock wave transition into detonation, which was performed in this work, permitted to check the validity of approximation of a single curve (SCI), in accordance with which he transition of initiating shock wave transition into detonation is made according to the only one for this HE curve in a plane  $P-x_0$  (plane Pop-plot) regardless of the value of initial pressure and initiating SW profile. The validity of the latter is usually proved by coincidence of x-t diagrams brought in one coordinate system with the center in a point  $(x_0, t_0)$ —shock wave transition into detonation. Detailed analysis performed in this work showed that SCI approximation is not met for HE studied in this work. SCI approximation is not met for all initial HE porosities investigated in the work. Detailed processing of trajectories of shock wave transition into detonation permitted to build Pop-plot only on the basis of data obtained with the help of radio interferometer, i.e. without attracting the data obtained by piezo resistive method. Presented diagrams for various porosities of HE under study have physically correct asymptotes. On the top, the diagrams are limited by detonation velocity. In the bottom, they are limited by the velocity of shock wave propagation at Hugoniot elastic limit. Initiation can not occur lower than this value, as far as mechanism of hot points at lower velocities can not be realized.

#### DIFFRACTION STUDIES OF TATB

Ten K.A.,<sup>\*1</sup> Pruuel E.R.,<sup>1</sup> Lukyanchikov L.A.,<sup>1</sup> Tolochko B.P.,<sup>2</sup> Shmakov A.N.,<sup>2</sup> Zhulanov V.V.,<sup>3</sup> Shehtman L.I.,<sup>3</sup> Aminov Yu.A.,<sup>4</sup> Muzyrya A.K.,<sup>4</sup> Kostitsyn O.V.,<sup>4</sup> Smirnov E.B.<sup>4</sup>

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Detonation characteristics of explosives are in strong dependence on internal parameters of initial compositions. Conditions of initiation, as well as crest values in the cumulative process, depend on the presence of voids (pores) and their size distribution. Monitoring of such parameters as irregularity size distribution and variation of lattice parameters as a function of temperature are a topical task. Diffraction techniques allow one to find out internal parameters of TATB explosives in a nondestructive way. The object of the study were new explosives, promising from the industrial point of view, which were manufactured on the base of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). TATB has high effective temperature resistance and ability to decompose (without explosion) under further heating. This paper gives an account of diffraction studies of TATB-based explosives, carried out with the use of synchrotron radiation from the VEPP-3 accelerator complex. Presented are the results of the measurements of SR small-angle X-ray scattering and determination of irregularity distribution in the range of 2 to 10 nm at temperature variation from 27 to 240°C. The paper also presents the results of measurement of TATB diffraction reflections under heating to 240°C and compression in diamond anvils to a pressure of 6.5 GPa.

#### STRUCTURE OF CONDENSED HETEROGENEOUS EXPLOSIVES

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Applied methods of nondestructive survey of HE structure are reviewed. Currently available basic results are provided. The molecular structure of individual explosives having characteristic sizes of 0.1-1 nm was studied with the help of directions methods (XRD) (including the case with the changing temperature and the applied static pressure) and the diamond any limit method. The obtained results allow the isobaric and isothermal curves to be constructed as they are needed to construct the equation of state. In addition, these investigations give valuable information how the molecular structure changes under external stimuli (temperature and pressure) including the case when they approach the critical level. The small angle X-ray scattering method (SAXS) was used to study the structure of heterogeneous explosive charges. This method registers scatter for randomly distributed voids in an explosive material. The structure sizes registered in our experiments range from 1 nm to 10 nm. The structures with the size ranging from 1 um to 10 mm were studied with the help of Xray computer micro tomography that uses synchrotron radiation (XRCT). Sizes in the range from 10 nm to 1 um will be studied with the help of the ultra small angle X-ray scattering method (USAXS) being currently developed. In order to gather quantitative data on the in homogeneities distribution from small and super small angle X-ray scattering results, we need information on actual topology of air inclusions inside an explosive material. The raster electron and optical microscopy methods were used for this purpose. These methods helped to determine, first, the shape and size of in homogeneities in an explosive, as well as the size of in homogeneities in an explosive in the range from 100 nm to 10 um. As a result, the study provided quantitative characteristics of the structure morphology of the test explosive material and these data will be used to construct mathematical models for the kinetics of condensed heterogeneous explosive decomposition.

## ABOUT APPLICABILITY LIMITS OF EMPIRICAL RATIOS FOR A VELOCITY OF NONIDEAL DETONATION OF RDX

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The generalized empirical dependence of a detonation velocity of cylindrical RDX charges in nonideal regime  $D(\rho, d)$  can be taken from a file of experimental data  $D(\rho, d = const)$  and  $D(d, \rho = const)$ . Here  $\rho$ —RDX density of a charge; d—RDX diameter of a charge. The standard ratios of a detonation velocity in ideal  $[D_{as}(\rho) = D_{bp} + M_{as}(\rho - \rho_{bp})]$  and nonideal  $[D(d) = D_{as}(1 - K/d)]$  regimes can be used as base. Here  $D_{bp}$  and  $\rho_{bp}$ —a detonation velocity and RDX bulk density in a charge with big section size;  $D_{as}$  and  $M_{as}$ —a detonation velocity and dimensional factor of proportionality for charges with indefinitely big section size; K—dimensional factor.

We have produced two masses of experimental data of RDX detonation velocity of a charges with thin polypropylene and glass cylinders (thickness of walls of 0.5–1.0 mm) in a range of parameters of  $\rho = 1.0-1.4$  g/cm<sup>3</sup> and d = 9.5-36 mm. Unfortunately, the technology of hand compaction of RDX powder in such cylinders does not allow to observe precisely the condition  $\rho = const$  for a charges of different diameters. Therefore the data for a finding *i* of necessary dependences  $D(d, \rho_i = const)$  we took from dependences  $D(\rho, d = const)$ .

The last one are received by linear approximation of experimentally found values of a detonation velocity of a charges with different values of parameters  $\rho$  and d as  $\Delta D(d_k) = M(d_k)\Delta\rho$ . It has allowed to use in the further procedures a values of detonation velocity  $D(d_k)$  at arbitrarily picked values  $\rho_i$ . The mass of values of a detonation velocity for its approximation *i* by dependences  $D(d, \rho_i = const)$  as  $D(d) = D_{as}(1 - K/d)$ has been determined in such a way.

These dependences are constructed separately for charges with both polypropylene and glass shells. The constructed dependences give closely spaced values of  $D_{as}$  and  $M_{as}$  for experimentally tested sizes of a charge diameters (9.5, 12.5, 15 and 19 mm for polypropylene and 10, 16, 24 and 36 mm for glass shells) for any density  $\rho_i$ . However, it turned out that dimensional factor K depends on density of a charge. From dependence  $D(d) = D_{as}(1 - K/d)$  follows, that values of factor K < 1 mm define certain sizes on an axis d in coordinates D - d at value D=0. At the same time it is known, that the detonation as process takes place starting only from some value  $D_{cr}$ , when  $d > d_{cr} > 1$  mm. Therefore values of factor K cannot have physical sense.

#### EXPLOSIVE COMPACTION OF THE MIXTURE OF Ni-Al POWDERS IN CYLINDRICAL AMPOULES

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Some variants of explosive assemblies with cylindrical ampoules of preservation for dynamic compaction of powder mixture and initiation of chemical synthesis intermetallic Ni-Al are tested experimentally.

The scheme of realization of dynamic initiation of chemical synthesis in cylindrical ampoules is based on a longitudinal detonation of a cylindrical HE charge. An ampoule was placed on axis of HE charge. Sliding of detonation wave on a surface of an ampoule drives in it a wave of compression. Character of pressure change upon surfaces of an ampoule depends on design features of explosive assembly which influence the expiration of detonation products. HE charge had diameter of 57 mm and length of 70–100 mm. Diameter of a cavity of an ampoule was equal 5–8 mm, the length was equal 30 mm. Thickness of a wall of an ampoule was equal 2.5 mm. The weight of a HE charge was equal 160–300 g.

The analysis of shock-wave dynamics in designs of different explosive assemblies has shown, that dynamic acting on a wall of an ampoule proceeded more than 30 mcs and had variable value in a range up to 25 GPa. The estimation of postshock temperature of ampoules of preservation has given value 400–450 K according to measurement of rate of its decrease after dynamic acting.

As an initial material powders Ni and Al with the size of particles  $1-10 \ \mu m$  are used. A powder of an initial material in mass parts of 0.7Ni+0.3Al was pressed in a cavity of an ampoule up to relative density 0.55-0.70. Porosity of pressed powder was been in range of 0.31-0.42.

X-ray structure analysis of compacted samples and distribution of porosity along their length were been made after dynamic influence on ampoules. X-ray structure analysis has shown presence of some quantity intermetallic phases of Ni-Al. Distribution of porosity has shown obvious correlation with time change of pressure upon surfaces of an ampoule. Porosity of compacted sample has shown value of 0.22–0.35 in relative measurement from initial porosity on the average section of a cavity of an ampoule. The final relative density of compacted sample has shown value of  $0.87{-}0.93.$ 

Thus, experience of designing of cylindrical ampoules of preservation and explosive assemblies is received for carrying out experimental works in the field of of new materials and research of properties of substances.

## METHOD OF DETERMINATION OF SHOCK WAVE EXPLOSIVE SENSITIVITY

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Well known that the critical pressure of initiation and critical diameter are both connected with shock wave sensitivity [1]. Other parameter which influence to initiation pressure and critical diameter is speed of destruction wave which could be determined by formula [2]

$$C_0 = C_{PD} \left(\frac{\rho}{\rho_0}\right)^3,\tag{1}$$

where  $C_0$ —sound speed in explosive;  $C_{PD}$ —sound speed in detonation products;  $\rho$ —density of detonation products;  $\rho_0$ —density of explosive. Sound speed in explosive directly depends on the starting sound speed in explosives. In this case initial pressure and critical diameter have to influence to both parameters, moreover increasing of explosive energy  $(U^2)$ decreasing initial pressure and increasing of sound speed in other way increasing both values. The better way is choosing the well known explosive HMX as a standard and comparing to it a lot of other well known explosives. On the basis of the foregoing is offered to compared critical pressure P in the following correlation

$$\left(\frac{\frac{C_x}{U_x^2}}{\frac{C_{HMX}}{U_{HMX}^2}}\right)^{\mu} = \frac{P_{HMX}}{P_x},\tag{2}$$

where index HMX—standard material (octogen); index x—explosive; C—sound speed in explosive; U—mass speed of explosive.

In addition, factor  $\mu$  is around  $\approx 1.7$ . Verifying of the correlation with several explosives shows a small difference in results of calculation. Absolute value of initial pressure criterium could be calculated without any

difficulties from correlation of known sensitivity HMX and other explosives.

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## CALCULATION OF EFFICIENCY OF EXPLOSIVE TOSSING ENERGY FOR METHODS M-60 AND T-20 Reut I.I.,\* Krivchenko A.L.

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For practice usage of dynamic loads effects you have to know following characteristics: sound speed in explosive and in tossing material, detonation and mass speed and etc. Development of theoretical methods of predictive modeling of tossing speed are need a full analyzing of shockwaves processes during dynamic loads. For calculation of widening speed of copper cylindrical confinement  $W_c$  for method T-20 following expression are offered:

$$W_c = \frac{C+U}{2.6+\beta},\tag{1}$$

where C—sound speed in explosive; U—mass speed of detonation products;  $\beta$ —loading factor. Results of calculation were compared with experimental data of 30 explosives. The mean-square deviation is  $\Delta = \pm 51$  m/s (2.6%). For calculation of relative tossing speed of tossed element  $W_e$  by abutment tossing method M-60 method of equivalent mass are developed:

$$W_e = U \sqrt{\frac{4}{3} \frac{r\rho_0}{h_p \rho_p}},\tag{2}$$

where r—basis radius;  $\rho_0$ —density of explosives;  $h_p$ —thickness of tossing plate;  $\rho_p$ —thickness of tossing. Results of calculation were compared with experimental data of 30 explosives. The mean-square deviation is 3.5%. Offered methods of calculation of abutment tossing speed by method of equal mass and method of approximate calculation of widening speed of copper cylindrical confinement are gave the similar results as experiments and could be used for preliminary valuation of tossing power. 1. Physics of Explosion. T.1. Under the editorship of Orlenko L.P. Moscow: FIZMATLIT, 2004. 832 p.

## NUMERICAL ANALYSIS OF AUTO-IGNITION AND DETONATION OF HIGH-ENERGETIC MATERIALS UNDER EXTERNAL TEMPERATURE CHANGE

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Using mathematical modeling the problem of thermal explosion in the samples of heat-resistant high–energetic materials—RDX and HMX was solved. The focus is on the effect of external temperature fluctuations on the development of self-heating in the samples of different sizes. The diameters of the samples—12, 15, 50 cm. A case of axial symmetry is considered.

High–energetic materials after manufacture in industrial enterprises and various tests laid down for storage in warehouses. Storage of explosives experience shows that their sensitivity to external influences increasing over time, due to change of properties, which kitted explosives.

Various chemical and physical properties of explosives and their sensitivity to thermal effects, as well as the serious consequences for both the human and for the environment from their explosions, the real question about its safety under external thermal effects, such as oscillations of ambient temperature.

The problem was solved on the basis of the classical theory of thermal explosion [1] in two-dimensional axisymmetric unsteady formulation, during the flow of the first order reaction in the medium filling the area substance height of h and diameter d. The boundary between the explosives– environment, is the boundary on which the influence of heat the ambient temperature changing a sine curve [2].

The calculation results suggest that the heat-resistant explosives (HMX and RDX), included in the ammunition could catch fire due to external temperature fluctuations. The induction period can be very short and does not reach the stage of cooling, it is an explosion occurs in the stage of seasonal heating. Given that the storage of ammunition are in places where the risk of fire, the ambient temperature can reach high values, sufficient to lead to self-ignition of explosives [3].

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#### MECHANISM OF HYDRODYNAMICAL PERTURBATIONS EVOLUTION IN THE FLOW UNDER THE MOVING PISTON

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The studies of perturbations evolution and turbulence origins in the gas flows remain relevant for a decades. Studying the features of the dynamical processes can provide an information on the turbulent flows classification and their roles in these processes. Thus a developed phase of turbulence corresponds to the homogeneous isotropic turbulence for which there are no structure formation of the perturbations by definition. At the same time the dynamics of axisymmetric flow [1] on the stage previous to the isotropic does not contradict to the formation of sustained connections between perturbations. This paper is devoted to reveal and analyze the emergence and evolution of such connections. The study is based on the example of the axisymmetric flow in a chamber under a moving piston and carried out using 2D and 3D direct numerical simulations. The emergence and evolution of the structures in the flow under the moving piston is obtained from the visualization of the perturbations fields at the different time instants. While the flow fields under the moving piston represents identical slightly curved vertical lines going from the piston surface to the opposite end approximately during the whole phase of compression stroke the perturbations of these flow fields creates a complex pattern permanently changing over time. Analyzing the pattern evolution it is shown that the basic pattern for the evolution of the perturbed flow field is independent on the spatial dimensionality of the problem: randomly oriented weak perturbations merge into vortical structures which corresponds to the dynamics of entropy vortices. Further the spatial scales of these structures increase due to the vortecies interaction and diffusion. It allows us to conclude that the observed formation of the vortical structures in the chamber under the moving piston primary is caused by a non-linear dynamics of vortical fields.  Breuer S., Oberlack M., Peters N. // Flow, Turbulence and Combustion 2005. V. 74. P. 145.

## MECHANISMS OF CHEMICAL REACTION WAVE IGNITION BY TRANSIENT ENERGY SOURCE

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The features of the ignition of different combustion regimes is studied numerically for stoichiometric hydrogen-oxygen mixture using detailed chemical kinetics and transport models. It is shown that depending on the parameters of localized transient energy deposition there are two main mechanisms of reaction wave initiation: the Zeldovich gradient mechanism [1] and the volumetrical thermal explosion (which actually represents one of the asymptotics of the Zeldovich mechanism for the gradient of zero steepness). For practically important time scales the principal scenarios of ignition are: 1) for sub-microsecond pulses the volumetrical explosion takes place inside the hot spot; 2) for microsecond pulses the gradient of temperature and pressure arises on the profile created by the rarefaction wave and ignition starts via Zeldovich mechanism on the gradient of induction time; 3) for millisecond pulses gasdynamical expansion gives rise for a temperature gradient at approximately constant pressure, and the ignition starts according to the Zeldovich mechanism with all the features inherent to chain-branching chemistry disclosed in [2]. In three-dimensional case the spherical expansion of the hot spot weakens shock wave in favor of the intensified rarefaction wave. It results in sufficient drop in temperature and pressure in the hot spot on the time scales of the order of acoustic time. Thus, for the same conditions as in one-dimensional case the less intensive combustion regime arises. The deflagration regimes are less sensitive but to obtain detonation one should sufficiently increase the power of the energy source. The obtained results give the values of energy and power required for ignition of one or another regime of combustion wave, which is important for the practical use and for risk assessment.

<sup>1.</sup> Zel'dovich Ya. B.// Combust. Flame. 1980. V. 39. P. 169.

Liberman M. A., Kiverin A. D., Ivanov M. F.// Phys. Rev. E. 2012. V.85. P.056312

## ROLE OF SPATIAL FACTOR ON FLAME ACCELERATION AND DEFLAGRATION-TO-DETONATION TRANSITION IN RECTANGULAR CHANNEL

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The features of flame acceleration and deflagration-to-detonation transition (DDT) in channels are investigated using high resolution numerical simulations of three-dimensional reactive Navier-Stokes equations, including the effects of viscosity, thermal conduction, molecular diffusion and a detailed chemical reaction mechanism for hydrogen-oxygen gaseous mixture. Results obtained in two- and three-dimensional simulations are compared to emphasize fundamental features inherent to the flame propagating within rectangular channel with no-slip walls. In both cases flame acceleration process has four distinctive stages. Initial stage of flame expansion develops into the stage of exponential increase of flame velocity determined by the non-linear evolution of the wrinkled flame front. On the next stage flame acceleration is determined only by the stretching of the flame and the rate of flame acceleration decreases. On this stage compression waves generated by the flame steepen into the shocks close to the flame front. As a result a pressure peak arises inside the reaction zone causing sharp increase of the flame velocity and actual transition to detonation. In 3D case the run-up distance is shorter because of the higher acceleration rate determined by the features of three-dimensional evolution of the non-stationary flow. The qualitative pattern of flame acceleration and DDT is independent on the specific features of initial conditions and geometry of the channel.

## COMBUSTION REGIMES OF HYDROGEN-BASED MIXTURES IN GAS-FUELED RECIPROCATING ENGINES Smygalina A.E.,\* Ivanov M.F., Kiverin A.D., Zaichenko V.M.

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One of the most actual topics in power generation is utilization of renewable sources of energy including hydrogen energy. Hydrogen as a fuel for gas reciprocating engines has a set of advantages: it provides high efficiency factor and low level of pollutant emission. At the same time hydrogen has low antiknock level and its utilization is connected with high probability of detonation onset during engine cycle. To avoid overloads and destruction of the combustor associated with detonation we assume dilution of the hydrogen-air mixture with another less energetic gaseous fuel (e.g. methane or natural gas) or with recycled combustion products. On the other hand such mixtures containing  $H_2$ ,  $CH_4$ , CO,  $CO_2$  etc (so called mine gases) are of great interest themselves as renewable sources of energy.

This paper represents the results on the determination of composition for mixtures H<sub>2</sub>-Air-H<sub>2</sub>O, H<sub>2</sub>-Air-CH<sub>4</sub> providing the most optimal combustion regimes obtained by means of direct numerical modeling. Here we assumed two criteria of optimal regime: the detonation absence and high magnitude for effective work during the fuel combustion. The research was performed using direct numerical simulation of the combustion process under the moving piston in a cylindrical chamber filled with gaseous mixtures of different compositions. Mathematical model included gasdynamical equations with account of convection of compressible viscous gas, multicomponent diffusion, heat transfer and energy release due to the chemical reactions. Two detailed chemical kinetics mechanisms were chosen to describe the combustion of hydrogen and methane. An output data for each computation represents so-called "indicator diagram" providing information about combustion regime and the diagram for efficient work versus crank angle estimating the efficiency factor of an engine. Depending on the composition gaseous mixture the following combustion regimes were obtained: classical detonation characterized by the sharp pressure increase, slow combustion giving a smooth indicator diagram and intermediate regimes of a "stiff" combustion with sequential sharp peaks of pressure caused by the non-linear flame evolution and compression waves generation within closed chamber. Analysis of the results gave the following compositions of optimal mixtures: 26.5% H<sub>2</sub>-3.0% CH<sub>4</sub>-70.5% Air, 17.0% H<sub>2</sub>-12.5% H<sub>2</sub>O-70.5% Air.

