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The book consists of the abstracts of oral and poster contributions to the XXVII International Conference on Equations of State for Matter (March 1–6, 2012, Elbrus, Kabardino-Balkaria, Russia). The reports are devoted to the present-day investigations in the field of physics of extreme states of matter. The following questions are covered: equations of state and constitutive equations for matter under extreme conditions at high pressures and temperatures; shock waves and detonation physics; experimental methods of diagnostics of ultrafast processes; interaction of intense laser, x-ray and microwave radiation, powerful ion and electron beams with matter; techniques of intense energy fluxes generation; low-temperature plasma physics; issues of physics and power engineering, technology projects.

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═══════════      **EQUATIONS OF STATE**      ═══════════  
**FOR MATTER**

**EXTREME STATES OF NUCLEAR EXPLOSION**

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Physics of extreme states of nuclear explosion is discussed.

**SEMICLASSICAL METHOD IN PROBLEMS  
OF QUANTUM PHYSICS**

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We consider a recent semiclassical approach that has been developed during the last decades to describe the properties of interacting many-electron system. Its applications to a treatment of some quantum physics problems are discussed. The basis of the method is a statistical Thomas-Fermi model. Additive corrections to the model take into account the different physical effects including the electron spectrum shell structure. We pay attention to the matter and finite system behavior.

The analysis of the electron characters in 1D and 2D quantum dots, evaluation of the conductivity in the metal-insulator-semiconductor structures, description of the spacial oscillations of the radial electron density in the atom and atomic cluster, electron spectrum in 1D and 3D crystals, field ionization of the quantum systems, stepped dependence on the temperature of the ionization state and energy of the Boltzmann plasma, semiclassical evaluation of the free ion ionization potentials and partition functions, calculation and explanation of sodium and aluminium cluster mass spectra distinctions are presented.

This work was supported in part by the Russian Foundation for Basic Research (project 11-01-00267a).

## COLD CURVE CONSTRUCTION BY USING ABINIT AND QUASIZONE MODEL

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Cold curves of aluminum, iron, titanium, tungsten, xenon and other materials in a crystalline state were constructed by using a software package ABINIT and quasizone model. There were also calculated normal density, bulk modulus and heat of sublimation for these substances. To obtain the dependence of the pressure and the internal energy in a wide range of densities we used special sewing of data. Comparison of reference and calculated data shows that an appropriate choice of pseudopotential can give accurate results. This, in turn, makes possible using the proposed method to calculate a wide range equation of state and get reasonable results.

## POTASSIUM UNDER PRESSURE: ELECTRONIC ORIGIN OF COMPLEX STRUCTURES

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Recent high-pressure x-ray diffraction studies of alkali metals revealed unusual complex structures that follow the body-centered and face-centered cubic structures on compression [1]. The structural sequence of Potassium under compression to 1 Megabar is following:

*bcc – fcc – host-guest (tI19\*), hP4 – oP8 – tI4 – oC16.*

We consider configurations of Brillouin zones and the Fermi surface within a nearly-free-electron model in order to analyze the importance of these configurations for the crystal structure energy [2], containing two main contributions: electrostatic (Ewald) and electronic (band structure) energies. The latter can be lowered due to formation of Brillouin zone planes close to the Fermi surface opening an energy gap at these planes. Under pressure, the band structure energy term becomes more important leading to a formation of complex low-symmetry structures [3]. The stability of the *post – fcc* phases in K is attributed to the changes in the valence electron configuration implying the overlap of valence band with the upper core electrons. This effect has been considered for Na [4] and



offers an explanation of structural complexity of all alkali metals under strong compression.

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## LATTICE DYNAMICS OF HAFNIUM AT HIGH PRESSURES

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Group IV transition metals (Ti, Zr, Hf), which crystallize in the hcp structure at ambient conditions, transform under pressure to an omega phase and then to a bcc structure. Not much information is known concerning hafnium behavior under pressure: reported transition to an omega phase has started near 46 GPa and has completed near 60 GPa [1]. Lattice dynamics of the hcp hafnium show anomaly in the LO phonon branch near the zone center at ambient conditions [2]. Phonon anomalies may play an important role in the phase transitions at high pressures but so far no such data exist for hafnium.

Here we present the first Raman measurements of lattice dynamics in hcp phase of hafnium at pressures up to 50 GPa.  $E_{2g}$  optical phonon mode and the coupled elastic shear modulus  $C_{44}$  were found to show an anomalous pressure behavior. The second-order Raman spectrum of hafnium was also observed at high pressures giving the possibility to study pressure dependence of the phonon density of states.

This work was supported by the Russian Foundation for Basic Research (grant no. 11-02-00306.)

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# MULTIPHASE EQUATION OF STATE FOR TITANIUM AT HIGH PRESSURES AND TEMPERATURES

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A new wide-range multiphase equation of state for titanium with taking into account the polymorphic phase transformations, melting and evaporation is proposed. Calculated thermodynamic characteristics of different phases ( $\alpha$ ,  $\omega$ ,  $\beta$  crystalline modifications and liquid) are in a good agreement with available experimental data for the metal at high pressures and temperatures.

## MELTING CURVES OF METALS IN QUASI-HARMONIC APPROXIMATION

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In this work we present melting curves of metals calculated in quasi-harmonic approximation. The VASP [1, 2] and PHONOPY codes are used to determine the phonon spectrum of crystals and phonon density of states. This information is used to compute the mean-square displacement of atoms. Then the generalized Lindemann criterion is used to determine the position of melting curve at different pressures. We compare the results for aluminum and silver with existing multiphase equations of states. We also investigate the behavior of melting curves at different temperatures of ions and electrons, in particular, at high electron temperatures (several electron-volts). It is found that for silver the melting temperature for the crystal with hot electrons may be significantly higher than that for the equilibrium case. The ways to take this effect into account in two-temperature equations of state are discussed.

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## AB-INITIO SIMULATION OF ISENTROPIC COMPRESSION OF DEUTERIUM

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In this work we present our calculations of the compression isentrope of deuterium. We use a pseudopotential density-functional-theory (DFT) code VASP [1] with the plane-augmented-wave pseudopotential and generalized-gradient-approximation exchange-correlation functional. The quantum molecular dynamics approach which is based upon the Born-Oppenheimer approximation is applied to calculate pressure and internal energy of dense deuterium plasma. The calculations were made in the range of temperatures 293–25000 K and densities 1–3 g/cm<sup>3</sup>. We use Zel'dovich's approach to restore the isentrope and compare the results with experimental data and other theories [2]. The position of the calculated isentrope slightly depends on the initial point but agrees with the initial part of the experimental isentrope. However, we didn't find the density jump registered experimentally [2].

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## FIRST-PRINCIPLE CALCULATIONS OF TRANSPORT AND OPTICAL PROPERTIES OF ALUMINUM AND SILVER

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This work is devoted to the *ab initio* calculation of dynamical electrical conductivity and optical properties of aluminum and silver. The calculation is performed using quantum molecular dynamics (QMD) and density functional theory (DFT).

QMD simulation is used to calculate ionic trajectories. Independent ionic configurations are selected from the equilibrium section of the molecular dynamics run for the calculation of conductivity. Detailed zone structure calculation is performed for each of these configurations. Electronic energy levels and wave functions are obtained and then used to calculate the real part of dynamical electrical conductivity using the Kubo-

Greenwood formula. The values of conductivity for different ionic configurations are averaged. The imaginary part of electrical conductivity is obtained via the Kramers-Kronig transformation. Then optical properties are calculated: complex dielectric function, complex refractive index, reflectivity and opacity.

QMD simulation and electronic structure calculation are performed using Vienna Ab initio Simulation Package (VASP) [1, 2].

The calculation is performed for aluminum at different temperatures and densities in solid and liquid phase. Particular attention is devoted to the normal isochor for temperatures from normal up to 20000 K. The convergence of the results with the parameters of the calculation is examined. The results are compared with data of other authors, reference and experimental data. Similar results for silver at normal density are also discussed.

The calculations of this work were used to calibrate the semiempirical model of dielectric function, necessary for the simulation of femtosecond laser interaction with matter.

This work is supported by the FAIR-Russia Research Center grant for master students (2011–2012).

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## **REGION OF APPLICABILITY OF THE THERMAL CONTRIBUTION TO THERMODYNAMIC FUNCTIONS IN THOMAS–FERMI MODEL**

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The Thomas-Fermi model at finite temperature [1] becomes invalid at low temperatures because of the prevailing contribution of quantum and exchange corrections [2].

The quantum effects are known to determine thermodynamic properties of matter at zero temperature. Therefore, if we subtract the value of a thermodynamic function at zero temperature from the same value at finite temperature, we could expect that the region of applicability for this thermal contribution would be significantly extended. That's why it is interesting to check this by direct calculation.

In this work the region of temperatures and densities, in which the thermal contribution to the Thomas–Fermi model is applicable, is determined. The criterion, as proposed at [3], is the comparison of a thermal contribution to thermodynamic functions with their thermal quantum and exchange corrections. We discuss the regions of applicability for energy and pressure and their thermal parts and consider examples for different elements.

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## WIDEBAND TWO-TEMPERATURE EQUATION OF STATE FOR METALS AT HIGH ENERGY DENSITIES

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The description of matter at high pressures and temperatures is of great importance for the investigation of high-intensity electro- and thermophysical processes in the absence of complete local thermodynamic equilibrium in a system.

The objective of the work is to develop the phenomenological two-temperature equations of state (EOS), containing minimal number of constants, for solid metals (Cu, Al) at high energy densities.

Within our model any metal is considered to be a plasma-like medium, where conduction electrons appear to be single-particle excitations, complying with the Fermi-Dirac statistics within the equilibrium conditions. The developed model consistency while specifying metal dynamic and thermal-energy properties variables is achieved via defining EOS as a thermodynamic potential – free energy as a function of temperature and density. To describe a solid body we apply the Debye model, where considering both crystal lattice anharmonicity and electrons thermal excitation. The model free parameters for Cu and Al are estimated. The shock Hugoniot curves for Cu and Al, obtained within the one-temperature approach, are in agreement, both qualitative and quantitative, with available experimental data.

The relations at the front of a shock wave inside the solid body in equilibrium between electronic and lattice components absence are obtained. The theoretical shock Hugoniot curves for Cu and Al for various electronic and lattice temperatures ratios are estimated.

The work is carried out under the partial financial support of the RFBR (project No. 10-08-00691-a) and the Presidium of the Ural Branch of Russian Academy of Science within the integration projects, carried out by joint efforts of UB, SB and FEB of RAS (project No. 09-C-2-1002), and also within the Programs for basic research of the Presidium of Russian Academy of Science “Thermal physics and mechanics of extreme energetic interactions and physics of strongly compressed matter” (project No. 09-II-2-1016) and “Matter at high energy densities” (project No. 12-II-2-1005).

## “PHASE FREEZEOUT” IN ISENTROPICALLY EXPANDING WARM DENSE MATTER

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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 ions) are under discussion. The situation is considered when (i) – thermodynamic trajectory of such expansion crosses binodal of liquid-gas phase transition, and (ii) – expansion within two-phase region is going on along *equilibrium* (but *not metastable*) branch of two-phase mixture isentrope. It is known for the flat case [Anisimov, Inogamov and Rethfeld] that because of sharp break in the expansion-isentrope (in  $P - V$  plane) at binodal (boiling) point, i.e. because of significant jump in sound velocity at this point, there appears *extended zone* (layer) of *uniformity* for expanding material with constant thermodynamic and kinematic parameters, which corresponds just to thermodynamic state on this binodal of boiling liquid. It is important that because of self-similarity of such expansion (in flat case) this zone contains significant and *finite* portion of whole material, involved into the process of isentropic expansion. Even more, in the case of expansion of *semi-infinite* WDM sample the size of this uniform layer of boiling liquid formally *tends to infinity*. This remarkable property makes it possible [Iosilevskiy, 2011] to discuss (at least formally) this type of isentropic WDM expansion as a tool for generation (and subsequent diagnostics) of *extended uniform state* of the matter just

on binodal (in particular, at critical point!) of unexplored states of matter, when parameters of this binodal (and/or thermophysical properties on it) are not known. It is natural to use the term “phase freeze-out” for this regime of expansion. It is similar to the terms “chemical freeze-out” and “kinetic freeze-out”, which are widely used in interpretation of quark-hadron transformations during the expansion of products for ultra-high energy ionic collisions in supercolliders. Perspectives of appearance of such phase “freeze-out scenario” are discussed in connection with isentropic expansion of “fireball” of quark-gluon plasma, created by mentioned above relativistic ionic collision in supercolliders.

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## SEMI-ANALYTICAL CALCULATIONS FOR PARAMETERS OF BOILING LAYER IN ISENTROPIC EXPANSION OF WARM DENSE MATTER WITH VAN DER WAALS EQUATION OF STATE

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Features and parameters of “boiling” liquid layer, which arises under conditions of isentropic expansion of warm dense matter (WDM), 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. Idealized self-similar case of behavior of matter on interception of equilibrium (not metastable) isoentropic curve and boundary of gas-liquid coexistence curve (binodal) is analyzed. The possibility of formation of such “liquid layer” was studied previously in [1] during solving the problem of ablation of metal surface under the action of strong laser radiation. Peculiarity of such “freezing” of finite portion of expanding matter in the state, which corresponds to the binodal of gas-liquid or/and other phase transitions—so called “phase freezeout”—and prospects of applications of this phenomenon for intended generation of uniform and extensive zone of previously unexplored states of matter were discussed in [2].

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**BOUNDARIES OF THERMODYNAMIC STABILITY  
FOR WIDE-RANGE ANALYTIC EOS OF FULLY IONIZED  
ELECTRON-IONIC PLASMAS**

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Boundaries for thermodynamic instability are studied for well-known wide-range analytic equations of state (EOS) of non-ideal fully ionized electron-ionic plasmas (Potekhin & Chabrier), which is widely used in astrophysical applications. It was found that for one-element electron-ionic plasmas ( $Z:e$ ) this thermodynamic instability region looks as 1<sup>st</sup>-order phase transition of gas-liquid type with upper critical point, which is well described by simple relation:  $T_c(Z) \approx T_c(1)Z^\gamma$  (here  $\gamma \approx \frac{3}{2}$  and  $kT_c(1) \approx 1.49$  eV. Structure and parameters of discussed phase transition proved to be very close to those for similar phase transition(s), which were studied previously by Iosilevskiy and Chigvintsev for so-called Double-OCP model i.e. for superposition of two OCP-models for ions and electrons without electronic screening effects. In particular both phase transitions predict highly asymmetric phase diagrams with remarkably low values of critical compressibility factor for all values of  $Z$ . Parameters of mentioned above thermodynamic instability have been calculated for global and local instability conditions (i.e. binodals and spinodals). Calculations were provided for plasmas of single elements and for mixtures in Linier Mixing Rule approximation. Validity of several well-known semi-empirical rules for phase diagram is discussed. In particular new variant for the rule of “rectilinear diameter” was discovered for compressibility factor. This new variant appends standard variant of the rule for density-temperature phase diagram. Perspectives for calculation of simplest variant for noncongruent phase transition are discussed for the model of “binary ionic mixture” with the use of present and previous approximate equations of state.