## ALCOHOL SUPPRESSION EFFECT ON SOOT FORMATION IN SHOCK TUBE PYROLYSIS OF BENZENE

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The limitation of fossil fuels as well as soot and greenhouse gases emissions are the great problems in combustion. The ethanol is widely produced from biomass and it is a promising substance as an additive to the

fuels, besides that it can also be utilized as a fuel. The oxygenated additions are expected to decrease a soot formation. The influence of ethanol addition on soot formation was studied in shock tubes [1] and flames [2]. However, no attention was paid to the temperature behavior during soot formation. The aim of this work is to get new experimental data on the temperature effects during soot formation in pyrolysis of ethanol-benzene mixtures behind shock waves. Originality of this work is the simultaneous particle sizing by the laser-induced incandescence and gas-particle temperature measurements by emission-absorption spectroscopy together with the usual observation of soot volume fraction of condensed phase by the laser light extinction technique. The experiments were performed in the temperature range of 1650–2400 K and pressure range of 3–5 bar. The following mixtures were investigated:  $1\% C_6H_6 + Ar$ ,  $1\% C_6H_6 +$  $1\% C_2H_5OH + Ar$ ,  $1\% C_6H_6 + 3\% C_2H_5OH + Ar$ . The decrease of the optical density of condensed phase and the soot particle size with the increasing amount of the ethanol addition was observed in spite of the total carbon atom concentration increase in the mixture. The decrease of the initial temperature behind shock wave was detected during the pyrolysis of all mixtures. The drastic temperature drop due to the decomposition of benzene increasing toward higher initial temperatures and the following temperature rise due to the condensation process were observed. For the low initial temperatures  $T_5=1600-2000$  the behavior of the temperature during the pyrolysis is similar to the pure benzene and benzene-ethanol mixtures. Whereas for higher initial temperatures  $T_5=2000-2400$  K it was found the essential difference in the temperature behavior. The kinetic mechanism of the influence of ethanol addition to benzene pyrolysis is discussed.

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## OBSERVATION OF THE SHOCK WAVE PROPAGATION IN He DILUTED BY Xe

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Shock wave front structure was investigated in high vacuum shock tube "Jashma". The insident shock waves propagated in He diluted by small Xe concentration at conditions: Mach number M = 2.4-3.1, equilibrium pressures 0.3–1.1 bar, temperatures 980–1640 K. The laser-schlieren method of high time and space resolution was employed to study the incident shock waves structure. Simultaneously the emission spectra of heated gas at 200–650 nm region were detected. The density profiles were received. The affect of Xe small admixture on density profiles in shock wave front was established. The Xe-spectra in incident shock waves at low temperatures (1000 K and higher) was measured and analyzed.

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## A RAPID COMPRESSION MACHINE INVESTIGATION OF AUTO-IGNITION AND COMBUSTION OF LIQUID FUELS WITH ULTRADISPERSE ADDITIVES

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The uses of ultra disperse additives of energetic materials offers a promising means of adjusting the reactivity and improving the combustion properties of liquid fuels. This work outlines the development of a rapid compression machine technique for studying the impact of different ultra disperse additives on reducing the ignition delay time and increasing the combustion rate of liquid fuels. Ethanol with nano sized carbon particles produced by electric discharge treatment and n-heptane with aluminium nanoparticles were studied under different experimental conditions: heterogeneous and homogeneous fuel-air mixtures. In the first case a specimen of liquid fuel was placed in a bowl put into the combustion chamber before compression event. It was found that the rate of fuel combustion after electrical discharge treatment can be increased substantially (about 10%). On other hand addition of aluminium nanoparticles (1%-weight) not effect on combustion rate of n-heptane at these experimental conditions. In the second case the homogeneous fuel-air mixture was generated using simultaneous charging of fuel by a nozzle and air to the initially evacuated chamber. At these conditions addition of aluminium nanoparticles can increase the maximum pressure in the test chamber after combustion (up to 20%). In both cases any significant changes of ignition delay time were not observed.

## DETONATION ACCELERATION INVESTIGATION IN THE PULSED COMBUSTOR

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Nowadays many scientific laboratories and aerospace research centers have a reasoned interest in developing absolutely new engines so-called "Pulsed Detonation Engines" (PDE) based on the use of detonation for combustible mixtures combustion. PDE is a semienclosed tube which fills up with the combustible mixture, where a detonation wave triggers. Reaction products flowing out of the open tube end at a high speed, create the jet thrust.

This work describes the features of the deflagration-to-detonation transition at a weak initiation in the pulsed combustor (PC), i.e. the model of the pulsed detonation engine. Also the work presents the evaluation of the possibility and degree of acceleration of the DDT under the same conditions of initiation in the PC fitted with an obstacle of different porous structures prior to the flame front propagation.

The hydrogen / oxygen / air mixture is used as a working charge in different fuel / oxidizer ratios.

## INVESTIGATION OF BOUNDARY LAYER BEHIND THE SHOCK WAVE FRONT

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Currently the shock tube is used more and more frequently in the study of the kinetics of chemical reactions in the gas phase and in the heterogeneous transformation of matter. An important advantage of the shock tube is the simplicity of obtaining the required thermodynamic conditions behind the incident and reflected shock waves. In the experiments, it is assumed that the flow behind the shock wave is uniform and undisturbed, or, at least, is that the effect of the perturbation caused by the boundary layer is small. To study this phenomenon visualization of the flow structure behind the incident shock wave was made by the averaged Talbot-interferometry method [1].

The shock tube with a square cross section was used to generate shock waves in the air with M=1.3–1.6. Grids with square cells  $(12 \times 12 \text{ and } 3.5 \times 3.5 \text{ mm})$  were used to initiate turbulence in the flow behind the shock wave. Interaction of the incident shock wave with the turbulizing grid creates velocity and density pulsations after the shock wave passage. Flow pulsations cause fluctuations of the local refraction index, which can be measured by Talbot-interferometer [2].

Distributions of time-averaged density of the air throughout the whole flow field were calculated for the  $12 \times 12$  and  $3.5 \times 3.5$  mm grids. It is found that the thickness of the boundary layer in the observation area is about 7–9 mm, and the density in the boundary layer behind the shock front raises sharply. This leads to an increase of 6–7% of the average density of the flow at  $\approx 3$  mm from the shock tube wall. The area occupied by the boundary layer reaches half the cross sectional area of the shock tube.

<sup>1.</sup> Talbot F. // Philos. Mag. 1836. V. 9. Pp. 401–407.

Doroshko M. V., Penyazkov O. G., Rankin G., Sevruk K. L., Khramtsov P. P., Shikh I. A. // J. Eng. Phys. Thermophys. 2006. V. 79. Pp. 937–942.

## EXPERIMENTAL INVESTIGATION OF SHOCK WAVE/BOUNDARY LAYER INTERACTION IN HEATED RAMP SURFACE

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The phenomenon of shock wave/boundary layer interaction (SWBLI) emerges on the curved surfaces of the supersonic vehicles. The shock wave appeared in front of an obstacle makes the pressure disturbance in boundary layer of the vehicle surface. This phenomenon is able to cause the boundary layer detachment which leads to energy loses and difficulties in controling. Importance of this problem encourages researchers in their investigations. Over the 50 years of numerical simulations and experiments resulted in crucial similarity equations [1]. Still these equations need to be improved. In order to provide real flight conditions in the laboratory experiments one should not forget about friction heating, as heat transfer affects greatly on the SWBLI [2]. Present work is dedicated to experimental investigation of heated ramp boundary layer behavior in the supersonic flow M=2. Particle Image Velocimetry and Schlieren was used for flow visualisation. Ramp angle was altered from 15 to 45 degrees and temperature of the surface achieved amount of 500°C. Experimental results have shown a good agreement with similarity equations of previous studies.

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# ON VARIOUS TYPES OF REFLECTION OF SHOCK WAVES AS A FUNCTION OF THE ADIABATIC INDEXES

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In the earlier papers of the authors it has been shown that in a steady supersonic flow apart from two well known modes of reflection (regular and Mach), there is another type of reflection—irregular reflection with a negative angle of reflection. It occurs at low rates of adiabatic indexes.

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In this paper the complete picture of different types of reflection of shock waves has been presented as a function of the value of the adiabatic index. It has been shown that the area formerly known as dual solution region, where there may be as a regular and as a Mach reflection, increases with the decrease of adiabatic index. It has been also found that at Mach numbers greater than 3 and the adiabatic index less than 1.4, there is another area of dual solutions. In this area, a regular reflection and various subtypes of unstable configuration with a negative angle of reflection are possible. It has been shown that the configuration with a negative angle may take different subtypes depending on the transition—from Mach reflection or from regular reflection to the configuration with a negative angle of reflection. In the transition from Mach reflection three shock configuration occurs with a negative angle of reflection and the bending on the reflected wave. In the transition from regular reflection, a new form of reflection—a reflection with a negative angle and the second triple point on the reflected wave (double Mach reflection with a negative angle of reflection). All the subtypes of configurations with a negative angle of reflection are unstable: their appearance leads to the disruption of the stationary flow pattern. The results obtained can have wide practical application. At supersonic flight in the atmosphere, when behind shock waves physical and chemical transformations occur, the adiabatic index decreases. In the atmosphere of Mars, which is composed of carbon dioxide, the adiabatic index is less than 1.4. In supersonic jets of products of combustion at high temperatures which outflow from rocket nozzles, the adiabatic index has a value much lower than 1.4. The appearance of the configuration with a negative angle of reflection can critically affect the operation of the aircraft and rocket engine. The defined boundaries of the negative angle of reflection are the boundaries of instability, the appearance of any subtypes of this configuration in this area will lead to the disruption of steady state flow pattern.

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## PRECHAMBER INFLUENCE ON DEFLAGRATION-TO-DETONATION TRANSITION IN CHANNELS SUBCRITICAL DIAMETER

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To reduce the deflagration-to-detonation transition is known to use the expansion at the beginning of the detonation channel. In connection with the acceleration of the flame front in the channel due to expansion of combustion gases into the settling chamber, the initial phase shift in the balance achieved between the released during the reaction and the dissipated energy in a positive way.

The absence of deflagration-to-detonation transition at lower pressures is explained by significant thermolosses to a wall and by low flame velocity at initial stage [1].

In the paper had been achieved the formation of gas detonation of hydrogen-air and methane-oxygen mixtures at lower initial pressure in a channel with subcritical diameter at short distance by transition of combustion from the forechamber of bigger diameter into the narrow channel. The effect of geometrical parameters of the forechamber on the deflagration-to-detonation transition in the subcritical diameter channel had been investigated. There were observed several scenarios of combustion propagation in narrow channel with the forechamber and it was proposed a non-dimensional criterion defining these scenarios. This criterion defines an effectiveness of forechamber effect on deflagration-to-detonation transition in subcritical channels and takes into account the energy release in the forechamber and relative distance passed by flame front in the forechamber.

<sup>1.</sup> Hsu Y.C., Chao Y.C. An experimental study on flame acceleration and deflagration-to-detonation transition in narrow tubes. In Proc. of the 22nd ICDERS, Minsk, Belarus. 2009.

## INVESTIGATION OF INFLUENCE OF EJECTOR ON GAS FLOW AT PULSE DETONATION ENGINE

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High thermal efficiency of the pulse detonation engine attracts researchers to apply it as a new technology for the aerospace propulsion. One of the main features of the pulse engine is that the nozzle produces a variable thrust. One stage of combustion can be effective, other is regressive. Thus, it is necessary to investigate each stage of the detonation combustion for the thrust to be maximal during the period. It was shown that there are an optimal dimensions of nozzle for the case of direct initiation of detonation in one-impulse regime in [1, 2].

One way to improve thrust is ejector. The increase in thrust is due to the growing mass of the working gas. Thus, while the gas velocity decreases, the thrust can be increased. It was showed that the using of the ejector can lead to increase the specific impulse up to 35% for the engines at a constant rate of gas flow in [3]. In [4] it is assumed that for the pulse engine the gain of thrust could be much higher.

Aim of the work was a numerical investigation of influence of an ejector on the thrust of a pulse detonation engine. Axisymmetric model was used. Equations of Navies-Stokes were solved using finite-difference scheme Roe of the second order of accuracy. The profile obtained experimentally was used, as a profile of the thermodynamic quantities at the combustion chamber.

The results of the math-simulation show that the initial velocity of the ejected air is in opposite directions on the velocity of the ejecting gas. Thus the using of ejectors for pulse motors with high frequency is ineffective. Dependence of the average thrust on ejector motor frequency was investigated.

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## ON USAGE OF GAS DETONATION IN THIN TUBES FOR NEEDLELESS INJECTIONS

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The object of research was the transition to detonation in hydrogenair and hydrogen-oxygen mixtures in narrow channels with a diameter about the critical diameter of existence steady detonation, as well as the possibility of using hydrogen mixtures detonation in devices for needleless injection [1, 2]. The purpose was to create the layout needleless injector that uses detonation energy.

As a result, the work was designed and manufactured model of the injector, which generates under the action of detonation a thin stream of liquid, capable of penetrating human covering tissue and produce a needleless injection.

Using a detonation in hydrogen-air mixtures will allow to replace less efficient sources of energy to accelerate the drug in devices designed for needleless injections. That will simplify, reduce the cost and make the needleless injection devices portable, and avoid the emission of toxic products which appear as result of using solid fuels.

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#### BIFURCATION OF MICRO JETS UNDER ACOUSTIC INFLUENCE

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A large number of theoretical and experimental studies devoted to research of jet instabilities. It is theoretically and experimentally proved that the free shear flow, which has a point of inflection in the velocity profile, is absolutely unstable. Its perturbations grow exponentially downstream, forming vortexes, which are combined with each other in the form of large coherent structures. However during the transition to smaller scales (when jet diameter becomes < 5 mm) the mechanism of jet development is change. In [1] shown that the micro jet with a parabolic and top-hat velocity profile remain laminar at distances of 10 calibers of jet diameter. In this case there are no Kelvin-Helmholtz ring vortexes, and the loss of stability is carried out at the expense of the asymmetric (sinusoidal) oscillation modes of the jet as a whole. The importance of this research is obvious both for science and for many technical applications, including MEMS technologies.

The object of research in this work is the jet of gas expiring into the ambient air, and its response to external acoustic influence. Gas flowed out into the ambient air from the tubes with various internal ( $\sim 1 \text{ mm}$ ) and external (from 1 to 100 mm) diameter. Exhaust velocity was set so that in the pipes was installed classical Poiseuille flow with a parabolic velocity profile.

Experiments with shadow visualization of the gas jet were performed. The dependence of the acoustic frequency which there is a bifurcation of the flow on the flow rate was obtained. Similar dependences were obtained for jets of different geometries, as well as for jets of various gases.

The same experiments were performed using the PIV diagnostic. As a result, a three-dimensional velocity field of the jet in the longitudinal section was obtained. Experimentally shown that asymmetric (sinusoidal) instability mode develops in the jet under the acoustic influence, the growth of which downstream leads to the bifurcation of the jet.

## INFLUENCE OF IGNITION DELAY TIME AND DIFFERENT GEOMETRY OF HYDROGEN JET ON PRESSURE LOADS IN A LARGE SCALE EXPERIMENTS

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## Hydrogen safety development requires detailed data on hydrogen distribution processes, explosive mixtures formation, ignition conditions, and possible combustion regimes. The objective of the present work is to investigate experimentally the influence of hydrogen release from nozzles of different configuration and volume geometry on pressure loads. Four different

Kozlov V.V, Grek G.R., Litvinenko Yu.A., Kozlov G.V., Litvinenko M.V., Subsonic round and plane macro and micro jets in transverse acoustic field// Vestnik NGU. Physics, V. 5, No. 2, P. 28–42.

jet nozzle configurations and different level of congestion and confinement of experimental volume were tested. Initial jet pressure was approximately 150 atm., the mass of ejected hydrogen in experiments varied from 100g to 1000g and release time was from 0.5 to 6 s, the ignition delay times varied from 0 to 10 s.

## THE EFFECT OF AKM INHIBITOR ON PARAMETERS OF COMBUSTION OF HYDROGEN-AIR MIXTURES OF DIFFERENT COMPOSITION

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Experiments were conducted in volumes about 7 m<sup>3</sup> in size that were bounded by thin rubber envelopes located inside 13Ya3 explosion chamber 12 m in diameter. AKM inhibitor developed in Institute of Structural Macrokinetics and Materials Science RAS represents propane with added 17% propylene. In experiments the pressure in the shock front was measured by PCB pulse pressure sensors, and the velocity of the flame front was measured by the use of ionization detectors. The combustion process was recorded by high-speed camera. Investigations were made of the hydrogen-air mixture with 30, 22 and 16% (Vol.) content of hydrogen, in which was added AKM inhibitor in amounts from 1.5 to 7.5% (Vol.). Initiation was carried out by 2.7 g of PETN (15600 J). The addition of AKM inhibitor in amounts of 4, 5 and 6.5% (Vol.) in the hydrogen-air mixture with 30, 22 and 16% (Vol.) content of hydrogen respectively prevents ignition of the mixture during its initiation by energy of 15600 J.

#### INFLUENCE OF METHANE ADDITIVES ON DIFFUSIVE SELF-IGNITION OF HYDROGEN

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Features of hydrogen self-ignition discharged into channel filled by air were experimentally investigated. Required condition for hydrogen selfignition is to maintain the high temperature for a time long enough for hydrogen and air to mix on the contact surface and inflammation to take place. Hydrogen self-ignition occurs owing to the formation of a shock wave in front of a high-pressure hydrogen gas propagating in the tube. Temperature is increased, as a result of this shock wave. It leads to the ignition of hydrogen-air mixture formed on contact surface [1]. But duration of diaphragm rupture may influence on self-ignition of hydrogen [2], because of appearing system of shock waves that may form areas with temperature and pressure exceeding one-dimensional approximation.

Adding into hydrogen small amounts of other gases can significantly slow down the diffusive inflammation if ignition delay for this additives on the order of magnitude greater than that of pure hydrogen. And given the fact that in the pulsed jets gas dynamics of burning is largely determined by the shock wave, the contact surface and the duration of shock-wave configurations with the boundaries of the system. In this case a slight change in the ignition delay can significantly change the character of the process, for example to repay burning.

Found as impurities of methane on the ignition delay. It was shown that increasing the concentration of methane increases the ignition delay. At the same dependence of ignition delay on the duration of diaphragm rupture is monotonic.

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## PROMOTION OF SHOCK-INDUCED METHANE DETONATION BY FIRE SUPPRESANTS

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The various halogenated hydrocarbons are widely used as fire suppressants and were suggested in recent works as a species which could prevent ignition and detonation of combustible mixtures [1]. It was also noticed, though, that at certain conditions the halogenated species do not inhibit combustion, but even accelerate an ignition of hydrocarbon-oxygen mixtures [2]. In most recent works it was shown that at elevated temperatures many fluorinated hydrocarbons are combustible themselves and, moreover, their induction times are shorter than one for propane [3, 4]. Thus, possibility of practical using of halogenated hydrocarbons as detonation inhibitors is still quite questionable and thorough studies in wide range of conditions are required. The goal of present work was the experimental investigation of the influence of  $CCl_4$  and  $CF_3H$  admixtures on shock-induced detonation development in methane.

Experiments were carried out in a shock tube of standard design in the mixtures 3%CF<sub>3</sub>H/CCl<sub>4</sub> + 6.7%CH<sub>4</sub> + 13.3%O<sub>2</sub> + Ar at the temperatures 1350-1850 K behind the reflected shock waves. Investigated section was equipped with five pressure gauges and rectangular sapphire windows which allowed obtaining the time-resolved emission images of shock-heated flow. The induction time of detonation development was determined as the moment of a pressure rise at the end plate of the shock tube.

It was observed that both CF<sub>3</sub>H and especially CCl<sub>4</sub> dramatically promoted the development of detonation and reduced the induction time by approximately one order of magnitude. Rough kinetic modeling of the obtained data indicated that the promoting species formed by admixtures pyrolysis were correspondingly CF<sub>2</sub> and atomic chlorine, which produced active radicals in reactions CF<sub>2</sub> + O<sub>2</sub>  $\rightarrow$  COF<sub>2</sub> + O and Cl + CH<sub>4</sub>  $\rightarrow$  CH<sub>3</sub> + HCl and initiated chain combustion mechanism, while chain termination reactions proved to be less effective.

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#### INFLUENCE OF HALOGENOALKANE ADMIXTURES ON DETONATION OF ACETYLENE

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The halogenoalkanes were widely considered a species that may prevent the explosion and detonation of various combustible mixtures [1, 2]. At certain conditions (particularly at elevated temperatures), though, the halogenated species do not inhibit combustion, but, moreover, even accelerate ignition of hydrocarbon-oxygen mixtures [1, 3]. Such effects could be explained via the interaction of the products of admixture pyrolysis with the initial compounds, resulted in accelerating of active radicals formation during the induction time. The goal of present work was the experimental investigation of the influence of  $CCl_4$  and  $CF_3H$  admixtures on formation of shock-induced condensation detonation wave [4] in acetylene.

Experiments were carried out in the mixtures 3%CF<sub>3</sub>H/CCl<sub>4</sub> + 30%C<sub>2</sub>H<sub>2</sub> + Ar in shock tube of standard design equipped with five pressure gauges and unique elongated windows which allow to obtain time-resolved emission images of shock-heated flow and detect the formation of condensed particles by laser light extinction. The induction time of detonation development was determined as the moment of a pressure rise at the end plate of the shock tube. Obtained values of induction times at various pressures and acetylene concentrations were normalized to carbon concentration [C] in the investigated mixtures as described in [4].

No significant inhibiting or promoting influence of  $CF_3H$  was detected. On the other hand, the admixture of 3% CCl<sub>4</sub> essentially promoted the development of detonation and reduced the induction time by approximately one order of magnitude. An analysis of the obtained data indicated that the promoting species is atomic chlorine formed by  $CCl_4$  pyrolysis, which interacts with acetylene and produces the  $C_2H$  radical, initiating a chain mechanism of acetylene decomposition.

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## STUDY OF KINETICS OF SMALL CARBON CLUSTERS C<sub>2</sub> AND C<sub>3</sub> FORMATION IN ACETYLENE DETONATION BEHIND SHOCK WAVES

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The study of the carbon nanoparticles formation in the process of detonation of explosives is an important research for many scientific problems. Specific importance has the initial stage of detonation, which is quite complex and uncontrolled process. Recently, new knowledge about the development of detonation in acetylene [1–2], as well as the role of quantum corrections in the induction times of acetylene condensation at the temperatures of 800–1600 K [3] were acquired. Therefore the study of initial stage of formation of small primary carbon clusters during acetylene decomposition in the gas phase is very actual.

This paper presents experimental and kinetic studies of small clusters  $C_2$  and  $C_3$  formation in the pyrolysis of acetylene behind shock waves. The experiments were performed in a shock tube with an inner diameter of 108 mm, consisting of a low-pressure section length of 6 m and high-pressure section 2 m long, separated by an aluminum diaphragm. Measuring of the radical  $C_2$  and  $C_3$  concentrations were performed using molecular resonance absorption spectroscopy (MRAS). As a light source for MRAS the diode lasers at the wavelengths of 405 nm and 473 nm were used.

Several series of experiments with the mixtures from 500 ppm to 9000 ppm  $C_2H_2$  in argon in the temperature range of 2600–4000 K and pressure range of 1.2–3.0 bar were carried out behind reflected shock waves. The effective activation energies of  $C_2$  and  $C_3$  radicals formation were determined. The numerical simulation of  $C_2$  and  $C_3$  concentration profiles was performed by kinetic modeling in the standard package CHEMKIN. A comparison of experimental data with the results of kinetic calculations of  $C_2$  and  $C_3$  concentration profiles is presented. The conclusion about the need to improve the kinetic scheme for the successful modeling of the experimental results of  $C_2$  and  $C_3$  radicals formation is expressed.

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## CHARGING OF CARBON NANOPARTICLE IN SHOCK-HEATED PLASMA DURING PYROLYSIS OF C<sub>6</sub>H<sub>6</sub> Bronin S. Ya., Emelianov A.V.,<sup>\*</sup> Eremin A.V., Khrapak A.G., Mikheyeva E.Yu.

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This work continues the study of charged carbon nanoparticles formed at pyrolysis of various carbon-containing substances behind shock waves [1–4]. The experimental results and computer simulation of the electrical charging of carbon nanoparticles produced during the pyrolysis of  $C_6H_6$  in shock waves are presented. Particle charging was studied in the mixtures initially containing 1%  $C_6H_6$  in argon. The measurements of nanoparticle charge by electric probes, as well as their temperature by emissionabsorption spectroscopy and size by LII, were performed simultaneously. In the presence of condensed carbon nanoparticles produced during pyrolysis  $C_6H_6$ , the concentration of free electrons is reduced by two orders of magnitude, while the concentration of positive ions changes slightly.

The concentration of soot particles during the calculations was varied within  $10^{11}-10^{12}$  cm<sup>-3</sup>. In fact, at any time moment there is some distribution of soot particles over size and the total concentration of soot particles can vary with time. Therefore, calculations were based on the experimentally measured particle size. The formation of soot particles is accompanied by the growth of the enthalpy of the mixture due to the heat release during condensation. Quantitative account of the heat, based on temperature measurements, was carried out. Soot particles formed under present conditions influence the ionization equilibrium in the plasma, since an additional mechanism of recombination of ions and electrons on the surface of the particles appears. The proposed modeling of the kinetics of particle charging in the process of their formation provides a satisfactory agreement between the calculation results and experimental data.

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## TREATMENT OF LII MEASUREMENTS OF CARBON PARTICLES FORMATION IN THE PYROLYSIS FLAMES Emelianov A.V.,<sup>1</sup> Eremin A.V.,<sup>1</sup> Jander H.,<sup>2</sup> Tsirlina E.A.,<sup>\*1</sup> Wagner H.Gg.<sup>2</sup>

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The formation of carbon nanoparticles in so-called "pyrolysis flames" was experimentally studied. Experiments were performed in the flows containing 10-30% C<sub>2</sub>H<sub>2</sub> and 0-4% C<sub>3</sub>O<sub>2</sub> diluted in N<sub>2</sub>. Laser extinction, scattering, laser-induced incandescence (LII), visible and infrared (IR) temperature measurements were carried out in different flame conditions and flame heights, varied between H = 60-240 mm above the burner. The measurements of particle radiation by LII technique were carried out simultaneously at two wavelengths, providing the measurements of the particle temperature and volume fraction from the signal intensities and particle size from the rate of their cooling. For statistical analysis of the data of LII measurements a set of special programs has been developed, including the evaluation of reliability of recorded data, depending on their amplitude, and recovery of LII intensity time profiles for distorted signal records. In result of LII measurements and developed programs the size and volume fraction of carbon particles in pyrolysis flames of  $C_2H_2$  and  $C_3O_2$  have been obtained. Based on analysis of these data the main kinetic parameters of particle formation—the effective rate constant of soot mass growth and the formal rate constant of particle coagulation have been extracted.

## THE PROSPECTS OF USING DETONATION IN THE MULTISTAGE MODE FOR COATING OF FINE PARTICLES

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Currently, there is a need to provide deposition of micron and submicron particles with a complex structure. Thanks to them, various properties of materials the principal are expected to be improved fundamentally.

There is the possibility of organizing a detonation regime in valveless mode to increase the resource of the equipment. [1] The development of such devices requires a study of the multistage mode of detonation process, because this mode has high efficiency and allows increasing of detonation parameters. A number of papers is aimed at numerical simulation of this process and it is important for expanding the use of technology. [2]

Gasdynamic method of creating composite materials based on the method of detonation spraying is considered. Justification of using this method for the deposition of advanced composite materials is produced

The method has a high power density and a significant simplification of the energy conversion into useful work. An experimental system for the study of this method and investigation of the main parameters that influence the process is proposed.

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Nikolaev Y.A., Vasiliev A.A., Ulianitsky V.Y. Gas detonation and its application in engineering and technologies (Review) "Physics of combustion and explosio". 2003, V.4. P. 22–54.

## SELF-ORGANIZING OF THE REACTIONARY ZONES OF THE ENERGETIC MATERIALS AND CONCEPT OF THE SMART SOLID MICRO-PROPULSION SYSTEM

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For more than ten years, micro-propulsion has been an active worldwide field of research. The level of thrust and the precise impulse required for micro-satellite maneuvers cannot be achieved with conventional solid propulsion systems. Because in the combustion chambers of micropropulsion systems of the small-sized orbital maneuvering vehicles, the scale factor has the significant influence, the micro/nano- structures arising in energetic material reactionary zones has a significant influence on physical and chemical processes and on controllability of processes of ignition and combustion. The analysis of experimental data shows that in a number of cases, the macro-scale phenomena at the energetic material combustion are result of self-synchronization of the magneto-dipole micro/nano-structures in the reactionary zones.

In the paper the new hypothesis of excitation of some anomalies of burning that connected with collective interaction of the self-organizing magneto-dipole micro-structures in the reactionary zones is suggested. The hypothesis is supported by the experimental data provided by Japanese research team. This data has been obtained during study of oscillation and synchronization in the simple experimental system containing a set of paraffin candles. Research of self-organizing and self-synchronization of the micro/nano- structures in the reactionary zones opens a new possibility for development of the smart solid propellants that allow variable thrust at minimal cost. In the paper the extensive experimental data showing excitation of micro/nano- structures of electric field and magneto-dipole micro-structures in the reactionary zones are discussed. The new possibilities for effective control by combustion processes opens in connection with possibility of initiation of self-organizing of the reactionary zone by use of the electric fields and electric discharges. Self-organizing of the reactionary zones is essentially new level of self-organizing which is determined by achievement of critical spacial concentration the micro/nano- structures. In particular, application of an electric field, changes the burning surface roughness, i.e. modifies the process of excitation of the micro/nanostructures in the reactionary zones. The concept of the smart solid micropropulsion system includes integration of the propellant reactionary zones

both into the control system by combustion mode, and into the general control system of the small-sized orbital maneuvering vehicle.

#### WHY THERE ARE NO CRATERS ON THE EARTH DUE TO GALACTIC COMETS?

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Galactic comets are a previously unknown class of large cosmic bodies, which intensively bombarding the Earth and other planets in periods of presence the Solar system in jet streams of the Galaxy. These comets are moving relative to the Sun with speed 450 km/s, composed primarily of water ice density 1 g/cm<sup>3</sup> and diameter of their nucleus is 100–3000 m. Fallings of galactic comets on atmosphereless celestial bodies (Mercury, Moon and, partly, Mars) and on planets with a dense atmosphere (Venus, Earth) differ significantly in its consequences. In the first case these comets form large craters with a complex morphology, and in the second they lead to lifting surface on large areas as well as to emergence of long-term functioning seamounts (Earth) and shield volcanoes (Venus) [1].

To understand the reason for absence of craters on the Earth from galactic comets, we conducted calculations on base of hydrodynamic theory proposed by M. A. Lavrentiev [2] for bodies moving at cosmic speeds. According to this phenomenological theory, a fall galactic comets on the Earth can be seen as an inelastic collision of two ideal incompressible fluids. This task was solved in the one-dimensional approximation for galactic comet by diameter of 300 m, which falls vertically Earth's surface at a speed of 450 km/s.

It is shown that falling comet creates narrow-focused shock wave. In course of its distribution, this shock wave vaporizes layer of surface rocks and creates cylindrical crater by diameter and depth of 600 m. However this crater is largely leveled owing to volume expansion of underlying rocks in result their melting and heating. A layer of molten rock below the bottom of the crater reaches 2 km, and total length of rocks column, heated to a temperature above 100 K is of 14 km. The evaporating material is ejected from the crater at a speed of 70 km/s. And, therefore, may leave the planet.

When galactic comet falls in ocean or in the case high water saturation of rocks, shock wave, apparently, can experience focusing, which will lead to a decrease in diameter and lengthening column of strongly heated rocks.

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## AMBIGUOUS REPRESENTATION AND SPLITTING OF RELATIVISTIC SHOCK WAVES

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The behavior of relativistic shock waves under conditions of ambiguous representation of the shock wave discontinuity is investigated numerically. The relativistic hydrodynamic code based on ENO scheme with reconstruction in terms of primitive variables is elaborated. Scaling of the internal energy in the model equation of state [1] is provided transition from non-relativistic case to relativistic one:

$$e = \xi (1 - \exp(-p^2/\xi^2))(4 - \exp(-(4 - V)^2)).$$

Here, the thermodynamic parameters refer to the rest system, and  $\xi$  is a scaling factor permitting to vary the pre-shock velocity  $u_0$ . The shock waves with the initial state ( $p_0 = 0.1\xi$ ,  $V_0 = 5.491$ ) are considered. At values of  $\xi$  close to zero velocity  $u_0$  is small with respect to light speed c, and the problem under consideration reduces to non-relativistic case analyzed earlier in [2]. With growth of  $\xi$  the role of relativistic effects increases (for example, at  $\xi = 0.3 u_0$  equals to 0.74c), and the equations of relativistic fluid dynamics should be solved.

The Taub adiabats are built and analyzed to check the fulfillment of the relativistic shock wave instability conditions [3]. The series of calculations at different values of  $\xi$  is performed. The boundaries of Taub adiabat fragments with shock splitting are determined and compared with theory. The results obtained are visualized and discussed.

The analysis of the problem considered is important in connection with suggested phase transitions in quark-gluon plasma in the process of collision of heavy relativistic ions. Another aim of the work is to compensate for the lack of test solutions for relativistic hydrodynamic codes with arbitrary equation of state. 1. Ni A. L. et al. // Teplofiz. Vys. Temp. 1986. V. 24. No. 3. P. 564.

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## NUMERICAL SIMULATION OF RELATIVISTIC JETS Konyukhov A.V.

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Numerical simulations of supersonic relativistic jets are able to explain some structures observed in astrophysical objects. However, there is a lack of simulations of jets with a large value of Lorentz factor which can be explained by numerical difficulties that arise in modeling of the highly relativistic flows. In the present work high resolution two-dimensional code is developed to solve the special relativistic hydrodynamics equations  $\partial_{\alpha}(\rho u^{\alpha}) = 0, \ \partial_{\beta}T^{\alpha\beta} = 0$ , where  $\rho$  is the rest-mass density,  $u^{\alpha}$  is fourvelocity and  $T^{\alpha\beta}$  is the energy-momentum tensor [1]. The code is based on the essentially non-oscillatory scheme and the local characteristic approach. The numerical algorithm is validated by the comparison with some numerical and analytical solutions to Riemann problems for the equations of relativistic hydrodynamics ([2], [3]). Supersonic jet with specified diameter d is injected into the half space through the part of the boundary. Corresponding initial boundary value problem for the equations of relativistic hydrodynamics is posed and solved numerically. The equations have been solved in normalized form by setting the light speed c, beam diameter d and reference rest-mass density. Dependence of solution to the problem on governing dimensionless parameters is studied. Cases of under and over expanded jets are considered. Relativistic effects in the obtained flow structure are revealed and discussed.

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#### EQUATIONS OF STATE FOR MATTER

## EQUATIONS OF STATE FOR MATERIALS OVER A WIDE RANGE OF PRESSURES AND TEMPERATURES

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An equation of state of matter over a wide range of pressures and temperatures is necessary for numerical simulations of physical processes under intense pulsed influences. Accuracy of calculation results is determined mainly by adequacy of description of thermodynamic properties of materials in question. In the present work, different approaches to equationof-state calculations are considered. A model of thermodynamic potential free energy with taking into account polymorphic transformations, melting and evaporation is presented. On the basis of this model, equationof-state calculations are carried out for some metals, alkali halides, oxides and polymers in a broad region of the phase diagram. Obtained results are compared with available experimental data at high energy densities.

### LOW MELTING POINT OF ALKALI METALS UNDER PRESSURE: ELECTRONIC ORIGIN

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Group I elements—alkali metals Li, Na, K, Rb and Cs—are examples of *simple* metals with 1s electron in the valence band with the bodycentered cubic structure. Under pressure these elements display unusually complex behaviour transforming first from bcc to fcc and then to low symmetry open structures including an incommensurate host-guest structure in Na, K and Rb [1]. Unexpectedly complex form was found for melting curves of alkalis under compression with initial increasing (according to the Lindemann melting criterion) and further decreasing to very low melting point. The lowest point of melting was found to be 300 K at 120 GPa for sodium and 200 K at 50 GPa for lithium [2, 3]. Heavier alkalis have also non-monotonic behaviour of the melting curve on T-P diagrams. To understand complex and low symmetry structures in compressed alkalis a transformation of the energy levels was suggested which involves an overlap between the valence band and outer core electrons [4, 5]. Within the model of the Fermi sphere—Brillouin zone interaction the Na-oP8structure above 117 GPa can be stabilized assuming that sodium is divalent metal at such compression [5].

Similar electron transfer in compressed alkalis may occur also in liquid state and even at lower pressure, leading to the increase of stability for the liquid state. The well known example of the only one liquid metal at ambient conditions is mercury—the divalent metal. Experimental diffraction data on liquid alkalis display non-simple behaviour on compression suggesting the essential changes of the electron state in the valence band.

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#### INVESTIGATION OF MELTING IN AB INITIO CALCULATIONS

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In this work we suggested two melting criterion which allow to determine melting transition in *ab initio* calculations (VASP [1]). Within the first method the rotational invariants (RIs) of both second  $q_i$  and third  $w_i$  order are calculated for each particle in the system. The calculated rotational invariants  $q_i, w_i$  are then compared with those for ideal lattices (e.g., [2–4]). The destruction of the local orientational order can be easily seen as a sharp shape change of the associated probability distribution function (PDF). To construct the melting indicators based on the PDFs we applied the approach developed in [3, 4]. The second method uses quasiharmonic appoximation and Lindemann [5] criterion to determine the melting curve and the region of stability of crystals. This approach allows to calculate free energe, so it can be used to determine all thermodynamic properties for the crystalline state. Results of calculations were compared with experimental data.

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# SHELL EFFECTS IN FREE IONS CHARACTERS Shpatakovskaya G.V.

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The semiclassical method [1], [2] is applied to analyze some properties of the free ions at zero temperature. The statistical Thomas-Fermi model with additive corrections is compared with the self-consistent statistical model and empirical data. The shell effects contribution is discussed.

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## REGION OF VALIDITY OF THE THERMAL CONTRIBUTION TO THE THERMODYNAMIC FUNCTIONS OF ELECTRONS IN THOMAS–FERMI MODEL WITH QUANTUM, EXCHANGE AND SHELL EFFECTS

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The Thomas-Fermi model [1] at low temperatures is not valid for calculation of thermodynamic functions of electrons because of quantum, exchange and shell effects [2, 3]. For this reason, the model cannot represent correctly the physical reality.

However, it is known that the main influence of quantum effects appears at zero temperature. It was shown [4] that if one subtracts thermodynamic parameters at zero temperature from the thermodynamic functions at finite temperature, the region of validity to this thermal contribution expanded to the region of low temperatures. In that case only quantum and exchange effects were considered. For conditions of validity of the Thomas-Fermi model to be defined more exactly, one should calculate shell correction.

In this work the region of validity of the Thomas-Fermi model was refined. It was done in the similar way to [5], by comparing the thermal contribution to the thermodynamic functions in the Thomas-Fermi model without corrections with the thermal contribution to the corrections to these functions. In this case all the effects were taken into account: quantum, exchange and shell. The precision of calculations was controlled to evaluate the error of the calculation of the thermal contribution to the thermodynamic functions and corrections to them.

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## THERMODYNAMIC AND TRANSPORT PROPERTIES OF STRONGLY COUPLED QUARK-GLUON PLASMA BY COLOR PATH-INTEGRAL MONTE-CARLO SIMULATIONS

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Based on the quasiparticle model of the quark-gluon plasma (QGP), a color quantum path-integral Monte-Carlo (PIMC) method for calculation of thermodynamic properties and—closely related to the latter—a Wigner dynamics method for calculation of transport properties of the QGP are formulated. The QGP partition function is presented in the form of a color path integral with a new relativistic measure instead of the Gaussian one traditionally used in the Feynman-Wiener path integral. A procedure of

sampling color variables according to the SU(3) group Haar measure is developed for integration over the color variable. It is shown that the PIMC method is able to reproduce the lattice QCD equation of state at zero baryon chemical potential at realistic model parameters (i.e. quasiparticle masses and coupling constant) and also yields valuable insight into the internal structure of the QGP. Our results indicate that the QGP reveals quantum liquid-like (rather than gas-like) properties up to the highest considered temperature of 525 MeV. The pair distribution functions clearly reflect the existence of gluon-gluon bound states, i.e. glueballs, at temperatures just above the phase transition, while meson-like  $q\bar{q}$  bound states are not found. The calculated self-diffusion coefficient agrees well with some estimates of the heavy-quark diffusion constant available from recent lattice data and also with an analysis of heavy-quark quenching in experiments on ultrarelativistic heavy ion collisions, however, appreciably exceeds other estimates. The lattice and heavy-quark-quenching results on the heavy-quark diffusion are still rather diverse. The obtained results for the shear viscosity are in the range of those deduced from an analysis of the experimental elliptic flow in ultrarelativistic heavy ions collisions, i.e. in terms the viscosity-to-entropy ratio.

#### ENTHALPIC AND ENTROPIC PHASE TRANSITIONS IN HIGH ENERGY DENSITY NUCLEAR MATTER

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Features of Gas-Liquid (GL) and Quark-Hadron (QH) phase transitions (PT) in dense nuclear matter are under discussion in comparison with their terrestrial counterparts, so-called "plasma", dissociation and de-polimerization PTs in shock-compressed hydrogen and nitrogen etc. Both, GLPT and QHPT, when being represented in widely accepted T- $\mu$  plane, are often considered as similar, i.e. amenable to one-to-one mapping by simple scaling. We argue that this impression is illusive and that GLPT and QHPT belong to different classes: GLPT is typical *enthalpic* (VdW-like) PT while QHPT ("deconfinement-driven") is typical *entropic* PT (like hypothetical ionization- and dissociation-driven phase transitions in shock compressed hydrogen and nitrogen in megabar pressure range). Fundamental differences of enthalpic and entropic phase transitions are discussed and illustrated.

Hypothetical possibilities of mesoscopic scenario for GLPT and QHPT

in simple ("mixed phase") or complicated ("structured mixed phase") forms are discussed also in connection with another hypothetical peculiarity of GLPT and QHPT—their non-congruency [1], [2].

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## BINODAL LAYER IN ISENTROPICALLY EXPANDING SLAB TARGET WITH VAN DER WAALS EQUATION OF STATE

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Features of isentropic expansion of warm dense matter (WDM) created by intense energy fluxes (strong shock compression or instant isochoric heating by laser or heavy ion beams) are under discussion in situation when (i)—thermodynamic trajectory of such expansion crosses binodal of liquid-gas phase transition, and (ii)—expansion within two-phase region is going along *equilibrium* (not metastable) branch of the isentrope for two-phase mixture. It is known for the case of plane geometry (Anisimov, Inogamov et al. 1999) that because of sharp break of the expansion isoentrope at boiling point (in P-V plane) there appears extended zone (liquid layer) of uniformity for expanding material with constant thermodynamic and kinematic parameters, which correspond exactly to the state on binodal. General properties of such boiling ('binodal') layer were claimed and discussed at [1] for the cases of isentropic expansion of finite plane and spherical samples (slab and ball) as well as for the system of well positioned slabs (stuck target).