# THERMODYNAMIC EQUATION OF STATE USED TO DESCRIBE THE BEHAVIOR OF A POROUS MIXTURE

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The work is devoted to a problem of the description of behavior of multispecies mixtures of various powders under shock-wave loading. The actuality of similar researches is caused as wide representation of heterogeneous systems in various branches of a science and engineering, and wide spectrum of tasks facing to a science at the present stage. If the mixture is thermodynamically equilibrium and the motion of the species relative to each other is ignored, its motion can be described as the motion of one continuum with a special equation of state, which takes into account the properties of the species of the mixture and their concentrations. As a result, the number of equations is substantially reduced. The method implies that the equations of state of the species are similar to the equations for these substances in the free state. Equations of state of condensed species and air filling the pore space and an equation of state of the mixture are presented in a unified manner (in the form of the Mie–Grüneisen equation). Applicability of such an equation of state for air in the range of high pressures and temperatures is validated by comparisons of shock adiabats calculated with the use of this equation and available data in the literature. The numerical calculations of shock adiabats for porous substances and porous mixtures of the condensed species are performed with use of various models of the equation of a state of a mixture taking into account: a) only elastic pressure and elastic energy; b) both elastic, and thermal terms with constant specific heat of substance and Grüneisen coefficient; c) elastic and thermal terms with specific heat of substance the dependence on the temperature and variable Grüneisen coefficient. The thus-derived equation of state of a thermodynamically equilibrium mixture offers a fairly accurate description of the behavior of a porous medium.

**EXPERIMENTAL SETUP FOR INVESTIGATION  
OF THERMOPHYSICAL PROPERTIES OF CONDUCTIVE  
REFRACTORY MATERIALS AROUND ITS MELTING  
POINT BY PULSE HEATING METHOD**

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The method and the experimental setup for investigation of thermophysical properties of conductive refractory materials are described. The method allows to investigate set of properties, e.g.: enthalpy  $H_p(T)$ , heat capacity  $C_p(T)$ , melting temperature  $T_m$ , melting heat  $\Delta H_m$ , resistance of refractory metals, carbides and graphite in the vicinity of the melting point and in a liquid phase, which are the most perspective at the creation of innovative high-temperature power-plants and gas-cooled nuclear reactors. Nowadays the pulse heating method is the most essential in the modern experimental physics technique for researching the properties of matter at the high temperatures up to 10000 K. Electrical pulse heating has the significant advantage (to a laser impulse) in a volumetric thermal emission that allows to measure specific properties of the matter. Feature of the method is that at the high velocities of heating the specimen has no time to interact with a surrounding medium, has inappreciable losses of heat by radiation and transpiration and maintains geometry in a fluid state at high rates of energy inserting. A key role at the method realization plays precise and reliable temperature measuring of the sample surface. Measuring of a specimen temperature by pyrometers through the inert gas allows to use all potential of the modern methods of an optical pyrometry that is inconvenient while using the capillaries or opaque intermediate medium. However the small sizes of specimens ( $\sim 1$  mm) and high rates of heating (up to  $10^{11}$  K/s) complicate temperature measuring and do not allow using pyrometers, submitted in the market. Therefore a necessity of development of a temperature measuring procedure and creating of the special optical pyrometer suitable to measuring in such requirements occurs. Novelty of the suggested approach consists of high static pressures of inert gases that allows to use all the modern optical diagnostics—an optical pyrometry, high-speed digital visualization, and also high metrological precision of the electrical quantities measuring, provided at the duration of the experiment about 100–1000 microseconds. Results of preliminary experiments on the example of technically pure tantalum specimen are discussed.

# STUDYING OF MICROPOROUS STRUCTURE OF CARBON MATERIALS AND THEIR APPLICATION IN SUPERCAPACITORS

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The growth of energy consumption and industry development negatively influences on ecological situation in the world. Creation of new ecological energy sources not polluting environment is very actual now. Nowadays electrochemical sources and energy accumulators find the wide application. Electrochemical double-layer capacitors (EDLC) are considered to be the perspective working out. Various carbon materials with high specific surface such as the carbon fabric, activated coals, etc. are used at manufacturing EDLC electrodes. Carbon fabric Uvis-Ak-T-0.4 was investigated in the present work. Uvis-Ak-T-0.4 is a part of the pulse EDLC with sulfuric acid as electrolyte. It has shown good electrochemical characteristics during tests. It can be connected with the presence of microporous and their accessibility to molecules of sulfuric acid, forming a double electric layer.

In the given work other types of carbon materials have also been investigated: some samples of carbon black and the serial of activated coals. Researches were made using the Limited Evaporation Technique (LET) with benzene and water as adsorbates. We do not cope to identify pores which radius is less than 7 angstrom unit using benzene as an adsorbate. Nevertheless residual volume of a benzene at desorption proves the existence of these pores. The use of water as an adsorbate has allowed us to receive micropores size distributions in an explicit form (from radius 4 angstrom unit). The residual volume of benzene is a consequence of surface "roughness" of a carbon material. Surface defects create the centers with raised adsorption energy. Benzene molecules are kept on a surface of an adsorbent and do not evaporate at relative pressure equals to a corresponding pore radius.

Pore size distributions of carbon fabric Uvis-Ak-T-0.4 have been received. The micropore volume  $0.4 \text{ cm}^3/\text{g}$  is concentrated in pores, which radius is 4–10 angstrom unit. The mesopore volume  $0.25 \text{ cm}^3/\text{g}$  is concentrated in pores  $r = 10\text{--}500$  angstrom unit. The total pore volume  $0.82 \text{ cm}^3/\text{g}$  includes basically micro- and mesoporous. The contribution of macroporous is insignificant. Good correlation between pore size distributions using benzene and water as adsorbates was established.

LET allows us to investigate the structure detailed. It facilitates selection of porous materials with certain structure and properties that is of the great importance for supercapacitors.

## DIAMOND CRYSTALLIZATION FROM SUPERCOOLED LIQUID CARBON

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Diamond growth was predicted earlier in the framework of the thermodynamic approach from liquid carbon supercooled below the diamond melting point, estimated as  $T_{DM} = 4160$  K [1]. This possibility should exist even when the fluid pressure is much lower than the pressure at the graphite–diamond–liquid triple point and without use of catalysts.

In the experiment different mass liquid carbon particles at the pressure of 30 MPa were quenched in contact with the flat surface of natural diamond monocrystal with record for the solid thermal conductivity of about 2000 W/m·K. Structure of the solidified particles with thicknesses of 10–15 nm and 120–150 nm was determined. White carbon particles of the first type diffusely reflected visible light, and represented splices of individual crystals, surrounded by diamond-like amorphous carbon. In the second case, transparent crystal fine-grained film was formed, in which the amorphous phase is presumably located directly in contact area with the substrate. Amorphous phase was identified using the Raman spectra. It was difficult to identify the particle crystalline component by Raman scattering because of the background scattering in the diamond substrate. However, according to atomic force microscopy single crystals and grains have octahedral and cubic faceting, what is sufficient evidence of the diamond structure of newly formed crystals in both cases. Partial amorphization of the particles, uniquely identified on the particles of 10–15 nm thickness, is the evidence the deep supercooling of the liquid before the crystal growth. Based on the known similarity of the short-range order of the liquid and quenched from it amorphous state it can be argued that the liquid carbon, high supercooled in contact area with the diamond, has the diamond-like short-range order. Such liquid structure along with the autoepitaxy mechanism is the advantage in the formation and growth of the nucleus with the diamond structure, in comparison with the nucleus with the structure of graphite, due to the lower interphase energy.

Present studies show promising of new direction associated with the investigation of structure and thermodynamics, as well as practical application of high supercooled liquid carbon. This work was supported by RFBR (grant 10-08-01-266-a).

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## **ATOMISTIC MODELING OF GRAPHITE MELTING**

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Process of graphite melting was studied using molecular dynamics simulations with the semiepirical bond-order potential AIREBO [1]. The software package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) was used. For the calculations of the temperature along the melting line the two-phase simulation method was used [2]. As a result the graphite melting line was obtained in the pressure range up to 8 GPa.