Thermodynamic and kinematic parameters of discussed binodal layer are studied with the use of simplest Van der Waals equation of state (EOS). Advantage of this EOS is possibility of demonstrable and semi-analytical description of thermo- and hydrodynamics of the process. Self-similar case of behavior of matter with VdW EOS on interception of equilibrium isoentropic curve and boundary of gas-liquid binodal was analyzed in [2]. Current work studies phenomenon in planar case of isentropic expansion of finite sized layer (*slab*) of VdW-matter.

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#### VALIDITY OF SEMIEMPIRICAL RULES FOR GAS-LIQUID PHASE BOUNDARIES IN SIMPLIFIED COULOMB MODELS AND REAL COMPOUNDS

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Validity of well-known semi-empirical rules for gas-liquid phase boundaries are discussed as applied (i) to strongly non-ideal fully ionized electron-ionic plasmas with well-known wide-range analytic equations of state (EOS) of Potekhin and Chabrier [1], which is widely used in astrophysical applications, as well as with EOS in previously used models  $OCP(\sim)$  and  $DOCP(\sim)$ , and (*ii*) to phase diagram of real hightemperature compound  $SiO_2$  as predicted by several theoretical models [2]. Four well-known and new such semi-empirical rules are compared and discussed: (1) Traditional rule of "rectilinear diameter" of Calliete–Matthias for density-temperature two-phase boundary; (2) Validity of Guggenheim formula for temperature dependence of boiling liquid density; (3) Socalled Timmermans-Fillippov's rule for correlation of asymmetry factor of density-temperature phase boundary and critical compressibility factor of gas-liquid phase transition; (4) Validity of linear extrapolation for saturation pressure in Arrhenius coordinates:  $\ln P \Leftrightarrow 1/T$ . Present comparison shows the evolution of these semi-empirical rules for the most popular models, which describes thermodynamics of fully ionized plasma also with the relation of accuracy of mentioned empirical rules with the ion charge Z. Besides this new variant of the rule of rectilinear diameter for compressibility factor, not for density, is considered for gas-liquid phase transition in Coulomb model and in high-temperature evaporation in  $SiO_2$ .

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# EQUATIONS OF STATE, COMPOSITION, CONDUCTIVITY OF DENSE VAPORS PLASMAS OF VARIOUS METALS

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In this work we suggested the chemical model of non-ideal gas-plasma compound for the description of dense metals vapor plasma, taking into account electrons, ions, atoms, molecules and molecular ions, and also twoand triple ionized atoms. This chemical model created by us being continue of work [1] for the calculation of composition, EOS and conductivity of large group of various metals (Al, Cu, Ag, Au, Ni, Ti, B) in the "warm dense matter" regime. In this sense our model is the universal. In previous work [1] we critically analyzed virial coefficients of charge-charge and charge-atom interactions available in literature. As a result we used BDapproach for description of Coulomb interaction. The modified Likalter's virial coefficient is used for ion-atom interaction. Scattering length approximation is used for an electron-atom interaction. Caloric and thermal equations of state and composition of metals vapors are obtained. The important role of molecules and molecular ions, especially in initial stage of metals heating is shown. Our results for the equation of state and conductivity of metals vapor are in good agreement with the recent experimental data available in literature [2], [3] in the field of applicability of model.

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## THE BOYLE AND BACHINSKY CURVE IN THE MODEL OF INTERACTING POINT CENTERS

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Our purpose is providing the adequate equation of state (EOS) based on a simple but realistic molecular model. At this stage we are realizing the potential of the model of interacting point centers (IPC). In the present work the possibility of the new EOS obtained by author is analyzed in the description of Boyle and Bachinsky (on behalf of the pioneers) curves (orthometric curve, curve of single compressibility; the ideal curve of zero order; the curve of ideal gas: under those different names we know the set of real gas (fluid) states, where the final configuration pressure is reduced to zero). The structure of the new EOS, in which are clearly identified two configuration contributions allows to enter two comparative parameters connected with the manifestation acting in the system of the attraction and repulsion forces in respect of the available volume and pressure. It is shown that the first parameter is the control parameter of the thermodynamic level. The case where both configuration contributions to the pressure are equal (but not necessarily small), leads to the Clapeyron-Mendeleev EOS (but not the ideal gas equation). Proceeding from these conditions was obtained and studied (analytically and graphically) the general equation of Boyle-Bachinsky linking the reduced temperature, the volume (or density) and the control parameter of the thermodynamic level. The value of the control parameter determines the reduced Boyle temperature for the calculation of which two analytical expressions are obtained. The first one for the case when the control parameter EOS remains constant, the second for the more general case. It is shown, that with increase of the control parameter the calculated value of Boyle temperature is growing, starting from 3.375 for van der Waals EOS. The calculated values of Boyle temperature for the investigated family EOS does not fall into the interval of known values for different substances: 2.7 for noble gases and methane; 2.57 for diatomic gases (nitrogen, oxygen, fluorine), 2.35 for carbon dioxide. However, a new family of EOS should not be excluded from the further search of more general adequate EOS, which is based on a number of reasons.

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## THE MODEL OF THE KINETICS OF DIRECT PHASE TRANSITION GRAPHITE TO DIAMOND UNDER SHOCK LOADING

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For the phase transition of graphite to diamond high pressure and temperature are required. Since the line of graphite–diamond equilibrium has a positive slope, the temperature increase would lead to the increase of pressure in the beginning of the phase transition, and this is inconsistent with the numerous experimental data. It has been found experimentally that lowering the density of graphite reduces the pressure of the beginning of transformation, increasing the initial temperature of the graphite also decreases the pressure of the beginning of the conversion. Also opinions differ widely on the nature of the mechanism of phase transformation: some authors believe that the transformation is of the martensitic type, others—by diffusion.

This work is devoted to the numerical study of the kinetics of phase transition of graphite into diamond. To determine parameters of the onset of transformation and kinetics of this transition several models were proposed. For the description of porous graphite, diamond and graphite– diamond mixtures the author proposed the equation of mixture state expressed in different approximations: a) with constant Grüneisen coefficient and constant specific heat capacity; b) with constant Grüneisen coefficient and specific heat capacity dependent on the temperature; c) with Grüneisen coefficient the dependent on the volume and constant specific heat capacity; d) with Grüneisen coefficient the dependent on the volume and specific heat capacity dependent on the temperature.

For all kinetics models shock adiabats with each approximation of the equation of mixture state were calculated. Results of the comparison of the calculated and experimental shock adiabats allow to conclude that the equation of state mixture, model of the kinetics of direct phase transition and the relationships used are applicable for describing the Grüneisen coefficient and specific heat capacity.

### STUDY OF DYNAMIC COMPRESSION OF POLYMERIC MATERIALS

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The high-molecular compounds are perspective materials which are extensively used in constructions bearing high heat and power loadings. The equations of state of polymers in broad ranges of energy densities and pressures are necessary for the solution of multiple problems of highenergy physics (such as modeling of processes of high-speed piercing of protective screens of spacecrafts, influence of beams of relativistic electrons on polymer targets and others) [1].

However, the number of experimental and theoretical papers, devoted to the study of the Gruneisen function of polymers and compositions in extreme conditions, is very few. This fact stimulated our research for the dependences of the Gruneisen function on density and temperature calculated according to the various models. It has to be taken into account that the glass transition temperature of polymers possessing complex macromolecular structures may change in respect to the speed of impact, and, as a consequence, the ratio between the intermolecular and intramolecular values of the Gruneisen function varies as well [2].

The Gruneisen function of polyethylene, synthetic butadiene rubber and their compositions has been studied in dependence on the density at different degrees of dynamic compression according to the acquired models. It has been shown that the best agreement between the calculated and the experimental values of the Gruneisen function in studied range of compressions is provided by the equation of A.M.Molodets, which involves the general fundamental properties of material and the deduction of which is not restricted by the assumptions on type of condensed matter [3].

The dependence of the Gruneisen function of polyethylene, synthetic butadiene rubber and their compositions on temperature has been found to be quite weak. The more the density achieved in impact tests the less is the dependence of the Gruneisen function on temperature [2].

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## THE INTENSIFICATION OF THE RESISTANCE TO DEFORMATION AT HIGH-RATE STRAIN AND ANOMALOUS THERMAL HARDENING OF ALUMINUM IN THE CUTTING

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Based on the analysis of experimental data on plastic shock waves in aluminum AD1 a viscoelastoplastic material model was constructed. The model describes the intensification of the resistance to deformation at high-rate strain (at  $10^3 - 10^4$  1/c) and anomalous hardening with temperature rise. In frame of the finite element method the two-dimensional problem on cutting the viscoelastoplastic workpiece with strain rate up to  $10^5$  1/c was considered. The comparative calculations were performed for different developed models of the material including standard (similar to Johnson-Cook) model. Some qualitative effects and quantitative estimates concerned about the influence of the resistance to deformation at high-rate strain and anomalous hardening on the cutting process were obtained.

# MOLECULAR DYNAMIC SIMULATION OF NANOINDENTATION OF TiC & Al<sub>2</sub>O<sub>3</sub>

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TiC-Al<sub>2</sub>O<sub>3</sub> ceramic is widely used for manufacturing wear-resistant materials due to their high hardness, high heat and wear resistance even at high temperature. Despite much research on the development of multilayer coatings, questions still remain about the mechanisms of deformation and wear. Nanoindentation is one of the best methods to measure such properties of materials. In such experiments an indenter of known geometry is pressed into the surface under a fixed load and the depth of penetration or the area of the resultant impression can be used as a measure of the resistance of the material to damage. Young's modulus, hardness, yield strength, etc. can be measured in one experiment. Atomistic simulation of nanoindentaion is necessary to link the macroscopically observed properties to the mechanical properties of the material on the microscopic level. Film thickness, indenter size and speed can be varied systematically to study their influence on the load versus indentation depth response. In this work we used molecular dynamic simulation for modeling nanoindentation processes of titanium carbide and sapphire ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>). Hardness and Young's modulus values are obtained from load-penetration curves. Mechanisms of elastic-plastic transition are discussed. Results are compared with experimental data [1].

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### THEORIES AND MODELINGS OF HOMOGENEOUS NUCLEATION

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The work covers various approaches to theoretical description and atomistic modeling of homogeneous nucleation in metastable media. The processes include nucleation of voids in liquids and solids, crystal in supercooled melts, dislocation loops.

The applicability of different approaches to nucleation study in molecular dynamics (MD) simulation is tested, including direct simulations, survival probability calculation, mean first-passage time analysis, transition interface sampling. At high degrees of metastability, direct MD simulations coupled with kinetics analysis provide detailed information about nucleation kinetics, nucleus size and structure and can give some insight into nucleation barrier shape. At lower degrees of metastability, indirect simulation using transition interface sampling methodology can be used to extend the time scales available for MD simulations.

The results of MD simulations of nucleation are discussed in the framework of the classical nucleation theory (CNT). Applicability of some approximations accepted in the CNT is analyzed.

# ATOMISTIC MODELING OF GRAPHITE MELTING

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Graphite melting properties have been the subjects of debate for many years due to discrepancy in experimental data. We report here molecular dynamic simulations of graphite melting with the semiepirical bond-order potential AIREBO. As a result in the pressure range up to 14 GPa the graphite melting line was obtained and properties of liquid carbon were investigated. For the superheated graphite the melting front velocity dependencies on temperature were calculated to verify the values of melting temperatures.

### GLASS TRANSITION CRITERIA AND CRITICAL COOLING RATES

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Molecular dynamics study of transition from liquid aluminum into amorphous solid state is carried out.

Aluminum is described by a form of embedded atom method potential. The system was first equilibrated at T = 1500 K, which is above the melting temperature of aluminum. Then the velocities of atoms were gradually rescaled until the system reached T = 300 K.

Two models are considered—isochoric and isobaric cooling. Isobaric process is carried out in a thin film of aluminum.

MD simulations were held for cooling rates from  $10^{13}$  K/s to  $10^{10}$  K/s. Different glass transition criteria are observed—splitting of the second peak of radial distribution function, changes on the self-diffision coefficient—temperature dependence and increasing the number of atoms with icosahedral environment.

Critical cooling rates related to the sharp increasing number of atoms with icosahedral environment and fomation different structures of these atoms are studied.

The results are compared with the common data.

# STATE OF LIQUID AT HIGH TEMPERATURES Vorontsov A.G.,\* Kuts D.A.

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It is known, that simple liquids expansion with heating is not an uniform process. Coordination number changes significantly, but the position of the first coordination sphere changes slightly. The biggest effect was observed in liquid alkali metals, where coordination number falls from 8...10 to 3...4 during expansion up to the critical point. Non-uniform expansion leads to the formation heterogeneous (non-uniform) structure of liquids at low densities. The low-density liquid and high-density liquid have essentially different properties because of change in interatomic interaction. At high density the repulsive part of the interatomic potential plays the main role, but at low density the attractive part does it. Moreover in some materials the nature of chemical bonding could change from metallic-like to covalent-like. Thus describing the expanding of liquids is not a simple problem.

MD simulation of the atomic structure of different liquids with model and realistic potentials was performed. Atomic positions were analyzed by Delaunay method after simulation and changes of the structure were pointed out. All models have basically the same transformation of local atomic arrangement during expansion. The temperature and density region of the transformation from high-density liquid to low-density liquid was observed being correlated with disappearing of the positive dispersion of the sound velocity in N, Ne, Hg [1], non-monotonic change of susceptibility in Hg, Cs [2, 3] and other peculiarities of properties of simple liquids.

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# MOLECULAR MODELING OF POLYMER SOLAR-CELLS Triandafilidi V.M,\* Stegailov V.V.

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21st century puts some really important problems to solve [1] One of them are the new perspective sources of energy. Polymer based devices seem to be the breakthrough. And as they are based completely on cheap organic they are cheap, easy to manufacture and the most important they are environment-friendly. Research [2] showed that one of the most important part in solar-cells manufacturing plays the exiton splitting. And to deep into this process the internal structure should be studied thoroughly. Also investigating of that process [2] elucidated the nature of that process and unveiled that polymer-nanotube self-assembly plays a crucial role in exiton splitting. This phenomenon is under investigation in this work. In this work we will perform a molecular-dynamics (MD) study of polymer self-assembly around the carbon nanotube(CNT). The polymer specimen is made of P(3HT) and the some different CNT (different chiralities, lengths, diameters).

Our numerical experiment will include the following parts:

- Building: Setting the molecular topology.
- Potential: Setting the interatomic potential—the forcefield.
- Simulation: The MD study of self-assembly process.
- Analysis.
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#### ON AN ALGORITHM FOR CALCULATING THE CONCENTRATION DISTRIBUTION OF ABSORBING MOLECULES ALONG THE LASER BEAM

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An algorithm for calculating the concentration distribution of absorbing molecules along the laser beam, when the absorbing layer is a medium with fractal geometry, is offered. The algorithm is based on a loaded partial differential equation of the second order that changes its type at a critical time moment, when the concentration of molecules in absorbing medium reaches its maximum. Under certain the physically admissible assumptions, this equation can be written in the form

$$\partial_{\tau t}^{\alpha+1} \upsilon(z,\eta) + \operatorname{sign}(t-\tau) |t-\tau|^m \frac{\partial^2 \upsilon(z,t)}{\partial z^2} = 0,$$
(1)

where  $0 < \alpha = \text{const} \leq 1$ ;  $\partial_{\tau t}^{\alpha+1}$  is the regularized Riemann-Liouville fractional derivative of order  $\alpha + 1$  with the origin at  $t = \tau$  with respect to the time variable t, or, that is the same, is the Caputo operator of fractional differentiation; v(z,t) is the concentration distribution of absorbing molecules in the point  $z, z \geq 0$ , and at the time moment t; m is a non-negative integer, [1]—[3]. Equation (1) coincides with the Tricomi equation, which is well known in gas dynamics of hypersonic flows, when  $\alpha = 1$  and m = 1, and with the Lavrent'ev-Bitsadze equation when  $\alpha = 1$  and m = 0.

The algorithm for calculating the concentration distribution of absorbing molecules provides to approximate equation (1) by the equation

$$\partial_{\tau t}^{\alpha+1} \frac{1}{h_{i}} \det \left\| \begin{array}{cc} \upsilon(z_{i},\eta) & z_{i}-z \\ \upsilon(z_{i+1},\eta) & z_{i+1}-z \end{array} \right\| + \operatorname{sign}(t-\tau)|t-\tau|^{m} \frac{\partial^{2} \upsilon(z,t)}{\partial z^{2}} = 0,$$

where  $z_i < z < z_{i+1}, i = 0, 1, \dots, n$ .

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# NON-EMPIRICAL CALCULATION ON TRANSPORT PROPERTIES OF GROUP 12 ELEMENTS (Zn, Cd, Hg)–RARE GAS SYSTEMS Meshkov V.V.,\*1 Fokin L.R.<sup>2</sup> <sup>1</sup>MSU, <sup>2</sup>JIHT RAS, Moscow, Russia \*meshkov@laser.chem.msu.ru

Rare gases and metals of group 12 (Zn, Cd and Hg) mixtures are of high interest due to their prospective use in excimer lasers, adsorption and catalytic processes. However, both theoretical and experimental results for these systems are rarely presented.

We present the results of high-level electronic structure calculations of the potential energy curves (PECs) for the ground state of van der Waals molecules MeRg (Me = Zn, Cd, Hg; Rg = He, Ne, Ar, Kr, Xe). The energies were calculated in a wide range of internuclear distance using the coupled-cluster method with single, double and approximate triple excitations CCSD(T), with the aug-cc-pVnZ (n = T, Q, 5) basis sets for both atoms augmented by the bound functions centered on a middle of internuclear distance. The extrapolation to complete basis set was performed and the full counterpoise correction technique was employed to remove basis set superposition error.

The derived *ab initio* point-wise potentials have been approximated by the closed form based on Chebyshev polynomial expansion, and then, the resulting analytical PECs were used to estimate transport properties of the Me-Rg pairs in the framework of classical and quantum statistical approaches. The present results are obtained in a wide temperature range and compared systematically with available experimental data and preceding calculations.

The work is supported by the Russian Foundation for Basic Research, through the grants 11–08–00821–a and 12–08–31407–mol–a.

### AB INITIO CALCULATIONS OF TRANSPORT AND OPTICAL PROPERTIES OF METALS: ALUMINUM AND SILVER

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This work is devoted to the first principle calculation of dynamical electrical conductivity, optical properties and static thermal conductivity of metals (Al, Ag) at different temperatures and densities. The investigation is based on the quantum molecular dynamics (QMD) simulation, density functional theory and the Kubo-Greenwood formula.

The main calculations are performed for the aluminum at the nearnormal densities and the temperatures from melting up to 20000 K. To verify the computational scheme the first calculations were performed at the points on the phase diagram where the results of the other authors, reference and experimental data are available. In general the results of this work are in satisfactory agreement with the results of other authors. The dependence of the results on the technical parameters was investigated. The static electrical conductivity calculation error was estimated for the aluminum at the normal isobar and the temperature 1273 K.

The calculations of the optical properties, static electrical conductivity and thermal conductivity were performed for aluminum at the normal density and the temperatures from melting up to 20000 K. The frequency dependences of the dynamic electrical conductivity possess the Drude-like shapes. The static electrical conductivity decreases with the growth of temperature, whereas the thermal conductivity increases.

The influence of the non-equilibrium excitation of the electronic subsystem on the optical properties and thermal conductivity was investigated. It was shown that in the temperature range under consideration the dynamic electrical conductivity is almost not affected by the excitation of the electronic subsystem. On the contrary, thermal conductivity depends considerably on the non-equilibrium excitation of the electronic subsystem.

Several calculations were also performed for silver. The preliminary results show that the curves of the dynamic electrical conductivity possess the shapes that differ form the Drude-like behavior. The work is to be continued. The influence of the non-equilibrium excitation of the electronic subsystem on the optical properties and thermal electrical conductivity of silver should be investigated. It is planned to create the semiempirical model of the optical properties of silver based on the results of *ab initio* calculations. This model is to be used during the simulation of the femtosecond laser heating of the metallic targets.

## RELATIVE EMISSIVITY USE FOR TEMPERATURE DETERMINATION VIA THERMAL RADIATION SPECTRUM OF OPAQUE BODIES

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It is known, that in the determination of the thermodynamic (true) temperature of opaque, emitted object via the registered thermal radiation spectrum, as a rule, the spectral emissivity is unknown and the number of equations is less than the number of unknown parameters, i.e., problem is ill-posed. To regularize the problem, additional communications relations are often specified by parametric approximation of the unknown object emissivity depending on the radiation wavelength and narrowing range of possible temperatures. However, even with a slight increase in the number of unknown parameters, the accuracy of their determination, in particular the desired temperature plummets. However, information on the spectral dependence of the emissivity and temperature of the object is contained in the spectrum and, in some simple cases can be determined. To determine the true object temperature of the thermal radiation registered spectrum is proposed to search for spectrum parts, where the emissivity (or its logarithm) is dependent on the wavelength linearly and solution of the corresponding system of equations. This spectral part can be found if the spectral radiance derivative on the wavelength is constant within the experimental error. To reduce the range of operating temperatures used relative emissivity, which is the ratio of the spectral radiance of the thermal radiation object spectrum to the spectral radiance of a black body at the temperatures expected. It is shown that using a relative emissivity, graphical interpretation of the solution set of the original system of nonlinear equations. If emissivity (or its logarithm) is a linear function of the wavelength, then the operating temperatures range can be determined from the change in the convexity (concavity) of the spectral relative emissivity dependence in the process of changing the values from permissible temperature lower than the true object temperature to large true temperature. To illustrate the proposed method uses experimental data known from literature.

## EXPERIMENTAL SETUP FOR INVESTIGATION OF THERMOPHYSICAL PROPERTIES OF REFRACTORY COMPOUNDS UNDER HIGH STATIC PRESSURE

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A technique and an experimental setup for complex investigation of thermophysical properties of matter: thermal expansion coefficient, heat capacity, melting temperature, melting heat, resistance of refractory metals, carbides (TaC, TiC, etc.) and graphite in the vicinity of melting point and in the liquid phase, the most perspective at the creation of innovational high-temperature power-plants and supersonic flying machines, are described. Nowadays the pulse heating method is one of the most essential techniques in the modern experimental physics using for research of matter properties at the extremely high temperatures. This method has the significant advantage (to a laser pulse) in a volumetric heating allowing to measure specific properties of matter. The feature of this method consists in fact that due to the high rates of heating the specimen has no time to interact with the surrounding medium, has inappreciable losses of heat by radiation and transpiration and maintains its geometry in fluid state. Structure (stoichiometry) changing of metallic carbides at high temperatures causes a necessity of carrying out the experiments under the high gas pressures. For this purpose the setup has been equipped by a high pressure system based on the diaphragm-type compressor. During the experiment gas pressure remains at the constant level that is controlled by the pressure monitor with an accuracy of 0.2%. Peculiarity of the suggested approach consists in an integration of the high static gas pressure technique and the modern technique of optical diagnostics—precise optical pyrometry, high-speed digital visualization of the specimen dimensions for the determination of expansion coefficient, provided at the experiment duration of about 100–1000 microseconds. Results of preliminary experiments on the example of tantalum specimen with typical size of approximately  $0.3 \times 1 \times 25$  mm melting are discussed.

#### HIGH PRESSURE INDUCED TRANSFORMATIONS OF SELENIUM NANOCOMPOSITES

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Selenium is the very interesting element, so it has many useful properties applied in electronics, photonics, medicine, pharmacology, etc. It has promising features can be applied for production of new materials. especially on nanoscale level. Nanosized selenium has the great perspectives now. There are some ways of its synthesis in the nanostate. We had obtained this element as a part of polymeric nanocomposites. It was interesting to study a behavior of these substances at high pressures as for fundamental knowledge and for practical applications. It is a good way to find structure stability parameters for our complex systems. Selenium nanocomposites were obtained on water solutions of polyvinyl alcohol with surfactants. Selenium nanoparticles were formed after reaction of reduction of ammonium selenite with hydrazine-hydrate. Polymeric films produced in result of drying of solutions on smooth surfaces were applied for the study. The sizes of nanoparticles were determined with ESM and optical spectral data. For investigation of high pressure transformations of our materials diamond anvil cell technique combined with Raman spectrofotometer were used. The pressure range was up to 10 GPa. Spectra obtained show changes of structure of our composites under pressure as compared with published data. The previous researches in high pressure were not devoted selenium nanocomposites.

## STUDY OF ELECTRIC PROPERTIES OF AMORPHOUS SILVER SULPHIDES WITH CONTENT OF CARBON NANOTUBES

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Multicomponent amorphous copper and silver chalcogenides have been known as promising materials for scientific and applied purposes, because they possess unique physical properties and exhibit a combination of interesting optical, electrical, ferroelectric, and other characteristics [1]. In order to obtain materials with a high ionic conductivity component, glassy silver chalcogenides  $AgGe_{1+x}As_{1-x}S_3$  with the addition of nanotubes were synthesized. In this work the results of the study of material with x = 0.4are presented. X-ray and Raman attestation of AgGe<sub>1.4</sub>As<sub>0.6</sub>S<sub>3</sub> with content of carbon nanotubes was carried out. Its electrical properties at a frequency of the alternating-current electric field varying from 200 Hz to 200 kHz in the cells with different electrodes (copper, silver, graphite) and on direct current were studied. The presence of polarization effects related to the ionic conductivity was established. The ion transport was confirmed by means DC measurements in cells with blocking ion component of conductivity electrodes. An evaluation of the proportion of ionic conductivity can make a preliminary conclusion that the ionic component of the conductivity of at least 98%.

Analyze of the baric dependences of AC properties have shown that the dielectric loss tangent and the real part of an admittance of the  $AgGe_{1.4}As_{0.6}S_3$  with carbon nanotube content compound exponentially increase with a pressure increase from 1 up to 30 GPa. The baric dependences of tangent of loss is approximated by function

$$\tan \delta = a + b \cdot \exp(P/c),$$

where P—pressure in GPa; a, b, c—constants.

The study was supported in part by the Ural Federal University development program with the financial support of young scientists; and by the Russian Foundation for Basic Research, project 12–02–31607.

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## ELECTRICAL RESISTANCE OF FULLERENE C<sub>60</sub>, GRAPHITE AND QUASI-GRAPHENE AT HIGH PRESSURE

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Comparative studies of resistivity of fullerite  $C_{60}$  and graphite were performed in the pressure range from atmospheric pressure to 29 GPa at room temperature. The resistivity of quasi-graphene (sample MSG-76), produced from synthetic graphite, was measured as well at pressures of 15 GPa to 48 GPa at room temperature. Samples of quasi-graphene were flakes with the number of layers from 5 to 20.

High-pressure chamber (HPC) of the "rounded cone-plane" form with anvils made of synthetic polycrystalline diamond (carbonado), was used for studies of electrical characteristics of the materials at high pressures. The measurements were performed for  $C_{60}$  and graphite samples at stepby-step increasing and decreasing pressure from atmospheric pressure to 29 GPa during several cycles of application of pressure. The measurements for quasi-graphene were performed at pressures from 15 GPa to 48 GPa. The pressure dependences R(P) was measured at different loading times for every P point to study the kinetics of resistance relaxation.

A hysteresis observed in the pressure dependences of resistance of  $C_{60}$ and graphite indicates the occurrence of metastable states. No hysteresis was observed for the resistance of quasi-graphene. The resistance of fullerene under pressure decreased by more than one order of magnitude, and the resistance of quasi-graphene decreased by almost 2 times. The features in the pressure dependences of resistance of fullerite and graphite corresponded to the known phase transitions in these materials, were also identified.

The resistance relaxation after changing pressure was studied for the fullerene, graphite and quasigraphene. The relaxation times for graphite are less than 1 min. The resistance of  $C_{60}$  samples did not reach the saturation at the time intervals used (up to 10 min.); that gives evidence of the existence of long relaxation times for this material. The relaxation times for quasi-graphene were about 3 min.

### NEW HIGH-PRESSURE PEROVSKITE-LIKE PHASE Dy<sub>0.75</sub>Cu<sub>3</sub>V<sub>4</sub>O<sub>12</sub> AT HIGH PRESSURES

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A-site-ordered perovskites with the general formula  $ACu_3B_4O_{12}$  (where A-rare earth or alkaline element and B-Jahn-Teller ion) show diverse and intriguing physical properties [1]. The purpose of this work is to study the effect of high pressures on the electrical properties of the new high-pressure perovskite-like phase Dy<sub>0.75</sub>Cu<sub>3</sub>V<sub>4</sub>O<sub>12</sub>. Dy<sub>0.75</sub>Cu<sub>3</sub>V<sub>4</sub>O<sub>12</sub>—oxide was prepared under high-pressure and high-temperature conditions in a toroidtype high-pressure chamber [2], and crystallized as an Dy-site-ordered double perovskite (space group Im - 3, Z = 2). The electrical properties were investigated on a direct current and by a method of impedance spectroscopy in the frequency range between 200 Hz and 200 kHz at temperatures between 10 and 300 K at a pressure up to 50 GPa. High pressure from 10 GPa to 50 GPa has been generated in the diamond anvil cell with anvils of the "rounded cone-plane" type made of synthetic carbonadotype diamonds [3]. In the temperature range of 10–300 K with direct and alternating currents (frequency-4 kHz) the temperature dependence on the conductivity exhibits metallic behavior. The baric dependences of the resistance of  $Dy_{0.75}Cu_3V_4O_{12}$  at 15–50 GPa and 300 K shows that the resistance first falls rapidly with the pressure increase (up to 23-26 GPa), and then the rate of the drop in resistance slows sharply (up to 50 GPa). The dependence R(P) can be approximated in the pressure ranges by two exponential functions with different exponents. Similar behavior of the resistance upon a change in pressure was described in detail [4] for  $Tm_{0.75}Cu_3V_4O_{12}$  and other compounds of this series. This work was supported in part by the Russian Foundation for Basic Research, project 12-02-31607. Also the research was carried out in terms of Ural Federal University development program with the financial support of young scientists.

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## HYDRODYNAMIC INSTABILITIES AND BOUNDARY VALUE PROBLEM

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For the first time, on the basis of conservation principles and thermodynamics laws, we derive the generalized Rankine-Hugoniot conditions that can be applied at unsteady and curved fronts. The conditions describe the dynamics of the interface (front) in an explicit and covariant form and can be applied in convergent or Cartesian system of coordinates for three-dimensional systems. The consideration is applied to the instabilities of Landau-Darrieus (LD), classical Rayleigh-Taylor (RT) and ablative Rayleigh-Taylor (ART). It is shown that in the case when if there is mass flux across the interface and no acceleration (LD), the front can be unstable only if three conditions are satisfied (1) bulk vorticity is generated; (2) energy flux across the front is imbalanced; (3) the energy imbalance is large enough. When acceleration is present (RT and ART), the dependence is obtained of the instability growth-rate on the mass flow and energy imbalance across the front. Connection between the ablative RTI and classical RTI is made. The obtained results provide a theoretical framework for design of experiments in ICF-relevant conditions.

## VORTEX CASCADES IN SHARE LAYERS AND RELAY-TAYLOR INSTABILITIES Fortova S.V.

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This work is a continuation of series of articles [1] devoted to study of vortex cascades formed in compressible non-viscous liquid under various hydrodynamic conditions. In this work we study how flow parameters influence the formation of a turbulent core in share layers and in RTI. Special attention is given to energy spectrum of kinetic energy. It is shown that as the flow transforms to the turbulent phase there emerge pulsations of velocity of various scale which leads to the formation of a vortex cascade.

Decomposition of kinetic energy on wave number reveals correspondence with the energy spectrum of Kolmogorov–Obukhov.The structure of the Kolmogorovs energetic cascade of the kinetic energy is well-known : for large Reynolds numbers there are three intervals of wave numbers for the spectral distribution of energy—energetic, inertial and viscous. The well-known Kolmogorov's "-5/3 law" is valid for the inertial interval.

Based on numerical experiments we investigate turbulent flow, analyze the scheme of formation of the turbulent core and the study the "-5 / 3 law" for share layers and RTI. Analysis includes evaluation of spectrum kinetic energy. We obtained a dependence of the kinetic energy on wave number by means of the Fourier expansion of the velocity components. Also we demonstrated existence of an inertial interval for the kinetic energy for both problems.

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# MATHEMATICAL MODELING OF HYDROCARBON MIXTURES FILTRATION PROCESS IN POROUS MEDIA

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A mathematical model is developed which enables one to calculate the hydrodynamic and thermodynamic characteristics of the process of filtration of hydrocarbons in the stratum. We consider the two-dimensional gascondensate reservoir consisting of a porous skeleton and two-component mixture of hydrocarbons methane-n-butane. Structurally, the model consists of two parts, namely, the hydrodynamic part, which describes the process of two-phase filtration in a porous medium in the Darcy law approximation, and the thermodynamic part, within which the equations of state for mixture are used to calculate the compressibility coefficients of the mixture and the parameters of phase equilibrium of the system in the vapor and liquid phases. A new numerical method for solving problems without the explicit separation of the jump phase saturation (front evaporation or condensation) to calculate the processes is developed. Qualitative and quantitative agreement is obtained between the experimental results and calculated relationships. The mathematical model and numerical method are implemented in a software product and patented in RF.

#### CAPILLARY OSCILLATIONS OF THE DROP IMMERSED IN A LIQUID WITH TAKING INTO ACCOUNT THE VISCOSITY

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The analytical solution of problem of capillary oscillations of drop immersed in a liquid with taking into account of viscosity is presented for the fist time. For the time dependence of the drop radius

$$r(t) = \sum_{n} a_n(t) P_n(\cos(\theta)),$$

the coefficients  $a_n$  are calculated, here  $P_n$  are Legendre polynomials. It has been shown, that the oscillation frequency of the drop with radius a depends on the viscosity

$$\omega_n^2 = \frac{\sigma}{\rho a^3} n(n-1)(n+2) - \left[\frac{\eta}{\rho a^2}(n-1)(2n+1)\right]^2$$

where  $\sigma$  is the surface tension,  $\rho$  is liquid's density,  $\eta$  is viscosity, n is the harmonic number.

The same type of expression has been obtained for oscillations of liquid surrounding the bubble.

### NUMERICAL SIMULATION OF DYNAMICS OF COMPOSITE DROPLET UNDER CONFINED SHEAR FLOW

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The liquid dispersion and emulsion is encountered in many engineering and biomedical applications such as mixing and dispersion processes, materials processing, microfuidics technologies, targeted drug delivery et al. This work is devoted to the numerical investigation of dynamics of 2D composite droplets in a continuous immiscible liquid phase under the confined simple shear flow. The fluids are incompressible and governed by the Navier–Stokes equations. Numerical solution of these equations has been carried out on the basis of the projection method along with the level set method tracking the interfaces of the composite droplets.

The following characteristics of the systems were considered. The core to shell viscosity ratio of the composite droplet were taken as 10, while viscosities of a core and dispersion medium were matched. The main goal of the present work is to investigate the influence of channel walls to the hydrodynamic behavior and steady state parameters of the composite droplet. With this end, numerical simulations for different ratios of initial radii of shell and core were performed. This made it possible to reveal the time sequence of droplet deformation along with velocity and pressure field in the system considered. The steady state Taylor deformation and orientation of a composite droplet for different ratios of its radius to the channel thickness were derived.

#### NANOSECOND ELECTRICAL EXPLOSION OF TUNGSTEN WIRE

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The experiments on electrical explosion of 25  $\mu$ m tungsten wire were carried out on the equipment with the following parameters: the charging voltage was  $U_0=20$  kV, the current amplitude was up to 10 kA; the current rise rate dI/dt was up to 50 A/ns; the capacitance was  $C=0.1 \ \mu$ F, the circuit inductance was L=600 nHn.

To analyze the processes accompanying generation and propagation of shock with constant velocity, we used a well-known model in which a mechanical impermeable piston moves uniformly with velocity u, generating a shock wave moving with constant front velocity D in a motionless ideal gas (non-viscous, non-conducting of heat). In the frame of reference in which the shock front is at rest  $(u_1 = u - D, u_0 = -D)$ , the equation of conservation of mass, momentum and energy at the wave front can be written in the following form (see, for example, /1/):  $\rho_0 u_0 = \rho_1 u_1$ ,  $P_0 + \rho_0 u_0^2 = P_1 + \rho_1 u_1^2$ ,  $h_1 + u_1^2/2 = h_0 + u_0^2/2$ , where h is the enthalpy,  $\gamma = c_p/c_v$  is the adiabatic index,  $c_v = iR/2$  and  $c_p = (i+2)R/2$ are the thermal capacities of gas for constant volume and pressure correspondingly, i is the number of degrees of freedom of gas molecules and Ris the gas constant. The parameters with indexes 0 and 1 refer to motionless gas before the shock front and to compressed gas behind the shock front, respectively. In the frame of powerful shock  $P_1 \gg P_0$  moving in a motionless gas, the expression for the parameters of gas behind the front can be written in the well-known manner:  $\rho_1 = (\gamma + 1)\rho_0/(\gamma - 1)$ ,  $P_1 = 2\rho_0 D^2/(\gamma + 1)$ ,  $u_1 = 2D/(\gamma + 1)$ ,  $T_1 = 2\gamma D^2/c_p(\gamma + 1)^2$ .

Therefore, without taking into account relaxation processes, the temperature behind the shock front will be  $T_1 = 4.2$  kK, pressures  $P_1 = 54$  atm and piston velocities  $u_1 = 2.5$  km/s in our case of explosion of tungsten.

According to the experiments the velocity of the region with maximum current density is 2.43 km/s. This velocity well agrees with the predicted piston velocity. Based on this fact, we can conclude that the region in which the current flows is the "piston" generating a shock wave.

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# THERMOPHYSICAL PROPERTIES OF IONIC LIQUIDS: MODELS AND NUMERICAL DATA IN INTERNET

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Different Internet resources containing information about thermophysical properties of ionic liquids are analyzed in the report. An information from Database No.147 of TRC NIST (National Institute of Standards and Technology, Boulder, CO, USA) is considered. Authors have made a research that includes: 1) an analysis of literature sources containing numerical data of properties; 2) a development of software tools those let us treat and save numerical data on thermophysical properties of ionic liquids; 3) a development of models and algorithms those devoted to fulfill online calculations connected with thermophysical properties of ionic liquids. A special server software is elaborated to work with thermophysical data offline in different common-used programs. Its demo version is available in Internet: http://www.irboc.com. IRBOC (Interactive Reference Books and Online Calculations) is a server software for working with thermophysical databases. IRBOC is multilingual: English and Russian languages supported. Thermophysical data may contain formulas/formulations and tables. IRBOC includes: 1) Search system; there are 3 search types: by a compound, by a property, by a reference. 2) Data review page; all data from a selected dataset is available on this page. 3) Online calculation page; It connects with online calculations of properties in given points. 4) Code generator page; a client can generate codes of functions and use different programming languages (Java, Matlab, VBA). 5) File generator page; a client can generate files containing functions for PTC Mathcad and datasets in different formats (electronic tables CSV, TXT textfile, XML datafile). A navigation is very simple. All pages contain information about dataset. A client always can return to a search result and reproduce it in future. IRBOC may work with different units.URL of every page and a situation is unique.

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#### PHYSICS OF LOW TEMPERATURE PLASMA

#### DUSTY PLASMAS AT LOW AND ELEVATED GAS PRESSURE

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Today the study of dusty plasmas is a focus of attention of many research laboratories [1-5]. In the present paper a comparative analysis of main processes in the dusty plasma at low gas pressure (for example, see [6]) and elevated gas pressure (for example, see [7]) is presented. Processes around a dust particle at low gas pressure about 1 Torr and lower can be considered in the collisionless approximation, and at elevated gas pressure about 1 bar and higher the collisional regime of electron and ion transfer takes place. Therefore, charging, conditions of levitation of dust particles, screening of their charge, ion drag force and friction force by neutral atoms differently depend on plasma parameters at low and elevated gas pressure. Charging theories and main forces acting on dust particles at low and elevated gas pressure are considered. Screening of dust particle charge in plasma is thoroughly considered and it is shown within the kinetic approach [8] how the screening is changed at the gas pressure variation. The screening is also considered within the Bogolyubov-Born-Green-Kirkwood-Yvon or BBGKY hierarchy [9, 10], the hydrodynamic approach and the integral-equation theories using Ornstein-Zernike relation and hypernetted-chain (HNC) approximation [10]. Directions of development of the dusty plasma theory and experiment are briefly outlined.

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ON QUANTUM BOUND OF SHEAR VISCOSITY OF STRONGLY COUPLED PLASMA Mintsev V.B.,\* Fortov V.E. IPCP RAS, Chernogolovka, Russia \*minvb@icp.ac.ru

String theory methods led to the hypothesis that the ratio of shear viscosity coefficient to volume density of entropy of any physical system has a lower bound [1].

$$\frac{\eta}{s} \ge \frac{\hbar}{4\pi k_B} = Q_L = 6.08 \cdot 10^{-13} \text{ K} \cdot \text{s}.$$

This work is devoted to analysis of the behavior of the shear viscosity of strongly coupled electromagnetic plasma. Systems with strong coupling have a small viscosity compared to weakly coupled plasmas in which the viscosity is proportional to the mean free path. Today a huge array of experimental data on the thermodynamic, transport and optical properties of strongly coupled plasma was received, but there are no direct measurements of viscosity. For our purposes experimental data on measurements of electrical conductivity of hydrogen, deuterium and rare gases under intense shock compression and under quasiisentropic compression in multistep loading up to megabar pressures are the most interesting. The data on hydrogen, deuterium and helium-hydrogen mixture, received in the region of "metallization" at  $P \sim 150$  GPa in different experimental systems by the method of quasiisentropic compression reach the values  $\eta/s \sim (0.3 - 10)Q_L$ . Thereby, the hydrogen plasma in the region of "metallization" possesses the lowest values of the shear viscosity to the entropy ratio. Note that in this case we have an extremely high value of the coupling parameter  $\Gamma \sim 20 - 80$ . It is shown, that the data on electrical conductivity of strongly coupled electromagnetic plasma, confirm the tendency of decreasing of the viscosity  $\eta/s$  with an increase in the correlation  $(\Gamma)$  and thus confirm trend of the transition of the physical system to the perfect frictionless fluid with the increasing of the interparticle interaction.