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## **MOLECULAR DYNAMICS STUDY OF CRYSTAL NUCLEATION IN ALUMINUM MELT**

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Kinetics of crystallization of supercooled aluminum melt is studied by molecular dynamics (MD) method. The melt is described by embedded atom method (EAM) potential. The dependence of crystal nucleation rate on pressure and temperature is obtained. Kinetics of near-critical nucleus formation is analyzed using mean first-passage time method.

Homogeneous crystal nucleation at constant temperature and density is considered. The nucleation rate is defined as  $J = 1/N\langle t \rangle$ , where  $N$  is the

number of atoms in the simulation cell,  $\langle t \rangle$  is the lifetime of homogeneous liquid averaged over multiple simulations for one and the same  $(T, \rho)$ .

The dependencies of the nucleation rate on pressure for temperatures ranging from 670 K to 900 K are obtained. They are fitted using the formulas of the classical nucleation theory (CNT) [1]. The values of crystal-melt interface free energies are fitted to have the best approximation of MD data by analytical expressions.

Kinetics of nuclei formation is analyzed using mean first-passage time (MFPT) method [2]. In the case of nucleation, the MFPT can be defined as the average time  $\tau(n)$  that a cluster takes to reach a particular size  $n$  for the first time. In the case of a single-maximum energy barrier  $\tau(n)$  is given by the expression

$$\tau(n) = \frac{\langle t \rangle}{2} [1 + \operatorname{erf}(b(n - n^*))],$$

where  $n^*$  is the critical cluster size.

For high undercoolings, this formula is found in good agreement with simulation results. For lower undercoolings, nucleation is found to proceed stepwise. This may indicate that there are several energy maxima on the reaction path in the case of crystal nucleation.

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## VITRIFICATION OF ALUMINUM MELT. MOLECULAR DYNAMICS STUDY

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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.

Influence of cooling rate on the final state of the system is studied. MD simulations were held for cooling rates from  $10^{10}$  K/s to  $10^{13}$  K/s. At cooling rates below  $10^{10}$  K/s the melt eventually crystallizes. At higher cooling rates the melt freezes into an amorphous structure.

Structural analysis of amorphous aluminum based on radial distribution function of atoms is performed. Splitting of the second peak is used as a criterion for the amorphous structure.

The results show the vitrifying temperature and final pressure in glass depends on cooling rate.

At cooling rate higher than  $10^{13}$  K/s the final amorphous state is nonequilibrium and relaxation time is approximately 100 ps.

Equation of state hysteresis takes place during cooling and heating. Phase transition from amorphous to solid state can take place at higher temperatures (800–900 K).

The results are compared with the common data.

## ATOMISTIC SIMULATION OF STRUCTURE AND PROPERTIES OF URANIFEROUS NUCLEAR FUELS

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Using atomistic simulation the structure and properties of pure uranium (U) and prospective uranium-molybdenum (U-Mo) fuel alloys are studied. Two new interatomic potentials for pure U and binary U-Mo system are developed in the frame of embedded-atom model [1] using force-matching method [2]. Both potentials are fitted to the values of interatomic forces, energies and stresses obtained from *ab initio* calculations. The potentials allow to reproduce structure of low-temperature  $\alpha$ -U, high-temperature  $\gamma$ -U, pure Mo and U-Mo alloys. The results obtained for elastic properties, thermal expansion, room-temperature isotherm and melting temperatures of U and Mo are consistent with the experimental data. The values of single defect (vacancy, self-interstitial atom) formation energies in pure U and Mo agree well with the results of *ab initio* calculations. The potentials developed are aimed to study in details the formation and evolution of radiation defects occurring in the fuel materials (U, U-Mo) under irradiation and heating and to investigate corresponding changes in fuel structure and strength properties.

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## TRANSPORT PROPERTIES OF GRAPHITE AND GRAPHENE AT HIGH PRESSURES

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Conductivity of graphite and graphene has been studied at pressures up to 35 GPa and room temperature, as well as magnetoresistance of these materials. The kinetics of resistivity at changing pressure was also studied. Transport phenomena were used as a tool for finding and interpretation of phase transitions arisen under high pressure.

High pressures have been generated in the high pressure cell with synthetic carbonado-type diamond anvils. The anvils are good conductors and can be used as electric contacts making possible to measure temperature and pressure dependences of resistance. The method used allows us to study the same sample at successive increasing and decreasing pressure and also to keep it loaded during a long time.

In the pressure range from 16 to 30 GPa, the sharp change in the thermo-EMF value of graphite was observed. It is consistent with the existence of phase transition in this pressure range, which was found earlier at our d.c. measurements. Impedance measurements of graphite were carried out by means of RLC-2000 impedance analyzer at room temperature in the frequency range of 1–200 kHz. The impedance features found for all samples at pressures of 18 to 32 GPa confirmed also the phase transition.

Baric dependences of resistance of graphite and graphene were of similar character, and the resistance of graphene was by almost one order of magnitude larger than that of graphite. Besides for graphene it is not revealed features at pressure above 20 GPa. The characteristic time of the change of resistance after the change of pressure for graphene was also larger than resistance relaxation times for graphite, it was  $\sim 10$  minutes. This time for graphite did not exceed 1 minute at all pressures used. In the vicinity of the phase transition (15–20 GPa) the relaxation times increased.

Magnetic field up to 1 T did not influence on the character of baric dependences of resistance. The resistances of both materials slightly (by 3–5%) decreased in magnetic field at the pressures below 30 GPa for graphite and 23 GPa for graphene. At higher pressures the magnetic field did not



influence on the resistance of both graphite and graphene.

Thus, the baric dependences of resistance of the investigated materials have similar character that is connected, most likely, with percolation mechanism of conductivity. This work was supported in part by RFBR grant 10-02-96036.

## **ELECTRICAL AND THERMOELECTRICAL PROPERTIES OF GLASSY CHALCOGENIDES OF COPPER AND SILVER UNDER DIFFERENT EXTERNAL EFFECTS**

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Investigations of the ionic and mixed electronic-ionic conductors in a broad temperature range and at high pressure are of practical and theoretical interest. The aim of this work was to investigate the electrical and thermoelectrical properties of the multi-component glassy chalcogenides of copper and silver with ion conductance at pressures up to 50 GPa and at normal pressure in the temperature range 10–400 K. The glassy materials from the systems  $\text{AgGe}_{1+x}\text{As}_{1-x}\text{S}_3$  and  $\text{Cu}_{1-x}\text{Ag}_x\text{GeAsSe}_3$  were studied. The compounds were synthesized by melting stoichiometric quantities of the elements in evacuated to  $10^{-4}$  Pa and filled argon or helium silica tubes at 1370 K and further quenching. X-ray diffraction experiments and qualification of materials have been performed by means with diffractometer Shimadzu XRD 7000. The radial-distribution functions of samples have been obtained. Electrical properties have been investigated by means of impedance spectroscopy in the frequency range of 0.1–200 kHz and on direct current. High pressures have been generated in the cell with synthetic carbonado-type diamond anvils of the “rounded cone-plane” type. For creation of temperature gradient one of the anvils was warmed. The baric dependences of thermoemf, impedance, a tangent of loss angle at increase and decrease of pressure were analyzed. The influence of the composition and temperature on the mean-squared displacement of silver mobile ions in the glassy chalcogenide ion conductors have been determined by means of Fourier analysis with the complex conductivity function. By the scaling of the ac conductivity at different pressures the baric ranges of noticeable changes of the electrical properties of materials were established.

The study was supported in part by the federal target program Scientists and Science Teachers of an Innovative Russia 2009–2013; and by the

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**EFFECT OF PRESSURE ON THE ELECTRICAL PROPERTIES OF THE NEW HIGH-PRESSURE PEROVSKITE-LIKE PHASES  $ACu_3V_4O_{12}$  (A=Gd, Tb, Er)**

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The perovskite-like oxides are of considerable interest due to their unusual electrical and magnetic properties [1]. The purpose of research was a study of the electrical properties of a new compounds  $ACu_3V_4O_{12}$ , where A-Gd, Tb, Er, at high pressure and at low temperature.  $ACu_3V_4O_{12}$ -oxides (where A-Gd, Tb, Er) were prepared under high-pressure and high-temperature conditions in a toroid-type high-pressure chamber [2], and crystallized as an A-site-ordered double perovskite (space group  $Im-3, Z=2$ ), the lattice parameters  $a=0.72939$  nm,  $0.7292$  nm and  $0.7266$  nm for compounds with A-Gd, Tb, Er respectively. 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 70 and 400 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 carbonado-type diamonds [3].

The ranges of significant change in the behavior of the electrical properties of the compounds as a function of applied pressure were determined. These ranges shifted toward higher pressures with decreasing ionic radius of lanthanide A, that may be associated with the effect of the chemical compression. The temperature dependencies of the electrical resistance at 80-300 K and atmospheric pressure have a semiconductor character for all three materials. Analysis of the temperature dependencies of the electrical resistance under different fixed pressures from 10 to 50 GPa have

shown that at pressures above 30 GPa the resistance of the compounds  $ACu_3V_4O_{12}$ , where A-Gd, Tb, Er decreases with decreasing temperature.

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## **ELECTRICAL AND MAGNETIC PROPERTIES OF $AgFeAsSe_3$ AT EXTREMAL CONDITION**

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The abstract is devoted the synthesis and investigation of electrical and magnetic properties  $AgFeAsSe_3$  in a wide regions of temperatures, pressures and magnetic fields. The researches of electrical properties carry out by a method impedance spectroscopy with use investigated-analyser of impedance RLC-2010 in the field of frequencies 1 kHz–1 MHz and temperature range 78–400 K. High pressures at 15–45 GPa have been generated in the cell with synthetic carbonado-type diamond anvils of the “rounded cone-plane” type [1]. Magnetization measurement carried out by SQUID-magnetometer MPMS XL7 in the temperature range 100–400 K and magnetic fields up to 7 T. Temperature dependence of electrical conductivity have activation type, the change of activation energy occurs in the temperature range 240–280 K. In the temperature region 220–250 K, anomaly of the resistance  $R(T)$  is observed, which is similar to that observed in measurements with continuous current in the temperature range 260–270 K [2], i.e. increase of frequency leads to decrease of temperature at the resistance anomaly domain. The dielectric constant increases with increasing temperature. Magnetization decreases in the temperature range from 78 to  $\sim$  310 K and remains practically constant with further increase in temperature. Perhaps this is due to the transition of the sample from the paramagnetic state to a state with magnetic order at temperatures below 310 K. These results are consistent with earlier studies at lower fields and

temperatures [2]. With increasing field, the magnetization increases, but does not reach saturation in fields up to 7 T. The curve of the field increase and decrease of the field at fields above 0.5 T are the same. With increasing pressure the resistance decreases up to 25 GPa and then remains virtually unchanged. Perhaps, in this pressure range there is a phase transition.

This work was partially supported by the Federal Program “Scientific and scientific-pedagogical personnel of innovative Russia” for 2009–2013 and RFBR grant 12–02–00987–a.

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## **INFLUENCE OF TEMPERATURE AND PRESSURE ON ELECTRICAL PROPERTIES OF $\text{CuGeAsSe}_3$**

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Multicomponent 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. The purpose of this work was to investigate the electrical properties of the polycrystalline chalcogenide  $\text{CuGeAsSe}_3$  (with tetragonal structure on sphalerite base [1, 2]) under a pressure in the range from 0 to 30 GPa, in the temperature interval from 10 to 300 K, at a frequency of the alternating-current electric field varying from 200 Hz to 200 kHz and on direct current.

It has been found that the temperature dependence of the conductivity exhibit anomalies that are characteristic of structural phase transitions. The dielectric loss tangent and the real part of an admittance of the  $\text{CuGeAsSe}_3$  compound exponentially increase with a pressure increase from 8 up to 30 GPa. The influence of the frequency on the electrical properties of the material has been analyzed.

The studied earlier polycrystalline chalcogenide  $\text{CuGeAsS}_3$  (crystallographic parameters are close to those of the studied compound  $\text{CuGeAsSe}_3$ ) is electron-ion conductor [2, 3]. When sulfur in  $\text{CuGeAsS}_3$

compound is substituted for selenium the conductivity rises by six orders of magnitude, ionic conductivity is not observed, the pressure range of substantial changes in the behavior of electrical characteristics shifts toward lower pressures. The last fact could be related to the effect of the chemical compression, connected with difference of the ion radii of sulphur and selenium.

The study was supported in part by the federal target program Scientists and Science Teachers of an Innovative Russia, 2009–2013; and by the Russian Foundation for Basic Research, project no 10–02–96036.

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## SUPERCONDUCTING STATES OF NANOSIZED Pb ISLANDS ON Si SURFACES BY SCANNING TUNNELING SPECTROSCOPY

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This report is dedicated to the scanning tunnelling microscopy and spectroscopy study of the quantum confinement effect of the superconductivity. For this study we have realized a original set-up. This ultra high vacuum device allows preparing the surface of the samples in-situ under the UHV conditions and at different temperatures with further controlling the created nanostructures by LEED and Auger spectroscopy. The superconducting nanostructures were studied by scanning tunnelling microscopy/spectroscopy in magnetic field (up to 1 Tesla) and at very low temperature (down to 280 mK). The growth of the nanometer size lead islands on the atomically clean surface of Si(111), and as well on vicinal Si(557) surface, was studied in details. After that, the superconductive properties of the islands in strong confined regime were studied by STM/STS at low temperature and in magnetic field. For such a study an isolated island was chosen. The island lateral size ( $L = 110$  nm) corresponds well to the strong confinement case:  $L \sim 3\xi \ll \lambda$ . It was ex-

perimentally shown, that in this island only three states are possible: the state without vortex, the state with only one vortex and the normal state. This case corresponds to a limit case: islands of a larger size may accept the multivortex states, while any-vortex state becomes energetically impossible for a little bit smaller islands.

**ANOMALOUS SCENARIO FOR SPINODAL  
DECOMPOSITION OF METASTABLE MELTING  
IN THE ZERO-TEMPERATURE LIMIT**

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Hypothetical scenarios for termination of deep metastable melting in Coulomb model at zero-temperature limit  $T \rightarrow 0$  are under discussion. Present analysis based on study of topology for combination of melting, boiling and sublimation boundaries in non-standard version of one-component plasma model on uniformly compressible background: OCP( $\sim$ ) [1] [2]. In contrast to the widely accepted scenario of metastable melting termination in rare gases [3] and metals [4], when metastable melting curve reaches actually isotherm  $T = 0$  (“cold curve”) of a matter, present work devoted to more plausible scenario of deep metastable melting, titled as “spinodal decomposition”. Its basic point is unavoidable intersection at finite temperature of metastable liquid melting boundary (liquidus) with spinodal curve of metastable liquid-gas phase transition. Metastable melting at lower temperature is impossible in this case since absolute instability of liquid phase, so that metastable crystal has no where to melt. Two non-standard and more exotic scenarios for metastable melting termination (MMT) are under discussion in addition to two mentioned above MMT scenarios. In the first one (A) hypothetical unique crystal-fluid global phase coexistence is realized as smooth superposition of boiling and sublimation curves (without gas-liquid phase transition and corresponding critical point). In second scenario (B) anomalous non-standard type of “spinodal decomposition” is realized, when metastable solid binodal (solidus) intersects gaseous spinodal of metastable gas-liquid phase transition. Features of all mentioned above variants of MMT are under discussion as well as hypothetical possibility of direct numerical simulations for such new, exotic MMT-s.