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#### ANGULAR DEPENDENCE OF S- AND P-POLARIZED REFLECTIVITIES OF STRONGLY CORRELATED DENSE PLASMA

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The research of transitive layer of explosively driven dense plasma can be carried out using the technique of inclined probing by polarized electromagnetic waves. 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 nonideal xenon plasma are presented. The measurements of polarized reflectivity coefficients of strongly correlated dense plasmas have been carried out at incident angles up to  $\theta = 75^{\circ}$  simultaneously for s- and p-polarization using laser light of frequency  $\nu_{las} = 2.83 \cdot 10^{14} \text{ s}^{-1}$  ( $\lambda_{las} = 1064 \text{ nm}$ ),  $\nu_{las}$ =  $4.33 \cdot 10^{14} \text{ s}^{-1}$  ( $\lambda_{las} = 694 \text{ nm}$ ) and  $\nu_{las} = 5.66 \cdot 10^{14} \text{ s}^{-1}$  ( $\lambda_{las} = 532 \text{ nm}$ ) at incident angles up to  $\theta = 45^{\circ}$ .

The plasma composition was calculated within a chemical picture [1]. During the experiments, the plasma density up to  $\rho_{pl}=3.4 \text{ g/cm}^3$ , pressure up to P = 16 GPa and temperature up to  $T = 33000^\circ$  K were realized. Under these conditions, the plasma is non-degenerate.

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# DENSITY FUNCTIONAL THEORY APPROACH TO CALCULATION OF SHOCKED XENON REFLECTIVITY

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The reflectivities of shocked xenon, measured in the experiments of Mintsev and Zaporoghets in 1989 for wavelength  $\lambda = 1064$  nm [1] and further for  $\lambda = 694$  nm and  $\lambda = 532$  nm [2] are worth to pay attention, because of difficulty of explanation of these results with the standard methods of nonideal plasma theory. As it was shown in [3], the Drude model, with collisional frequency in Born approximation, gives reflectivities that are 2.5–3 times larger than the experimental data at low densities. The results of other approaches to the collision frequency calculation also can't provide better explanation of slope reflectivity drop with decreasing of density.

In [3–5] it was shown that the non-ideal plasma theories give a reflectivity results, which are in a good agreement with the experimental data, only in case of an assumption of significant width to the shock front. The values of reflectivity of xenon plasma, calculated by Desjarlais [6], are obtained in frames of the approach of quantum molecular dynamics, based on the finite temperature density functional theory; Kubo-Greenwood formalism was used for calculation of the optical properties. In comparison with [3–5] in [6] shock has an ideal step profile.

The approach, used in this work, is approximately the same with method in [6]. However, the agreement of obtained reflectivities in this work with results in [1, 2] is better than in [6].

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# RECOMBINATION IN DENSE ION PLASMA Lankin A.V.,\* Norman G.E., Amirov R.Kh. JIHT RAS, Moscow, Russia

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The results for the rate of recombination in the ion plasma are studied in the work. It is obtained by processing the data of experimental studies of the afterglow of the gas discharge in the environment of the fluorine and sulfur hexafluoride. Slowing the rate of recombination in such media is more as compared to the standard formula for ideal plasma. Deceleration increases with growth the parameter coupling. In the analysis of the mechanism of this phenomenon is set a number of features of ion recombination in strongly coupled plasmas.

In describing the recombination of ions in medium of sulfur hexafluoride model (Lankin, 2008) suppression of recombination in strongly coupled plasma due to the formation of zones of many fluctuations, separating the region free of charged particles and the pair states, is applicable:

$$k^{\cdot}(P,T,\Gamma) = \begin{cases} k_0(T) & \text{for } \Gamma < \Gamma_0, \\ \beta \cdot k_0(T) \exp[-A/2(2\Gamma + \Delta/T)] & \text{for } \Gamma > \Gamma_0, \end{cases}$$
(1)

where  $k_0$ —recombination rate constant in the limit of an ideal plasma,  $\Delta$ —an additional contribution of ion-molecule interactions in the width of zone of many-width fluctuations,  $\Gamma_0$ —point change in the mechanism of recombination, A—model parameter,  $\beta$ —is determined from the continuity of function.

In this case, the coupling parameter  $\Gamma_0$  at which the change in the mechanism of recombination in the ion plasma is less than the electronion plasma, because of the increased width of zone of the fluctuations as a result of many-particle interactions of ions and neutral molecules. In addition, parameter A is reduced several because of the higher probability of large-angle scattering of ion-molecule collisions, compared with the electron-electron.

Recombination process of fluoride ions in the medium of  $F_2$  is slowing solvation n of ions and passes through the intermediate formation of a pair of cluster ions. Similarity of the recombination rate as the temperatures and pressures is explained. Dependence of the rate of recombination at low coupling  $\Gamma$  due to the dependence of the equilibrium concentration of loose cluster pairs of the activity coefficient of the ion, which is defined in this case the value of the coupling parameter  $\Gamma$ .

## STUDY OF ELECTRON DYNAMICS IN IONIZED NANOSIZED METALLIC CLUSTERS

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Irradiation of nanosized metallic clusters by femtosecond laser pulses of moderate intensities  $(10^{13}-10^{16} \text{ W/cm}^2)$  has been considered recently in both experiments and computer simulations [1]. It has been shown that the plasma generated by ionization of cluster atoms is nonideal which allows one to apply these studies to the development of nonideal plasma theory. Electron plasma oscillations, electron-ion collisions, relaxation rates in such nanoplasma are of particular interest in view the size effects essential for the cluster plasma [2, 3].

The method of molecular dynamics (MD) is probably the most suitable numerical technique to study dynamical processes in the cluster nanoplasma due to a small number of particles. In this work we propose to use the Graphics Processing Units (GPUs) to accelerate MD simulations of the nonideal nanoplasma. Contemporary GPUs are widely used for scientific computing and showed their high efficiency for a particular class of atomistic simulations [4]. In our case it results in the speedup of two orders of magnitude when comparing Nvidia Tesla M2050 GPU and a single core of Intel Xeon E5520 CPU. It allows us to increase the number of particles and observe the transition of the electron oscillation spectra in the cluster plasma ranging from 55 to  $10^5$  ions. The dependence of frequency and damping of different collective plasma oscillation modes including Mie and Langmuir oscillations are presented. Dependence of obtained results of the choice of the potential is discussed.

GPU-accelerated program is also suitable for other problems of strongly coupled plasma.

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# THE PRESSURE AND ELECTRONIC TRANSPORT COEFFICIENTS OF SILICON AND BORON PLASMA

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The thermophysical properties (equations of state, conductivity etc.) of various substances play important role in fundamental tasks and applications. As a consequence, there are many theoretical and experimental investigations of the considered properties for various densities  $\rho$  and temperatures T [1]. During past two decades the region of dense plasma  $(T > 5 - 10 \text{ kK} \text{ and } \rho < \rho_n, \rho_n \text{ is the normal density})$  has become accessible for the measurements in non-gaseous media [2–4]. In particular, the conductivity and the pressure along isochores have been measured recently for silicon and boron plasma [4]. These two elements are "bad" metals under normal conditions.

Earlier we have developed the model for calculation of electronic transport coefficients for various substances in plasma state within the relaxation time approximation [5, 6]. The ionic composition, necessary for this calculation, has been obtained within the generalized chemical model [1, 5]. The above techniques have been successfully applied to obtain the conductivity and composition in the plasma of noble gases and noble metals. Presently we have included intoour model the pressure calculation. Then we have calculated the pressure, conductivity, thermal conductivity and thermal power for boron and silicon plasmas under conditions of the measurements [4]. Our data are in good agreement both with experimental results and calculations of other researchers [7].

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# ANOMALOUS DIFFUSIVITY OF IONIC LIQUIDS. A CLASSICAL MOLECULAR DYNAMICS STUDY

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Ionic liquids are organic salts with melting temperatures below 100°C. Their organic nature makes it possible to adjust smoothly the properties of ionic liquid for a specific application.

Ionic liquids are used as electrolytes in supercapacitors and batteries. Along with high energy capacity comparable with energy densities of electrochemical cells supercapacitors possess short charging/discharging times as those of convenient capacitors.

Usage of ionic liquids as electrolytes for supercapacitors produces a series of research problems. Particularly, diffusive and viscous properties of ionic liquids in porous structure of the supercapacitor electrode have to be studied, because these are the factors defining charge/discharge times of the device. Systems with both ionic liquid and electrode are very difficult to describe and are to be studied using quantum approaches. In this work we apply methods of classical molecular dynamics to study diffusive characteristics of the system composed entirely of the ionic liquid.

Two types of ionic liquids were studied: 1-buthyl-3-methylimidasolium tetrafluoroborate ( $[bmim]^+[BF_4]^-$ ) and N-methyl-N,N,N-triethylammonium tetrafluoroborate ( $[tema]^+[BF_4]^-$ ). Bulk diffusion of ions in ionic liquid at room temperature was observed. Anomalous character of diffusive processes in given ionic liquids was discovered. Time dependence of the mean square displacement of centers of mass of ions does not obey classical Einstein—Smoluchowski relation until ~10 ns. A long subdiffusive transition is observed between ballistic and diffusive regimes. Crucial importance of averaging was shown in calculating properties of such complicated orgamic systems with Coulomb interactions as ionic liquids. Results are presented in detail in [1].

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#### SCREENING OF DUST PARTICLE CHARGE IN NONEQUILIBRIUM PLASMAS WITHIN THE AMBIPOLAR APPROACH

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The paper is devoted to the study of the dust particle charge screening in nonequilibrium plasmas taking into account nonlocality of the electron energy distribution function within the ambipolar approach. In papers [1, 2] it was shown that in a nonequilibrium plasma with one type of ions the dust particle potential distribution is described by two exponentials, and in case of two ion types the potential distribution is a superposition of three exponentials with three different screening lengths [3]. In paper [4] the electron energy distribution function (EEDF) nonlocality influence on the electrostatic potential distribution in the vicinity of a dust particle was considered in two-component plasmas of noble and nitrogen gases at atmospheric pressure. The plasma is generated by an external gas ionization source, the ionization rate is varied in the range of 1010– 1018 cm<sup>-3</sup>s<sup>-1</sup>. The EEDF non-locality was taken into account by the additional energy balance equation which connects the local value of the electron mean energy with plasma parameters in contiguous points [5].

It is shown that the ambipolar approach allows determining two of the three screening lengths different from the Debye one (a detail calculation of the three screening lengths is reported in [4]). Either of these two constants is defined by the inverse length of ambipolar diffusion of electrons and ions on the characteristic recombination time, the other coincides with the electron energy relaxation length in elastic and nonelastic collisions with neutral gas atoms. The effect of change of electric field sign is found in numerical simulations and is discussed in details.

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## 2D AND 3D SMALL DUST CLUSTERS IN PARABOLIC TRAPS

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In axially symmetric parabolic (electrostatic or magnetic) traps confining dust clusters and structures, forces acting in the z (vertical) axis, is usually stronger than the radial ones. Under terrestrial conditions, this is due, first of all, to the need to overcome gravity. In a cusp magnetic trap under microgravity conditions this is due to the magnetic field configuration. So, small dust clusters containing  $N \sim 10^1$  particles are flat and have shell structures. With an increasing N the number of shells and then the number of layers increases too, and a transition from 2D to 3D structure occurs. We have considered Coulomb clusters with 3 to 30 particles in a parabolic trap, assuming the potential of locking in the z directions increases by 4 times faster than that in the radial direction, which is typical for the cusp magnetic traps. We have assumed that the particles are the graphite ones (graphite has a maximum of the magnetic susceptibility for diamagnetic materials) of spherical radius of 100  $\mu$ m have charge  $4 \cdot 10^4$ elementary charges of the same sign. The calculations are performed by molecular dynamics, clusters were collected from randomly scattered particles by trapping field and Coulomb interparticle interaction. In addition for clusters of a small number of particles, as well as clusters with high symmetry the system of algebraic equations was written which is solved numerically or analytically in the simplest cases. Both methods lead to the same results with very high accuracy. We have found that the transition from 2D to 3D clusters begins at 13 particles in the cluster. We have compared the configuration of Coulomb clusters and flat clusters observed in RF discharges. Some differences have been noted that, apparently, is due to the screening of the Coulomb interaction in RF discharge plasma.

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### ELECTRON BEAM DUSTY PLASMA AND SUPER HIGH CHARGING PARTICLES

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The study of electron-beam dusty plasma is of interest for many applications, for example, thrusters, particle accelerators, etc.

In the present work the super high dust particles charge was investigated. The dust particles charge was  $10^4-10^6$  electrons for micron-sized particles, the electron beam with energy up to 50 keV and current of 10 mA was used. The charge of the particles was measured directly (by the oscilloscope and electrometer current measurements) and indirectly (by video frames and by means of numerical simulation of dust particles scattering) methods. The dependence of the particles charge on their size and the energy of the electron beam was obtained. We can make a conclusion that charge increases with increasing particle size nonlinearly. The reason may be recharging, which takes place for small particles due to the presence of electron beam discharge plasma in the chamber.

The some features of the charged dust particles motion in the electron beam were observed: the particles breakdown and spiral trajectories. According to particles breakdown tracks the independent charge estimation was made. One of the possible explanations of non-linear particle tracks is particle heating, partial evaporation, and the subsequent motion by reactive forces.

# FORMATION OF ANISOTROPIC NON-IDEAL DISSIPATIVE SYSTEMS IN AN ELECTROSTATIC TRAP *Lisina I.I.,\* Vaulina O.S. JIHT RAS, Moscow, Russia*

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Strongly anisotropic structures of interacting particles are of interest in different fields of science and technology [1], [2], [3]. In hydrodynamics chains of point vortices researches associated with the names of Kelvin and Karman. And in the 20th century, interest in the Coulomb chains linked primarily to progress in high-resolution spectroscopy, and attempts to use a chain of ultracold ions to create new frequency standards [3]. Chain structures form in experiments with dusty plasma as well [1].

Here we present the results of numerical and analytical investigation

of chain-like structures of charged particles, confined by electric forces in the gravity field. The analysis of chains (quasi-one dimensional systems) was carried out for the variety of different isotropic and anisotropic pairinteraction potentials most frequently used in modeling the kinetics of repulsive interacting particles. For studying a stability of chain systems we considered equations describing the reaction of a vertical configuration of particulates in their small deviations from equilibrium. Through the analytical investigation the relations between the parameters of the pair interparticle interaction potential, the number of particles and the electric field gradient trap were determined. Vertical electric field gradient in a stable existence of a finite chain is found by using the virial theorem. We offered the criteria for determining a violation of stable equilibrium and formation of new configuration of the system, initially representing a "quasi-one-dimensional" chain of particles.

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# GROWTH OF PARTICLES FROM SPUTTERED METAL IN AN RF MAGNETRON DISCHARGE PLASMA TRAP

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The trap for particles with size in the range of  $10-10^3$  nm was realized in the RF magnetron discharge plasma. During the magnetron sputtering of the target the trap was fulfilled by the particles that nucleated and grew in the plasma. The volume occupied by confined particles cloud was of  $10^2$  cm<sup>3</sup>. The mean size and concentration of the levitated particles were estimated with LLS method. The particles with the sizes larger than 100 nm were collected onto the substrates located in some regions of the vacuum chamber. The collected particles were analyzed by SEM methods. The analysis showed that the particle elemental composition coincided with one of sputtered electrode material, the copper in the case. The particles, deposed from different parts of the trap, had the different crystal structure. Some particles had large habit planes and much of these particles with the sizes in the range of 0.3–1 mcm were the monocrystals. Other particles were ball-shaped with polycrystalline surface structure. This may be explained by difference of the concentrations and energies of sputtered atoms that formed the particles in this study of the growth.

#### SPECTRAL DIAGNOSTICS OF LOW TEMPERATURE ATMOSPHERIC MICROWAVE PLASMA

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Using of plasma sources for biomedical applications as well as development and creation of the new ones causes the development of plasma diagnostic techniques and methods. Plasma treatment of biological tissues occurs because of an effect of flows of different active atoms and molecules and UV-radiation. Among active species that can exist in plasma, one should note  $O_3$ , NO and OH radicals. In addition, intensive flows of charged plasma particles, such as electrons, negative and positive ions, can reach the surface of biological objects.

To define active species the spectrometric techniques based on the analysis of radiation and absorption spectra can be used. However some techniques are not valid for low temperature plasmas at atmospheric pressure because of their low sensitivity. In this case measuring directly in the region of plasma generation in combination with further interpolation of the data of distribution of active elements in a plasma flow is needed.

We used different gas mixtures, among which are argon, air, carbon dioxide, helium when choosing the optimal conditions of operation of plasma generator for an effective killing of pathogenic bacteria and acceleration of processes of wound healing. In this work we present the results of spectral measurements of plasma generated in different mixtures. It should be mentioned that the use of a mixture of argon with air significantly increases the intensity of radiation in the area of the short ultraviolet waves related to NO group. At the same time, the generation of plasma in the helium-argon mixtures significantly increases the brightness of lines related to the hydroxyl group. It is important to obtain quantitative data on the concentration of OH group specifically, as it is hydroxyl which is responsible for the appearance of peroxides when reaching a wet wounded surface.

Metastable argon appears as a result of collisions with electrons in the plasma. And we can calculate the concentration of metastable argon according to the analysis of an absorption spectrum. In this work we obtained integrated absorption coefficient and calculated the concentration of metastable argon in the region of generation plasma. It should be mentioned that errors of method have strong dependence on stability of discharge, gas flow, position of laser focusing, etc.

## INVESTIGATION OF ORIENTATIONAL ORDER AND FORMATION OF TOPOLOGICAL DEFECTS IN TWO-DIMENSIONAL YUKAWA-SYSTEMS

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In this work we present new results concerned with a study of dynamics of formation of topological defects and orientational order in non-ideal systems of particles, interacting via a screened Coulomb potential. Numerical calculations were performed by Langevin molecular dynamics method with periodic boundary conditions in a wide range of parameters, corresponded to ones in real experiments in dusty plasma. We revealed a dependence between a number of defects and a value of effective coupling parameter. Also, new approximations, related to the description of spatial asymptotic behavior of a bond-angular correlation function  $q_6(r)$  in liquid and, so called, hexatic phases of the system are proposed, based on the analysis of numerical simulation results. One of the main results of the presented study is a conclusion about a dependence of the form of  $q_6(r)$  from a phase state of the system. It is shown that the form of the bond-angular correlation function is different for liquid and hexatic phases, but remains within the bounds of mentioned phases. And the values of functions  $q_6(r)$  are completely determined by a magnitude of occurring defects.

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#### BROWNIAN MOTION IN THE DUSTY PLASMA OF GAS DISCHARGES

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The Brownian motion is widespread in nature. The random wandering of separate grain between atoms/molecules or other particles of the surrounding medium is described by the equations of macroscopic diffusion. Nevertheless, the existing level of experimental physics is going beyond the scope of a diffusion approach and of an Einstein relation. In particular, a description within the limits of the macroscopic kinetics may be insufficient for the analysis of mass-transfer processes on physically short time-intervals, which is especially important for the investigation of fast processes and for the analysis of transport properties of strongly dissipative media.

Here we present the experimental study of Brownian motion of grains in the dusty plasma, which represents an ionized gas containing micronsized charged particles (dust or grains) of a substance. The laboratory dusty plasma is the unique object for studying the transport properties of the systems of interacting grains on the "kinetic level". The separate grains in dust structures, highlighted by a laser beam, can be easily observed with a naked eye. To register the motion of grains, a standard video camera may be used. Therefore, experiments with dusty plasma allow a simple direct determination of spatial positions of particles, which were obtained during the video recording of dust cloud, and a study of their dynamics (i.e. a study of various regimes of grain motion).

In this work, the results of experimental study of Brownian motion of charged dust grains in weakly ionized plasma are presented. The experiments were carried out in the plasma of RF discharge for the small clusters and extended dusty plasma systems, containing the interacting dust grains of various sizes. The influence of the number of grains and the magnitude of the friction coefficient on the formation of various regimes of their motion was studied. We present the new analytical model, which describes the transition from the ballistic to the diffusive regimes for the Brownian grains under different conditions.

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Education and Science of Russian Federation and by the Program of the Presidium of RAS.

#### LUNAR DUSTY PLASMA ENVIRONMENT: A RESULT OF INTERACTION OF THE SOLAR WIND FLUX AND UV RADIATION WITH THE REGOLITH

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One of the main challenges of future missions to the Moon is associated with lunar dust. American astronauts walked on the moon, noted that this dust sticks to any surface and reduces lifetime of mechanisms due to abrasive effect. In addition, it contaminates the optics and white coating of devices, causing them to overheat. Lunar dust is extremely dangerous to human health: the sharp particles of lunar dust smaller than 2.5–3 microns are not output from the lungs and are toxic.

The lunar surface is exposed to both the solar wind and solar UV radiation causing photoemission. As a result, there is a substantial surface change and a near-surface plasma sheath. Dust particles from the lunar regolith, which turned in this plasma as a result of any mechanical processes, can levitate above the surface, forming dust clouds.

In 2015–2017 Russia plans to launch the spacecrafts "Luna-Glob" and "Luna-Resource". For experimental investigations of the lunar dusty plasma exosphere, it is planned to equip "Luna-Glob" and "Luna-Resource" stations with instruments both for direct detection of dust particles over the surface and for optical measurements [1].