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## PROPERTIES OF HIGH-TEMPERATURE PHASE DIAGRAM AND CRITICAL POINT PARAMETERS IN SILICA

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In this paper the comparative study of the properties of high-temperature phase diagram and the parameters of the critical points in silicon dioxide (SiO<sub>2</sub>), predicted by various theoretical models in comparison with those few experiments and handbooks (see [1] and references therein) was continued. This paper compares the equilibrium vapor composition at the boundary of high-temperature boiling SiO<sub>2</sub>, predicted by the calculation of the chemical plasma model (code SAHA [2]) with the experimental data. Also the satisfiability of well-known semi-empirical rules that are widely used in estimating the parameters of the critical points, such as the rectilinear diameter rule and the applicability of the so-called Guggenheim formula for the  $\rho - T$  diagram of SiO<sub>2</sub>, Timmermans rules for the critical compressibility factor, etc. was tested for selected theoretical models. The applicability of the new version of the rectilinear diameter rule for spinodal compressibility factor identified by the modified Coulomb model [3] is discussed on the example of the phase diagram of SiO<sub>2</sub>. The first steps of the calculation of incongruent phase transition gas-liquid interface in silicon dioxide, predicted in [2–4] is discussed.

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**CALCULATION OF PHASE EQUILIBRIUM CURVE  
IN THE PHASE DIAGRAM OF SODIUM CHLORIDE  
AT TEMPERATURES BELOW THE CRITICAL**

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The purpose of this paper is to calculate the pressure for more accurate determination of the spinodal on the basis of theoretically a certain critical temperature and the constants of the van der Waals forces and the experimental data for sodium chloride [1].

Pressure at  $T_k$  of van der Waals equation for one mole (kmol) of the substance we write in the form of:

$$p = \frac{RT_k}{V - b} - \frac{a}{V^2},$$

where the parameters  $a$  and  $b$ —constants. This equation is a cubic equation with respect to  $V$ , and hence it has three roots  $V_1, V_2, V_3$ . Note that  $V_1$  and  $V_3$  define the binodal, and the combination of  $V_1, V_2$  and  $V_3$  (which allow you to find the parameters of  $V_4$  and  $V_5$ ) determine the spinodal.

The calculation results are given, for  $T = 1025$  K, we have:  $V_1 = 665 \cdot 10^3$  m<sup>3</sup>/kmol,  $V_4 = 437 \cdot 10^3$  m<sup>3</sup>/kmol and  $V_5 = 0.24$  m<sup>3</sup>/kmol, and  $p_1 = 0.013$  kPa,  $p_2 = 0.021$  kPa, and  $p_3 = p_{30}$  enters formally into the region of negative pressures. For  $T = 1136$  K, we have:  $V_1 = 71 \cdot 10^3$  m<sup>3</sup>/kmol,  $V_4 = 47 \cdot 10^3$  m<sup>3</sup>/kmol and  $V_5 = 0.21$  m<sup>3</sup>/kmol, and  $p_1 = 0.13$  kPa,  $p_2 = 0.26$  kPa, and  $p_3/p_{30} = 1.4$ . For  $T = 1287$  K, we have:  $V_1 = 80 \cdot 10^2$  m<sup>3</sup>/kmol,  $V_4 = 53 \cdot 10^2$  m<sup>3</sup>/kmol and  $V_5 = 0.18$  m<sup>3</sup>/kmol, and  $p_1 = 1.33$  kPa,  $p_2 = 2.41$  kPa, and  $p_3/p_{30} = 2.1$ . For  $T = 1489$  K, we have:  $V_1 = 930$  m<sup>3</sup>/kmol,  $V_4 = 620$  m<sup>3</sup>/kmol and  $V_5 = 0.15$  m<sup>3</sup>/kmol, and  $p_1 = 13.3$  kPa,  $p_2 = 25.3$  kPa, and  $p_3/p_{30} = 3.5$ . For  $T = 1738$  K, we have:  $V_1 = 143$  m<sup>3</sup>/kmol,  $V_4 = 95$  m<sup>3</sup>/kmol and  $V_5 = 0.12$  m<sup>3</sup>/kmol, and  $p_1 = 101.3$  kPa,  $p_2 = 201.1$  kPa, and  $p_3/p_{30} = 6.0$ .

So, the work done was calculated the pressure for more accurate determination of phase equilibrium curves for sodium chloride. It is shown that



the region below the critical temperature of the isotherm is characterized by extremes and sudden changes in pressure in the area  $V_5$ .

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## **EQUATION OF STATE OF RARE-GAS CRYSTALS**

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Development of equations of state of matter in a wide range of pressures and temperatures is an urgent task at present. Using pair potentials obtained in [1, 2], we calculated the equilibrium interionic distance  $r_0$ , the binding energy of lattice  $U_{cr}$  and bulk modulus  $B$  for the number of crystals of inert gases (CIG) [3]. Pair interaction potential is written in the form of Lennard-Jones (6–12). The binding energy is calculated by summing the pairwise IGCs Lennard-Jones (6–12) within all the pairs in the crystal atoms. The series converge rapidly and the nearest neighbors contribute most to the interaction energy of atoms in the CIG. On the basis of lattice energy, equation of state is constructed for CIG.

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## **IN SEARCH OF ADEQUATE FORMS OF EQUATIONS OF STATE**

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The problem of adequate simple equation of state (EOS) obtaining and the related problem of determining the optimal EOS remain relevant. Searches have got a special scope after occurrence of the van-der-Waals equation of state. A considerable quantity of private forms of the vdW type EOS is suggested; the general cubic equations are investigated. It is shown that at appropriate selection of parameters all known private forms can be obtained from the general EOS. However such transition itself doesn't give the answer to one of questions, which can be formulated

during the analysis. For example. What is the explanation of the fact that insignificant changes of the EOS form result in much best description of properties? How many parameters in the famous “two-parameter” EOS? What is the meaning of the third parameter in the EOS of different forms? Whether the sense of the parameter  $b$  is identical and what is the correct its values in the various EOS? Whether the parameters of EOS are independent quantities? Why among simple EOS there are no equations giving experimental values of the critical factor of compressibility? Why the vdW EOS badly describes properties of the rarefied gas and much better—solids? What a condition of EOS parameters constancy results in? Answers can’t be received at the standard approach to the equations of state as to empirical modifications of vdW EOS. At the same time it is clear that, only having given answers, it is possible to hope for progress in a solution of a problem of adequate simple EOS. The analysis showed that in the hierarchy of thermal EOS there is a gap: there is no EOS, based on a model of interacting point centers—the simple but realistic model of the molecular level. Our recent works (many can be found at [www.csmos.ru](http://www.csmos.ru)) are intended to bridge this gap, to get the new EOS, to investigate its properties and to link the results with the information known for vdW type EOS. Incidentally it is possible to answer many from listed above questions; the part of results is discussed in the present work.

**ON METHODS OF TRUE TEMPERATURE  
DETERMINATION OF OPAQUE HEATED BODIES  
VIA THERMAL RADIATION SPECTRUM**

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At interaction of intense energy fluxes with matter the true (thermodynamic) temperature of a free emitting opaque object cannot always be measured by the contact or black body methods. Spectral methods of true temperature determination of opaque heated bodies via thermal radiation spectrum are analyzed. Computer simulation measurements occurred in a narrow spectral window, which moved along the spectrum with the given step. In this way the search for spectral ranges at which the dependence of the emissivity (or its logarithm) on the wavelength is the simplest and fairly accurate in particular linear was carried out. In the case of the successful search for the specified spectral range the true temperature was determined in the spectral window with the least squares technique (LST).

If the emissivity (or its logarithm) is linearly dependent on the wavelength then the alternative assessment of the true temperature is possible. In this case the required temperature is determined via the change of the convexity of the relative spectral emissivity dependence in the process of selecting its numerical value from the values smaller than the true temperature value to values higher than the true temperature value. It is also proposed to choose the desired temperature at the least effective length of the relative spectral emissivity curve. This approach is simple, does not require the solution of the system of equations and can significantly narrow temperature range to which belongs to the true temperature.