In preparing of the space experiments "Luna-Glob" and "Luna-Resource" PIC calculations of the near-surface plasma sheath parameters are carried out on the basis of the KARAT code [2]. Here we present some new results of PIC simulation of the plasma sheath formed near the surface of the moon as a result of interaction of the solar wind and UV radiation with the lunar surface. The conditions of charging and stable levitation of dust particles in plasma above the lunar surface are also considered.

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#### DYNAMICS AND INTERACTION OF PARTICLES IN DUSTY PLASMA UNDER AN INFLUENCE OF EXTERNAL PERTURBATIONS

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The results of numerical and experimental investigations of the dynamics of interacting particles in cluster systems under the action of an external perturbing field on them are presented.

We numerically studied the dynamics of interacting particles in cluster systems under the action of an external perturbing field. Our calculations were performed in a wide range of parameters close to the conditions of experiments in a dusty plasma. We analyzed the relaxation rates and characteristic relaxation times of clusters both to a new (perturbed) state and to the initial equilibrium position (after the perturbation has been removed). We found that the characteristic relaxation time of a cloud including up to 100 interacting particles to its equilibrium state is determined by the trap frequency and the coefficient of friction of the particles and can be described in the approximation of a harmonic oscillator.

A new method for recovery a pair interaction potential between dust particles in plasma, based on an analysis of their movement after an external perturbation, is also presented. The technique consists in destruction of a dust structure by a short-term external perturbation (e.g., by a laser) and followed by an analysis of the system relaxation (recristallization) using the method of inverse problem [1]. Such an approach allows one to minimize the influence of random forces on the results of recovery the spatial distribution of the interparticle interaction potential, as well as to reduce the lower limit of the spatial range of the method [1].

An experimental study of dust grain's dynamics in plasma was carried out for cluster systems relaxing to their equilibrium state after an action of the laser beam. Influence of this external perturbation the potential between interacting dust grains was analyzed. For the first time different spatial asymptotes of pair potentials for the perturbed (disordered) and for the equilibrium (ordered) dust systems has been found out.

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 Vaulina O.S., Lisin E.A., Gavrikov A.V., Petrov O.F., Fortov V.E., JETP 110, 662 (2010)

## ENERGY TRANSFER IN DUSTY STRUCTURES IN GAS DISCHARGE PLASMA

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Dust particles in gas-discharge plasma gain high negative charge and may achieve high kinetic energy, which exceeds both own temperature of dust particle material and temperatures of ions and electrons under certain conditions. Dust particles oscillate along the vertical and horizontal axes differently under certain conditions. The mechanism of energy transfer from discharge to dust particles motion is divided into several parts. Warming up of dust particles vertical oscillations is considered separately from the heating of horizontal oscillation, as these processes are determined by several different phenomena due to near-electrode layer anisotropy. The mechanism of energy transfer from vertical to horizontal oscillations of dust particles is based on parametric resonance and other physical phenomena. The outflow of energy from the dust particles oscillations due to friction on the neutral gas is also taken into account. These steps of scheme of energy transfer have different characteristic and relaxation times.

Mechanism of energy transfer is studied and verified by simulation and experiment. The experiment published in [M.Y. Pustylnik, A.V. Ivlev, H.M. Thomas, G.E. Morfill, L.M. Vasilyak, S.P. Vetchinin, D.N. Polyakov, and V.E. Fortov, Physics of Plasmas 16, 113705 (2009)] is chosen for main comparison. Features of mechanism of energy transfer between vertical and horizontal oscillations allow us to divide the concept of temperature for two subsystems of vertical and horizontal oscillations. Reasons for using the concept of temperature for description of dust particles dynamics are discussed. The proximity of velocity distribution to Maxwell distribution is one of the main factors, which allows us to use the concept of temperature for such systems. Consideration of dust particles horizontal and vertical velocity distribution and mechanism of energy transfer between these subsystems reveals the possibility of two different kinetic temperatures of dust particles.

## THE SELF-CONSISTENT MECHANISM OF RADIAL SUSTENANCE OF DENSE DUSTY PLASMAS

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The numerical study of positive column of glow discharge was carried out with the aim to understand the mechanisms of plasma-particle interaction, resulting in self-sustenance of dust structures in dense dusty plasmas. The simulation was based on the drift-diffusion model developed for air [1] and neon. The formation, drift, diffusion and losses on the tube walls and the dust particle surface of electrons and ions were considered. In neon, the possibility of step ionization was considered through the low lying metastable state. The electron temperature, transport coefficients and rate coefficients for electron impact reactions were calculated using the electron Boltzmann equation solver BOLSIG+ combined with the SIGLO Database. For description of dust particle charging the OML approximation was applied. The numerical task was solved at discharge parameters where the most stable dust structures were observed experimentally. In free discharge undisturbed distribution of electrons (ion and metastable atoms) in the discharge cross section was close to theoretically predicted Bessel distribution. Dust structures arising in gas discharge plasmas cause additional electron losses on the dust particle surface, changing plasma ionization balance. This is followed by the increase of ionization frequency and electron temperature and result in increase of electric field strength. The absorption of electrons in the center of discharge tube filled with dust particles, leads to the case when the electron concentration on the outer face of the 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 that is becomes negative in some region inside dust cloud. The inversion of a radial electric field appears. Such self-organizing of dust structures results in appearing of additional electric force directed inside the dust structure. This force keeps dust particles in balance in a radial direction. The size of this force increases with the growth of concentration of dust particles. The absolute value of the critical dust particle concentration in neon is higher than in air at the identical set of parameters and is of about  $10^5$  cm<sup>-3</sup>.

 Polyakov D. N., Vasilyak L. M., Shumova V. V., Fortov V. E. // Phys. Lett. A. 2011. V. 375(37). P. 3300–05.

#### ON THE REDUCED ELECTRIC FIELD IN THE REGION OF PHASE TRANSITIONS IN CRYOGENICS DUST PLASMA OF GLOW DISCHARGE

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One of the principal features of cryogenic plasma is a significant influence of metastable atoms and molecules accumulated in the discharge, on the characteristics of the plasma and the associated processes of ionization. Metastable atoms are intense source of free electrons. These extra electrons interacting with the dust particles, change the direction of the processes of self-organization of dust structures, which is accompanied by structural transitions in dusty formations. The structural transitions characterized, for example, by a change in density of the dust particles, lead to self-consistent changes in the properties of the background plasma. The dependence of the reduced electric field E/N in the positive column of a discharge in neon at T = 295 K and 89 K on the pressure in the range of 0.1–1.4 Torr and discharge current 0.1–3.5 mA was experimentally obtained. It was found that at presence of dust particles the longitudinal electric field strength increases while maintaining the total discharge current at all temperatures of gas. The decrease of the reduced electric field with decreasing temperature of the gas was revealed. It was found that at the transition from the room temperature of the heavy plasma component to the temperature of liquid nitrogen, the transition area to the normal glow discharge shifts to smaller discharge currents for the same values of the reduced pressure, and approximately coincides with the boundary of the melting of structured clusters. When reducing the temperature of the gas, a change in direction and structural phase transitions in dusty plasmas was observed. At room temperature, the boundary of the structural transition is mainly determined by the discharge current, while at cryogenic temperatures, this boundary is determined by the density of the gas. There is also a different type of structural transition. At room temperature, with an increase of the discharge current the structural transition associated with the restructuring of the form the lattice was observed, and at cryogenic temperature, the decrease in pressure leaded to clustering. The phase diagram of a dusty plasma in neon at a temperature of 89 K with the isolines of the reduced values of the longitudinal electric field is obtained. It was found that the regions of existence of structured clusters and structural transition were characterized by higher value of the reduced longitudinal electric field strength than the regions of their melting and the regions with a homogeneous structure ( $E/N \leq 1.2 \cdot 10^{-16} \text{ Vcm}^2$ ).

## SELF-OSCILLATION, CRYSTALLIZATION AND DIFFUSION PROCESSES IN CRYOGENIC DUSTY PLASMAS

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It was found that cryogenic dust structure can consist of the twocomponents of one-sort dust where one component represents chain-like crystal, which is typical for dust structures in striations of the dc glow discharge at room temperature, and the second one is ensemble of the dust particles orbiting chain-like crystal particles. These two subsystems form a mixture (i.e. they are not separated) and are characterized by different two dust particle kinetic temperatures. This work is devoted to detailed consideration of this phenomenon in laboratory experiment at 77 and about 10 K. Possible mechanisms of the formation of two-component dust system are analyzed; in particular, it was shown that the nature of such behavior can be as a result of deformation of ion function distribution in the cryogenic discharge, similar to discharge in gas mixtures with big difference of atom weights. In addition, dust structure self-oscillations with frequency of about several Hz at discharge temperature decrease were observed at temperature increase from about 5 K with rate of 1 K per minute. The view of the oscillations was similar to tidal waves. These regular motions were damped after several minutes down to stable two-component structure as mentioned above.

#### AN EFFECT OF DUSTY CLOUD ON THE DISCHARGE PLASMA GLOW

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The effect of dusty cloud on the discharge plasma radiation in neon lines has been investigated in the "PK-4" experiments during ESA 57 parabolic flight campaign. The dusty cloud was formed by 6.9 mcm plastic grains in the 1 mA DC alternating polarity (250 Hz) discharge in neon at the pressure of 0.4 mbar. The plasma radiations in lines of 585 nm and 703 nm as well as a dust scattered illuminating laser radiation were recorded by overview camera. Specters in range of 564–737 nm were also recorded and analyzed. The plasma glow in neon lines was dramatically increased in the dusty cloud position. This effect is connected with an ionization rate increasing in the discharge with dusty component.

### POSSIBILITIES OF USING ELECTRODES OF A VARIOUS FORM FOR STABILIZATION DUST PLASMA STRUCTURES

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For stabilization dust particles it is necessary to organize a potential trap, rather deep that motes could be taken and collect in it. It is reached by introduction of the face electrode located perpendicular to a bunch of ions which experiences bombing by ions. The negative potential given on an electrode, on the one hand, pushes away negatively loaded dust particles (in close proximity), and on the other hand attracts the secondary positively loaded ions of plasma. These ions in collisions with motes transfer them an impulse as a result of which in the distance from an electrode there is power of ionic hobby which forces dust particles to be grouped near an electrode. So there is a stable trap of dust particles.

The bulk of experimental data was received when using flat electrodes. Such geometry allows the simplest treatment and processing of experimental data. To research the influence of the shape of the electrode surface on the conditions of formation of dusty plasma structures of a series of experiments with spherical electrodes (convex and concave), and also an electrode in the form of the cylinder of final length was carried out.

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### NON-SELF-MAINTAINED DISCHARGE IN INERT GAS FOR INVESTIGATING OF NUCLEAR-INDUCED DUSTY PLASMA

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In this work non-self-maintained discharge in inert gas with dust particles was qualitatively analyzed for the regimes when stationary and nonstationary ordered dust structures are forming. The discharge is maintained by a proton beam and is used to study dust structures in nuclearinduced plasma [1]. Estimates of the main plasma parameters as well as parameters of near-electrode discharge layers were obtained: electron temperature, concentrations of atomic ions, molecular ions and electrons, electric field, near-electrode potential jump, width of the Langmuir layers [2]. It is shown that sufficiently large negative voltage on the collector forms a trap for negatively charged dust particles in the near-collector area of the discharge. Also estimates of the forces, acting on dust particles in the discharge, are made.

Possibilities of creation of extended dust structures in non-selfmaintained discharge are considered. That might significantly enhance the ability to study their properties.

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#### COULOMB SYSTEM OF CHARGED DUST PARTICLES CONFINEMENT BY LINEAR PAUL TRAP

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Due to the Earnshaw theorem [1] trapping of a charged particle cannot be achieved with a static potential, because any static potential, which fulfills Laplaces law, lacks potential minima. To confine an charged particle it is necessary to create local in space a force of type  $F = -k \cdot \overrightarrow{r}$ . Since the electric field should be proportional  $U(r) \sim \alpha x^2 + \beta y^2 + \gamma z^2$ . The Laplaces law must obey that condition imposed on potentials where there is no free charge distribution, namely that  $\alpha + \beta + \gamma = 0$ . That type of field creates an potential saddle and by rotating of that potential with proper friquency particles inside can be captured near center of the trap. Also in 1989, further improvement of the ion trap technology appeared with the demonstration of the linear Paul trap [2]. The purpose of this work is to study the possibility and conditions of the dust structure confinement in linear Paul traps at an atmospheric pressure in a corona discharge plasma or in a nuclear-excited plasma. The behavior of dust particles is simulated by Brownian dynamics. Our simulation have been carried out for normal atmosphere conditions (pressure and temperatures) for reasonable choice of the dust particle parameters and the trap electrode voltages. Dust particle parameters and parameters of the traps needed for dust particle confinement have been found. The results of our simulations allow finding the regions of the dust particle confinement, the influence on these regions the particle masses and charges, applied to the trap electrodes voltages and its frequency. The results of our simulations also agree with results of dust particle confinement obtained in our experiments for linear Paul trap.

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#### THE COULOMB CRYSTAL OF CHARGED DUST PARTICLES IN A DYNAMIC TRAP IN AIR AT ATMOSPHERIC PRESSURE

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In this work the possibility of dust particles confinement by alternating electric field in quadrupole trap at atmospheric conditions is investigated. We used numerical simulations to investigate the possibility of the dust structures forming in dynamic electrical traps such as the Paul trap and the quadrupole trap. Numerical simulations of dust particle behaviour is considered. The influence of forces acting on dust particles was taken into account such as gas medium viscosity, electrical forces and random forces. In considered model the dust particle motion is described by the Langevin equation. Results of our simulations for Paul trap showed the appearance of standing waves of the dust particle density arising due to the dynamic effects of periodic electrical field of low frequency. We have determined electric field amplitudes and frequencies needed for levitation of dust particles in a quadrupole trap. The dependence of the equilibrium position of dust structures in a quadrupole trap versus the frequency of the alternating electric field was investigated. Our experimental results agree well with conclusions of mathematical simulations for quadrupole traps.

## MACROPARTICLES CHARGING MECHANISMS IN AIR AT ATMOSPHERIC PRESSURE

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The electrostatic filters are used for gas cleaning from dust. They are widely used because of the good performance, simplicity and reliability in operation. However, in some cases, the electrostatic filters can not provide a necessary degree of dust cleaning (e.g. atomic and electronic industry). To confine levitating charged macroparticles the electrodynamic Pauli traps and their modifications in which particulates are confined with alternating electric fields are used. Dynamics of these particles in such traps is described by the Mathieu equations. The analysis of these equations showed that electrodynamic traps are capable to confine levitating charged dust particles in a wide range of charge to mass ratio by changing frequency and amplitude of AC voltage at the trap electrodes. Theoretically, one can achieve better efficiency gas cleaning by using a filter, operating on the principle of the electrodynamic trap, in comparison with an electrostatic filter. To create an experimental installation for studying the electrodynamics particle confinement, a device to charge macroparticles in air at atmospheric pressure is needed. Computer modeling of the electrodynamic trap showed that a sufficient charge to capture particles could be obtained by using a corona discharge as a charging device. In this paper the macroparticles charge mechanisms in the corona discharge are analyzed, the calculated ratios are considered. It is shown that the dominant mechanism for charging large (> 1 micron) and small (< 0.1 micron) macro particles can be quite different ones.

#### EXPERIMENTAL INVESTIGATION OF TRACK DUSTY PLASMA INSTABILITIES

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The properties of dusty plasma obtained due to ionization of gas-dust mixtures in tracks of fission fragments and products of radio nucleotids decomposition have been studied up to the present time quite slightly in comparison with the gas discharge dusty plasma of different types. There are only individual experimental works where it has been demonstrated that under the action of the <sup>252</sup>Cf fission fragments and accelerated protons dusty microparticles formed the ordered dusty structures of different type in dependence of pressure of plasma forming gas, ionization degree and other conditions. The dusty structure in these experiments occupied a small volume of the experimental chamber, as a rule, not exceeding  $1 \text{ cm}^3$ . The excessive dust particles that did not find a place in the dusty structure precipitated on the chamber walls. The attempts to increase a size of the dusty structures encountered to a number of difficulties connected with the non-stable behavior of these structures. It has been revealed that for stationary ionization conditions (gas pressure and beam current are constant) the following instabilities appear in the dusty structures: oscillation of dusty structure boundaries, density waves, separating of the dusty cloud into two and more components, ejection of the dusty cluster

out of the cloud. We present results of the study of these instabilities. The experiments have been performed with the proton beam (electrostatic accelerator EG-2.5) and the beam of heavy ions (electrostatic overcharging accelerator EGP-15). The electrodes of different configuration were used. The proton energy reaced 1.5 MeV with a current from 1 up to 3  $\mu$ A. The energy of triple-charged carbon ions was about 10 MeV with a current of 1  $\mu$ A. It has been demonstrated that changing the electric field configuration it was possible to stabilize the dusty structures and suppress instabilities. The dusty structures formed in the beam of carbon ions were more stable.

## THE THEORETICAL MODEL FOR THE GENERATION OF LASER RADIATION IN NEUTRON IRRADIATED GAS ENVIRONMENTS CONTAINING URANIUM NANOPARTICLES

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The model of the kinetic processes during the generation of laser radiation in an argon-xenon active gas medium containing nanoparticles of uranium irradiated by neutrons was developed. Such active medium is excited by fission fragments due to uranium nuclei fission initiated by neutrons.

The model includes the evolution equations for the electron energy distribution function, concentration of the different components of the gas plasma and dust particles with different charges, as well as the generation of laser radiation.

The process of generation of laser radiation at a wavelength of 1.73 microns was studied when used as the active argon-xenon media containing uranium nanoparticles irradiated by neutrons during the time of the order of 100 microseconds.

For the first time using mathematical modeling was shown that the total conversion efficiency of nuclear energy in the energy of laser radiation in the neutron bombardment of uranium nanoparticles dusty gas argon-xenon environment is more than ten times higher than efficiency of heterogeneous nuclear pumping energy conversion.

#### EVOLUTION OF THE HIGH-CURRENT PULSED DISCHARGE IN A QUARTZ SAND OF DIFFERENT HUMIDITY

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The spreading of the pulse current in low conducting ground leads to the appearance of electric field is sufficient to ionize and the spark channel and is a fairly complex physical phenomenon. For example, spark discharges, sliding on the soil surface, can propagate for a distances of several hundred meters. The mechanism of formation of the spark channel differs significantly from the formation of the classical leader in the air. In this work the process of spreading of pulse kilo ampere currents with duration of the order of ten milliseconds in the wet quartz sand, characteristic for the lightning of positive polarity. Unlike; as distinct from the sliding discharge along the surface, experimentally was studied ohmic spreading of the current and formation of the breakdown from a spherical earth rod in the volume of quartz sand of varying humidity. It has been recorded that in a non-uniform electric field in the intervals of length of the order of ten centimeters discharge accompanied by a bright flash and can form in a rather weak electric fields, characteristic for the giant leader in the air. A noticeable decrease of the electric field breakdown associated with the polarization of sand particles, as well as the conductivity current provided by the presence of water essential changes the dynamics of the formation of pulsed discharge. It is experimentally shown that there is a critical current density above which ohmic spreading of the current with the grounded electrode is accompanied by the breakdown and formation of a plasma channel such leader channel. In this case redistribution and constriction of the current in the conductive channel are happened. Spark discharge is formed by different mechanisms in the short and long intervals. In the long interval, there is a very large time delay breakdown (until one millisecond), which leads to the reduction of the average velocity of discharge to 2 orders of magnitude in comparison with the speed of a classic leader in the atmosphere. The formation of a breakdown in the wet sand similar to the breakdown of liquid non-polar dielectrics, in which in the final stage of the breakdown is formed by the gas ionized channel, originated by intense local heating current of conductivity. Performed studies confirm the possibility of the formation in the volume of wet soil of ionized non-streamer leader channel, capable to pass kilo-ampere currents.

#### INVESTIGATION OF OSCILLATIONS IN HIGH CURRENT DISCHARGES AT SUPERHIGH PRESSURE

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Two types of channel oscillations in investigations of super-high pressure discharges at initial pressure of 80–160 MPa and current amplitude up to 500 kA are registered. It was established that this oscillations were responsible for voltage on discharge gap and pulsed pressure on discharge chamber wall by correlation analysis. In the work a dependency each type of oscillations via the pressure in the discharge chamber are considered. A comparison with results of study of MHD instabilities in dense gas environment uses for confirmation the hypothesis that one of the branches of the oscillations was connected with the alignment of the magnetic and gas pressures. It was justified a assumption that at super-high gas pressures the most part of the current flows in vapour of initiating wire. The second branch of the oscillations is analyzed on the basis of calculation of the acoustic oscillations that occur in the whole volume of the discharge chamber. Two methods of channel parameters measuring were designed by this oscillations analysis.

The work is partially supported by Russian Foundation for Basic Research (grant 12-08-01062-a).

#### A LOAD CURRENT MULTIPLIER FOR RESEARCH OF INTERACTION OF FAST RISING MEGAGAUSS MAGNETIC FIELDS WITH METALS

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Powerful pulsed current generators of a megaampere range are widely used in studies of explosion of conductors in strong magnetic fields. One of the most important parameters of a generator used in such researches is a load current amplitude. Implementation of a load current multiplier (LCM) allows increasing of the current amplitude in the regime of a constant low-inductance load.