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## IT TOOLS OF THERMOPHYSICAL CALCULATIONS: PROPERTIES OF SUBSTANCES AND METHODS OF DETERMINATION

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Some tables and algorithms can be found in the Internet to determine thermophysical properties,  $R$ , of substances. Internet tools can be divided on two groups: a) tabulated values  $R$  of some substances; b) Internet resources those can be used by a client to calculate  $R$  with help of a program and border conditions  $Y$ . There are following tools examined in the report: 1) TF-resources in the form of text files those contain tabulated values of  $R = (P, T, v, h, \dots)$ , 2) EF-resources or closed objects those contain exe-files, 3) OI-resources or open interactive objects. The tools can be involved in some thermophysical calculations (TC) connected with: a) thermophysical properties  $R$  of substances, b) thermodynamical characteristics of power plants. EF-resources (OIVT RAN, NIST) include exe-files those are used by clients in TC calculations of properties  $R$  of various working media. Our analyses shows: OI-resource is a complicated Internet object. For example, a client can calculate properties  $R$  in the Internet portal where OI-resource is placed; he should take following steps: 1) to introduce input parameters  $Y = (P, T, \dots)$  for a substance, 2) to start a

program, 3) to copy the result  $R(P, T)$ . The advantage of the OI-resource can be explained by step 4: to copy mathematical formulas (MF) and to use OI-resource as a clouds function. OI-resource is located in a special Internet portal and includes: 1) a program Code-OI-Property-R(Y) that is used to determine  $R$ , 2) some operators connected with Internet technologies. Code-OI-Property-R(Y) includes MF formulas written with a help of Mathcad. A set of OI-resources is analyzed, among them OI-resources based on such equations as: EOS  $P(v, T)$  of liquid and gas phases,  $v_l(T)$ ,  $v_g(T)$ ,  $P_s(T)$ , where  $v_l$ ,  $v_g$  and  $P_s$  are properties on the coexistence curve. We have created OI-resource named Data on thermophysical properties of substances and engineering calculations [1]. In the case a client put  $Y$  (a substance name, parameters  $P$ ,  $T$  etc.) and fulfills TC: for example, he can calculate properties  $R = (v, h, s, \dots)$  of the water. Some clouds functions can be found in the resource and are discussed in the report. The work is supported by Russian Foundation of Basic Research.

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## SPECTRUM ANALYSIS OF THE VORTEX CASCADES IN SHEAR FLOW

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This work is a continuation of a series of studies on the vortex cascades in a free shear layer. Earlier the initial stage of formation of the core in three-dimensional turbulent shear layer of a compressible ideal gas without the influence of viscosity and walls was investigated. The onset and development of the vortex cascade of hydrodynamic instabilities were traced by the direct simulation of the classical laws of conservation.

The purpose of this paper is a deeper investigation of this problem using spectral analysis. The structure of the spectrum of the kinetic energy is well-known. For large Reynolds numbers there are three intervals of wave numbers for the spectral distribution of energy : interval of small wave numbers (within which energy is produced), dissipation interval of large wave numbers (within which energy is dissipates) and inertial interval (within which energy is neither produced nor dissipated but only advanced to the larger wave numbers). For the inertial interval the Kolmogorov's low  $-5/3$  is true.

Based on numerical experiments this type of turbulent flow is investigated and the scheme of formation of the turbulent core and the law of  $-5/3$  is analyzed. Analysis includes evaluation of spectrum kinetic energy. We obtained a dependence of the kinetic energy on wave numbers by means of the Fourier expansion of the velocity components. Also we demonstrated existence of an inertial interval for the kinetic energy  $E_k \sim q^{-5/3}$ .

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## EXPERIMENTAL RESEARCH OF WAVE ACTION ON THE GAS CONDENSATE SYSTEMS

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The results of physical modeling of patterns of filtering hydrocarbons mixtures methane-propane and methane-propane-butane on the experimental facility PLAST under the thermobaric conditions of the real gas condensate and oil stratum are shown. Series of experiments on the formation of condensate plug during the flowing of the two-phase mixture methane-n-butane, and on destroying the plug with wave action were conducted. The purpose of the experiments was to specify the mathematical model, based on equations of two-phase liquid state and hydrodynamic flow. A mixture, containing 75% volume of methane, at a temperature of 286 K, filtered through the experimental area. Results of the experiments showed the possibility of the self-oscillations existence with a few tens of seconds oscillation periods. At the beginning of the experiment a mixture was in the supercritical region. During the experiment, under a pressure drop of 6 MPa in the experimental area, the formation of gas condensate plug was observed. Thereafter, periodic change of the output pressure with a 3 MPa amplitude and 70 second period during 300 seconds was made. As a result of wave action was the flow rate increasing for 35%. Experiments on filtering three-component mixture in order to establish typical flow rates and gas condensate plug formation times for methane-propane-butane mixtures were performed. The experimental re-

sults also showed the possibility of the self-oscillations existence with a few tens of seconds oscillation periods. On resonant wave action the flow rate increasing of methane-propane-butane mixtures was 210%. As a result of the conducted experiments, gas condensate plug formation times, and the periods of flow rate oscillations, depending on the concentration of methane in the mixture at the constant pressure drop in the experimental area, were determined. Work is supported by RFBR 10-08-00 595-a.

## MATHEMATICAL MODEL OF HYDROCARBON FLUIDS FILTRATION IN POROUS MEDIA

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The mathematical model of unsteady two-component two-phase filtration for three-dimensional geometry is presented. Two types of possible geometry are considered: polar and cylindrical with axial symmetry. Polar coordinate system allows to model the processes of mass transfer during filtration of a hydrocarbons mixture from a stratum to a well, taking account of the real geometry. In the cylindrical coordinate system the processes of hydrocarbons mixture filtration in the experimental apparatus are modeled, taking account of radial flows. A two-phase two-component system for isothermal conditions is considered. It is supposed that the condition of phase equilibrium is fulfilled and the pressures in the different phases are equal (characteristic times of phase transfers are much smaller than hydrodynamic times). The filtration equations (in the approximation of Darcy's) under the assumptions of chemical neutrality of the components are the mass balance equations for each component, written in divergence form for molar densities. Equations of state for gaseous and liquid phases are expressed in the terms of compressibility factors. It is assumed that the mixture is in a state of local thermodynamic equilibrium. The system of equations is supplemented with the boundary and initial conditions. The system of equations describes the space-time changes of pore pressure and concentration of components in the mixture. The numerical method for calculation of unsteady two-phase filtration processes of a hydrocarbons mixture in two-dimensional case is presented. The calculation of two-phase filtration processes of binary hydrocarbon mixtures with reference to the physical model [1] of gas-condensate stratum was carried out. A mathematical model is implemented by software package PLAST for calculation of processes of two-phase filtration of binary hydrocarbon mixtures in re-

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## **EFFECT OF SUPERHEATING ON STRUCTURE OF METHANE HYDRATE FROM MD SIMULATION**

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Gas hydrates are crystalline water-based inclusion compounds physically resembling ice [1]. Guest molecules such as CH<sub>4</sub>, Ar, CO<sub>2</sub> are trapped inside cavities of the hydrogen-bonded water network. Natural gas hydrates are classified into three structures: a cubic structure sI, a face-centered cubic structure sII and a hexagonal structure sH. The structure type is mainly determined by the size of guest molecules. Methane hydrate at normal conditions has a sI structure with a unit cell composed of six 5<sup>12</sup>6<sup>2</sup> and two 5<sup>12</sup> polyhedra with an O atom at each vertex and H atoms located at the edges.

First order phase transitions allow the formation of metastable states. Metastability of gas hydrates is considered in the context of applications [2]. A concept of the spinodal is introduced to denote the stability limit of homogeneous phase. The thermodynamic criterion of the spinodal is  $(\partial P/\partial \rho)_T = 0$ . However the thermodynamic spinodal can not be usually reached because of the kinetic instability caused by nucleation.

The kinetic stability boundary due to the homogeneous nucleation; the universal dependence of the kinetic stability boundary on the heating rate and the system volume; the effect of defects was determined for the sI structure. Dynamical structure factor was calculated to determine properties of superheated structure.