The MIG generator is a terawatt-level pulsed power generator that provides a load current amplitude up to 2.5 MA with a current rise time of 100 ns. For several years, the MIG generator is used to study interaction of fast megagauss magnetic fields with metals. A distinguishing feature of conducting experiments is that the inductance of a load, which is metal cylinders with a diameter from 1 to 4 mm, is almost constant during the current pulse rise. When the LCM is used, this would make it possible to avoid a drop in the transformation ratio during the power feed stage, which is caused by an increase in the load impedance.

A design of the load current multiplier has been developed, and its operation with a current transformation ratio of 1.75 has been demonstrated on the low-impedance MIG generator at the terawatt power level. The practicability of using the load current multiplier operating with a constant low-inductance load, for example in the studies of skin electrical explosion of wires and non-linear diffusion of megagauss magnetic fields, has been shown. The use of the LCM provides an 1.5-fold increase in the load current (the load diameter in this case is equal 10 mm) in comparison with the regular operation regime of the MIG generator. The reduction of load diameter leads to the falling of the current transformation factor and at the load diameter of 3 mm one comes nearer to unit. That fact does using of the LCM with such geometry (with the chosen relation of the circuit inductions) inexpedient.

## THE GENERATOR OF HIGH-POWER NANOSECOND PULSES ON THE BASIS OF INDUCTIVE ENERGY STORAGE AND TWO STEPS DYNAMIC OPENING SWITCH

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The generation of multiterrawatt power pulses of nanosecond duration is associated, first of all, with the problems of primary accumulation of energy and its transfer to the load. At present, in spite of their low density and high cost, the capacitor storages are the most widely used. This is due to the properties of the closing device which permits providing a high ratio of the times of energy accumulation  $t_a$  and extraction  $t_t$ , which achieves the value of  $t_a/t_t = 10^6-10^7$  and more. Though the inductive storages are perspective because of their simplicity in design, energy density and cost, the problems with their application are connected with the current breaking gap. Some modern breakers, at their best, at high powers ensure the ratio of  $t_a/t_t$  not in excess of 10–20 [1].

In a number of works, with the goal of using the inductive storage to generate nanosecond pulses, some solutions have been proposed including the combination of the vacuum interrupter and plasma opening switch [2, 3] and generator-amplifier [4]. These works did not shed more light on the efficiency of the energy extraction from the transformer inductive storage that depends on a special screen designed to reduce the impact of the electromagnetic field to the primary winding. The paper also offers a variant of the screen design which makes it possible to transfer the energy to the load in the period of a double path of the electromagnetic wave between the primary winding and screen. Such a screen, even at small diameters of the inductive storage, allows us to transfer the energy to the load, with low loss, by way of the plasma current interrupter, with the energy accumulated for several seconds. The phenomena and processes occurring in the screen during the energy extraction can be explained in terms of the electric circuit of the generator-amplifier which is simpler in design than that proposed in [4]. The combination of the generatoramplifier and the screen proposed enables the ratio  $t_a/t_t = 10^7$  to be obtained and used to generate terawatt powers [5].

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#### ABOUT CREATING INSTALLATIONS OF THE INGIR TO INPUT ENERGY IN PLASMA

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We have a project to create a series of installations of the INGIR to input energy into plasma using a pulsed inductive discharge at rapid recession of strong magnetic field. The installation includes electrical connection via the breaker an inductive energy accumulator with installed inside of it the discharge chamber. Transmission of energy in the plasma takes place in two phases. In the first phase, after the connecting of primary electrical circuit, energy initially is accumulated in the inductive accumulator in form of magnetic field, and in the second phase, after the disconnecting of primary electrical circuit, the energy of magnetic field is pumped in the plasma. The term INGIR is formed by the first letters of combination of Russian words: Induktcionnyi Nakopitel dlya Generirovanuya Inducthionnogo Razryada (Inductive Accumulator for Generating of Inductive Discharge). Now we are carrying out the first phase of work, we are creating an installation the INGIR-Mega-15 with a design capacity of the pump pulse at 15 MW. The current amplitude of the pump pulse in accordance with the technical requirements of 35 kA, in the inductive accumulator magnetic field may have the induction of 13 T with duration of the leading and trailing edges of the pulse 500 and 50 microseconds, respectively. The purpose of the first phase of research is the experimentally obtaining long-lived plasmoids 1. In test mode (20 percent of the capacity of the pump pulse) confirmed the results presented in 2. In the future, depending on the results, we plan to enlarge the installation, bringing the power of the pump pulse to the level of several gigawatts, which presumably will allow get the controlled fusion 3. In addition these systems can be used to study plasma-chemical reactions and to other applications.

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# ECR PLASMA IN A PULSED MODE Polushkin E.A.,\* Kovalchuk A.V., Shapoval S.Yu. IMT RAS. Chernogolovka, Russia

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To improve the efficiency of the electron cyclotron resonance (ECR) plasma processes taking was studied the pulse mode plasma in nitrogen. Pulse mode was reached by modulating the applied microwave power. Was determined dependence of the intensity the plasma emission and the value of the ion current from the fill factor of the microwave pulses at different operating pressures and at fixed integral power. Have been measured edges profiles of light and ion current, was studied emission spectra of the plasma.

#### ETCHING OF HIGH ASPECT STRUCTURES IN ECR PLASMA

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ICP and bosh-process are well known and have some advantage: high aspect ratio, high etch rate. But such methods are not applicable to form detached vertical structures (columns, walls, etc.). In present work the structures were etched by ECR plasma. During the experiment RF-bias allows to control the ion energy. Etching parameters were varied by change the power of the microwave, the chamber pressure, substrate temperature and self-bias voltage and gas flow rate. Were obtained detached vertical structures with height (depth) columns (walls) up to 150  $\mu$ m.

## SHADOWGRAPH PHOTOMETRIC METHOD APPLICATION FOR ELECTRON DENSITY DIAGNOSTICS IN COLLIDING COUNTER-FLOWS OF COMPRESSED PLASMA

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The aim of this work is research of qausi-stationary high energy plasma formations for practical applications in high thermal physics and diagnostic of materials under extreme conditions. Visual examination, high speed photography and shadow investigation are to be discussed in the paper. Shadow measurements were performed on an IAB-451 shadow device using knife and slit method [1]. Investigated colliding plasma flows were generated by high-current discharges of counter directed erosion plasma accelerators in vacuum. A source of light based on a pulsed spark discharge in argon at high pressure with light pulse duration is 3  $\mu$ s was used. Averaged free electron density in the interaction area was calculated from intensity distribution of shadow photographs.

Shadow photographs data processing revealed that the localized stable spherical plasma structure forms in a collision zone by  $15\mu$ s from accelerators operation start. An electron density inside this structure reaches a maximum value  $8.4 \cdot 10^{16}$  cm<sup>-3</sup> between 15 and 20  $\mu$ s from accelerators operation start, at this moment a discharge current tops. After 20  $\mu$ s electron

density decreases and plasma structure downsizing occurs. The results of electron density measurements are in good agreement with data obtained by spectral method [2]. Electron concentration measurements of the order of m<sup>-3</sup> have a measurement error ~ 0.02%. When colliding accelerated plasma flows diagnostics is made, main measurement error appears due to determination of geometrical dimensions of investigated plasma and inhomogeneity of initial distribution of light intensity in focal plane of shadow device. Thus, total inaccuracy of electron concentration measurements for the used method is  $\approx 18-20\%$ .

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#### FLASH LAMP FOR TOEPLER PHOTOMETRIC MEASUREMENTS BASED ON A PULSED SPARK DISCHARGE IN ARGON

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Shadow method diagnostics of bright plasmas is complicated by need of use more bright blinker than investigated plasma. That is why for obtaining shadow photographs of colliding compressed plasma, suitable not only for qualitative analysis but also for quantitative interpretation of experimental data, a flash lamp, based on pulsed spark discharge in argon at high pressure was developed.

This light source is based on a pulsed spark discharge in argon at pressure 2 atm in a discharge chamber. The lamp operating voltage was 20 kV and light pulse duration is 3  $\mu$ s (at the level of 0.7 maximum light intensity). Usage of this light source in a shadow device allowed registering time-resolved shadow photographs of plasma flows collision. Registration of discharge glow spectrum was made by spectrometer S150A-IV.

Method of the electron temperature in argon plasma determination under the assumption of local thermodynamic equilibrium is based on the fact that the densities of various excited states are proportional to the products of statistical weights to the Boltzmann factors of these states. According to this temperature is inversely proportional to the logarithm of the ratio of the total intensities of lines appear at transitions from different upper levels, on conditions that none of these lines are not subject to selfabsorption [1]. For the analysis two emission lines of doubly ionized argon atom (500.94 nm and 437.49 nm.) were used. The calculated temperature is 4 eV. The calculation of the electron density in plasma was carried out in accordance with the theory of spectral line broadening due to the quadratic Stark effect [2]. The half-width of argon line  $\lambda = 486.0$  nm is  $\Delta \lambda_{S,4} = 1.04$ nm. So, the electron density was amounted  $4.9 \cdot 10^{18}$  cm<sup>-3</sup>.

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#### INTERACTION OF COLLIDING COUNTER-FLOWS OF COMPRESSED PLASMA WITH EXTERNAL PULSE MAGNETIC FIELD

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With the purpose of magnetic plasma confinement and restriction of the compression plasma flows collision area magnetic trap of probkotron type was created. Investigated trap was a system of two uniaxial solenoids of copper wire of  $\emptyset$ 3.7 mm. The diameter of each turn of these tree-turn solenoids was  $\emptyset$ 47.5 mm, and the distance between the solenoids centers was 50 mm.

The magnetic trap operation started as the result of capacitor bank with total capacity of 600 microfarads discharge. The capacitor bank was made up of capacitors type IR 6–150 TC4 set. Charging of the capacitor bank to a voltage of 4 kV was made by a high-voltage supply.

The magnetic trap and the accelerators current was measured using a noninductive shunt. The measured magnetic trap current was 20 kA at voltage value of 4 kV. The voltage drop on the shunt was recorded by oscilloscope Tektronix DPO 7104 C.

The most intensive interaction of compressed plasma with the field of the magnetic trap was observed in the fast current rise which appeared in the period of time from 7 to 12  $\mu$ s from the plasma accelerators start. Synchronization of accelerators and magnetic trap start was carried out using a six-channel pulse generator.

The magnetic field of the magnetic trap was calculated by use of Matlab. In the center of the trap there was an area of zero magnetic field, surrounded by a barrier magnetic field of 0.1 T. The "barrier" parameter  $\beta$  for the investigated case equals to  $\beta \approx 0.25$  [1].

Visualization of the plasma flows collision was made by high-speed digital camera DIACAM-Pro and was carried out at absence and presence of external magnetic field. The results of such visualization showed that the magnetic trap field limits the plasma flows collision area by compressing the spherical plasma formations appearing under plasma flows collision while increasing the intensity of theirs glow. Visualization results were obtained for a period of time corresponding to the maximum intensity of the trap magnetic field.

#### INVESTIGATION OF HYDRODYNAMICS AND HEAT TRANSFER IN THE CURRENT-CARRYING FLUIDS IN ELECTROMAGNETIC FIELDS

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The work is in the area of magnetohydrodynamics and devoted to studying the effects of electromagnetic fields on the processes of hydrodynamics and heat exchange in the current-carrying fluids [1], [2], [3]. The significance of this research is in the solution of fundamental problems and applications related to improving the performance of technical systems for energy efficiency in energy and industry, as well as to the improvement of environmental conditions. The project aims to address the fundamental problems of a complex electro-vortex (EVT) currents in conducting media by electromagnetic fields. Focus is made on the study of the influence of own and external magnetic fields on the flow pattern in the amount of molten metal by passing an electric current. The emphasis is on the study of the structure and characteristics of the turbulent environment, sustainability of vortices, the process of discharge above the current-carrying fluid [4].

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## DEVELOPMENT OF PHYSICS AND ENGINEERING PRINCIPLES AND CONCEPT PLASMA SEPARATION SETUP OF SPENT NUCLEAR FUEL FOR TASK SOLUTION OF CLOSED NUCLEAR FUEL CYCLE

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This work examines the plasma separation of spent nuclear fuel, which effectiveness is due to the creation in the magnetized plasma of an electric field with the potential hole [1, 2] capturing heavy ions and doesn't almost capture the light ones. The feature of this approach is to use the accelerating potential to overcome power and angular spreads of the plasma substances ions entering the chamber of separator and potential hole for the spatial separation of ions of different masses. To explain there have been done the calculations of substances ion trajectories which modelling spent nuclear fuel. The calculations were made for azimuthal and axial magnetic and electric fields taking into account the geometry of the chamber of separator. It is shown that in magnetic fields with specific value of strength which is about 1 kG and electric potentials up to 1 kV in volume with linear size which doesn't exceed 100 cm the separation of substance of spent nuclear fuel ions with energies ranging from 0.2 to 2 eV is possible. The calculations are made for the collisionless regime in particle approximation. This work also presents the results of separate blocks of the experimental setup development including the separation chamber, fields generation system and the block of collectors.

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#### THE STATIONARY VACUUM ARC AS PLASMA SOURCE FOR TECHNOLOGY OF ION SEPARATION

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The stationary vacuum arc on hot cathode of spent nuclear fuel (SNF) has great prospects for the plasma technology of ion separation. This disharge generates the high-speed plasma flow of cathode material. To debug the elements of new technology of processing of SNF the model conditions can be used.

This work presents the results of experimental study of such an arc on gadolinium cathode. Choice of gadolinium as model substance is determined by the similarity of the disharge characteristics on gadolinium and uranium cathodes.

Gadolinium was placed in a heat-insulated molybdenum crucible. The crucible had electron beam heater (EBH) that was allowed to change the cathode temperature at fixed arc current. Power of the EBH with maximum voltage of 2 kV reached about 1 kW. Diagnostics system included the crucible temperature, volt-ampere characterictic of discharge, the heat flux from plasma to cathode and its rate of evaporation. In addition the plasma spectra were studied.

With arc current of up to 100 A the temperature of the cathode crucible was about 2 kK. Discharge voltage at fixed arc current (40 A), depending on power of EBH, changed from 3 to 50 V. Under high power of EBH the heat losses due to electron emission from the cathode exceeds the heat flow from plasma to the cathode, and discharge cools the cathode. In this mode the arc voltage was less than 10 V. The average evaporation rate of gadolinium was about 2 mg/s. Spectral analysis showed that the portion of multiple charged ions increases with the growth of arc voltage. Therefore, by changing the temperature of the cathode one can optimize the charge of ions in plasma and the evaporation rate of cathode.

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- ANL, IPNS Argonne National Laboratory, Intense Pulsed Neutron Source Division, Argonne, United States
- ANO SIC MST Autonomous Non-commercial Organization "Scientific Innovational Center for Missile and Space Technologies", Moscow, Russia
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- FGUP NIMI Federal State Unitary Enterprise "Research Institute of Mechanical Engineering", Leningradskoe shosse 58, Moscow 125212, Russia
- FIPCE RAS Frumkin Institute of Physical Chemistry and Electrochemistry of the Russian Academy of Sciences, Moscow, Russia
- FORC RAS Fiber Optics Research Center of the Russian Academy of Sciences, Moscow, Russia
- FSUE SRMI Federal State Unitary Enterprise "Scientific and Research Machinebulding Institute", Leningradskoe Shosse 58, Moscow 125212, Russia
- GIST Gwangju Institute of Science and Technology, Gwangju, Korea (South) (Republic)
- GPI RAS A. M. Prokhorov General Physics Institute of the Russian Academy of Sciences, Moscow, Russia
- GPL CIW Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC, United States

- GRIEM RAMS Gamaleya Research Institute of Epidemiology and Microbiology of the Russian Academy of Medical Sciences, Moscow, Russia
- GSI GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany
- GUN Goethe Universitat, Frankfurt, Germany
- *HMTI NASB* Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, Minsk, Belarus
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- ICCT Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia
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- ICMM UB RAS Institute of Continuous Media Mechanics of the Ural Branch of the Russian Academy of Sciences, Academician Korolev Street 1, Perm 614013, Russia
- ICP RAS N. N. Semenov Institute of Chemical Physics of the Russian Academy of Sciences, Moscow, Russia
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- IEP UB RAS Institute of Electrophysics of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia
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- JKU, ITP Johannes Kepler University, Institute of Theoretical Physics, Linz, Austria
- JSC Forschzungszentrum Jülich, Supercomputing Centre, Jülich, Germany
- JU Jadavpur University, Kolkata, India
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- KNUT Khaje Nasir University of Technology, Tehran, Iran
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- KraSC— Krasnoyarsk Scientific Centre, Kirensky Street 26, Krasnoyarsk 660074, Russia
- KrIRT Krasnoyarsk Institute of Railway Transport Filial of Irkutsk State University of Railway Engineering, Krasnoyarsk, Russia
- $\mathit{KRSCE}$  S. P. Korolev Rocket-Space Corporation "Energy", Korolev, Russia
- KubSTU NPI Novorossiysk Polytechnic Institute of the Kuban State Technical University, Novorossiysk, Russia

LANL — Los Alamos National Laboratory, Los Alamos, United States

LC — Louisiana College, Pineville, United States

- LHC Laboratoire Hubert Curien, Saint-Etienne, France
- LIH SB RAS Lavrentyev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, Lavrentyev Avenue 15, Novosibirsk 630090, Russia
- LLNL Lawrence Livermore National Laboratory, Livermore, United States
- LP3 Laboratory of Lasers, Plasmas and Photonic Processing, Marseille, France
- LPD— Laboratoire des Plasmas Denses, Universite P. & M. Curie, Paris, France
- LPGP Laboratoire de Physique des Gaz et des Plasmas, Universite Paris Sud 11, Orsay, France
- LPI RAS P. N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia
- LTU Lulea University of Technology, Lulea, Sweden
- LULI EP Laboratoire pour l'Utilisation des Lasers Intenses, CNRS-CEA, Ecole Polytechnique, Palaiseau, France
- MA SRT Military Academy of Stratigic Rocket Troops after Peter the Great, Kitaygorodskiy 9, Moscow 109074, Russia
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- NSU Novosibirsk State University, Novosibirsk, Russia
- OGRI RAS Oil and Gas Research Institute of the Russian Academy of Sciences, Gubkin Street 3, Moscow 119991, Russia
- OJSC FGC UES Open Joint Stock Company Federal Grid Company of the Unified Energy System, Moscow, Russia
- OSAF Odessa State Academy of Freeze, Odessa, Ukraine
- PCI PCNU Physical-Chemical Institute PreCarpathian National University, Ivano-Frankovsk, Ukraine
- PGU Persian Gulf University, Bushehr 75169, Iran
- PL KAE Technical University of Lodz, the Faculty of Electrical, Electronic, Computer and Control Engineering, Department of Electrical Apparatus, Stefanowskiego 18/22, Lodz 90924, Poland
- PM & IUSTI Polytech'Marseille & IUSTI, Marseille, France
- PTI NASB Physical-Technical Institute of the National Academy of Sciences of Belarus, Minsk, Belarus

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- RIAMA KBRC RAS Research Institute of Applied Mathematics and Automation of the Kabardino-Balkarian Research Center of the Russian Academy of Sciences, Scortanova 89, Nalchik 360000, Kabardino-Balkarian Republic, Russia
- RIE ShU Research Institute of Electronics of the Shizuoka University, Hamamatsu, Japan
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- RRC KI Russian Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia
- RRC KI, INS Institute of Nuclear Synthesis of the Russian Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia
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- RUDN Russian University "Peoples' Friendship", Mikluho-Maklaya 6, Moscow 115569, Russia
- SamSTU Samara State Technical University, Molodogvardeyskaya 244, Samara 443100, Samara region, Russia
- SFU Siberian Federal University, Kirensky street 26, Krasnoyarsk 660074, Krasnoyarsky kray, Russia
- SIAS Scientific Industrial Association "Sintez", Moscow, Russia
- SIBGUTI Siberian State University of Telecommunications and Infor-
- matics, Kirova 89, Novosibirsk 630102, Novosibirsk region, Russia
- SNL Sandia National Laboratories, Albuquerque, United States
- SOIBC RAS Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry of the Russian Academy of Sciences, Puschino, Russia
- SPbSPU Saint-Petersburg State Polytechnic University, Saint-Petersburg, Russia

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- SRC AVTEC Scientific and Research Center AVTEC Automatics Telemechanics Ecology, Ltd., Kozlova Street 62, Novorossiysk 353920, Krasnodarskiy Kray, Russia
- SRC RF TRINITI State Research Center of the Russian Federation – Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk 142190, Moscow Region, Russia
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- SSC RF IPPE Federal State Unitary Enterprise "State Scientific Centre of the Russian Federation – A. I. Leypunsky Institute for Physics and Power Engineering", Obninsk, Russia
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- STC "Industrial Safety" Scientific and Technical Centre "Industrial Safety", Moscow, Russia
- SUSU South-Ural State University, Lenin Avenue 76, Chelyabinsk 454080, Russia
- SUT Sharif University of Technology, Tehran, Iran
- SWCMRC KU Shock Wave and Condensed Matter Research Center, Kumamoto University, Kumamoto, Japan
- TAMU Texas A&M University, College Station, Texas, United States
- TC Schlumberger Technology Company Schlumberger, Moscow, Russia
- TISNUM Techonological Institute of Superhard and New Carbon Materials, Troitsk, Russia

- TPU Tomsk Polytechnical University, Lenin Avenue 30, Tomsk 634050, Russia
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- TUBAF Technical University Bergakademie Freiberg, Freiberg, Germany
- TUD Technical University Darmstadt, Darmstadt, Germany
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