This work was financially supported by the Russian Foundation for Basic Research grants 09-08-01116 and 11-01-12131-ofi-m. Simulations were carried out using the computing cluster 'Lomonosov' of the Moscow State University and the MIPT-60 cluster of the Moscow Institute of Physics and Technology.

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## **SIMULATION OF PECULIARITIES OF THIN-FILM NANOSTRUCTURE FORMATION AND THEIR BEHAVIOR UNDER HEATING**

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Molecular dynamics simulation of nanostructure formation and their behavior under impulse heating is carried out. These structures are formed by self-rolling of nano-thickness bilayer crystal films. The interatomic interactions are described by potentials obtained by the embedded atom method. The influence of formation temperature and the degree of mismatch of the lattice parameters of layers of separated bilayer metal film and the substrate on the kinematical parameters of simulated nanostructures is investigated. The mechanical stability of non-closed nanostructures in contact with obstacle is studied. The calculation data are shown that simulated nanostructures can transform the supplied thermal energy into the mechanical oscillations of its free edges. The influence of heating rate and its duration, medium viscosity properties on kinematical characteristics of simulated nanostructures is investigated. The influence of mass, size and fixation of bilayer nanostructures on their kinematical characteristics when heated is studied. The efficiency estimation of thermal energy transformation, supplied to nanostructures, into mechanical oscillations of their free edges versus nanostructure configuration, chemical composition and rate of impulse heating is carried out. The atomic mechanisms responsible for the peculiarities of local atomic structure transformations in bilayer nanofilm under its detaching from the substrate as well as mechanism of thermal energy conversion into mechanical one by nanostructures are investigated.

The work is supported by RFBR (project No. 11-08-00817-a).



═══════════      **SHOCK WAVES.**      ═══════════  
**DETONATION. COMBUSTION**

**STRAIN RATE AND TEMPERATURE EFFECTS  
ON THE FLOW STRESS AND STRENGTH OF METALS  
AND ALLOYS UNDER SHOCK-WAVE LOADING**

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Some new and obtained earlier experimental data on the elastic precursor decay and rise times of plastic shock waves in several metals and alloys at normal and elevated temperatures are systematized. The data on precursor decay include last measurements at micron and submicron distances where realized shear stresses are comparable with their ultimate values. Results of measurements have been transformed into dependences of plastic strain rate on the shear stress. It has been found the precursor decay may occur in several regimes which are characterized by different decay rates. Anomalous growth of the Hugoniot elastic limit with heating correlates with a fast decay regime and is not observed when the decay is relatively slow. An analysis of the rise times of plastic shock waves shows by order of magnitude faster plastic strain rates at corresponding shear stresses than that at the HEL. Results of measurements of the resistance to high-rate fracture show gradual increase of the later with increasing rate of tension and approaching the ultimate strength in a picosecond time range. The spall strength usually decreases with heating although in less degree than the strength at low strain rates does. In general, the temperature dependences of the spall strength do not correlate with dependences of the yield stress that points on larger contribution of the fracture nucleation processes as compared to the void growth. Requirements to constitutive models for high-rate plastic deformation and fracture are formulated on the base of experimental observations.

# THE STRUCTURE OF THE SUPERELASTIC&PLASTIC SHOCK WAVE

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Last year we reported the observation of elastic (moving with the “elastic” velocity) shock waves with the pressure behind the wave up to several times greater than the Hugoniot elastic limit (superelastic shock wave). The motion of a shock wave and the subsequent plastic shock is correlated. [1, 2] Now we present the structure of a superelastic-plastic shock waves.

The initial elastic shock wave begins to form well before the maximum of compression wave on the front of melting. The pressure on the elastic shock wave at this time is close to the Hugoniot elastic limit (HEL, for aluminum the part of GPa). Then the elastic shock quickly passes the front of melting. Emerging plastic shock overtakes and pushes the emerging elastic one. The pressure in the metastable elastically compressed material behind the elastic shock rises to a value several times larger than HEL (in aluminum up to tens of GPa). In the area of decay of a metastable superelastic-compressed material, an additional acoustic wave arises, moving from plastic to elastic shock. In the advanced stage long time elastic shock moves with its “elastic” rate (taking into account the contribution of shear stresses under uniaxial compression) and plastic shock moves almost simultaneously it, behind in time order of the decay of a metastable elastically compressed state of matter.

This work was supported by the RAS program “Thermophysics and mechanics of extreme energy action and physics of highly compressed matter” and RFBR grant 10–02–00434–a.

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# HIGH-RATE DISLOCATION PLASTICITY AND SHOCK WAVES ATTENUATION IN METALS

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In this work we develop the theoretical approach for high-rate dislocation plasticity proposed in [1–3]. Plastic strain rate is found out through the dislocations sliding. Equations for kinetics and motion of dislocations contain pseudo-relativistic terms. In papers [1–3] a good prediction for elastic precursor form and height has been obtained for a number of metals (copper, aluminum, iron, titanium), but the unloading wave form was not so good predicted in comparison with experimental data. As opposed to [1–3], more complex kinetic equations are used here, which take into account mobile and immobile dislocations. This complication of the model allows describing of structure of the plastic shock wave front, the unloading wave and the plastic shock wave attenuation in metal. The model equations and results of simulation and testing are presented. The parameters of the model are fitted to experimental data and presented for several metals. This work was financially supported by the Ministry of Education and Science of Russia.

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## MOLECULAR DYNAMIC STUDY OF PLASTICITY UNDER SHOCK WAVE LOADING

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The mechanisms of the plastic deformation under shock compression of single crystalline *fcc* metals (Al, Cu) and ceramics (sapphire Al<sub>2</sub>O<sub>3</sub>) are considered by means of molecular dynamic simulations. The structure of

defects formed after the shock front is analysed. The growth rates and critical stresses required for nucleation and multiplication of defects are estimated.

Both homogeneous and heterogeneous nucleation of dislocation loops with wide stacking fault area is observed in *fcc* metals. In some cases the propagation of the leading defect (which do not belong to a certain crystallographic slip plane) is observed. Later it splits into a number of regular dislocation loops and twins. In most cases the defects propagate slower than the shock wave front resulting in a lag between the fronts of elastic and plastic deformation.

Homogeneous nucleation and growth of rhombohedral twins are observed in single crystal sapphire. A fast mechanism of plastic deformation is revealed under shock-wave loading of sapphire with microcrack. Rhombohedral twins nucleate and grow as a result of a two stage process. At the first stage the formation of a new type of linear defect takes place in the shock wave front, which is initiated at the surface of the microcrack. At the second stage the rhombohedral twins grow from the primary linear defects and combine with each other. The results are confirmed by first principles calculations.

## INTERNATIONAL SHOCK-WAVE DATABASE

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In this work, we announce the start of a new project: International Shock-Wave data base (ISWdb). Shock-wave and related dynamic material response data serve for calibrating, validating, and improving material models over very broad regions of the pressure–temperature–density phase space. As a follow-on to our current on-line database, the ISWdb will include approximately 20000 experimental points on shock compression, adiabatic expansion, measurements of sound velocities behind the shock front and free-surface-velocity profiles for more than 650 substances that we previously collected. The ISWdb project objectives are: (i) to develop a database on thermodynamic and mechanical properties of materials under conditions of shock-wave and other dynamic loadings, selected related quantities of interest, and the meta-data that describes the provenance of the measurements and material models; and (ii) to make this database

available internationally through the Internet, in an interactive form. The development and operation of the ISWdb will be guided by an advisory committee. The database will be installed on two mirrored web-servers, one in Russia and the other in USA. The database will provide access to original experimental data on shock compression, non-shock dynamic loadings, isentropic expansion, measurements of sound speed in the Hugoniot state, and time-dependent free-surface or window-interface velocity profiles. Users will be able to search the information in the database and obtain the experimental points in tabular or plain text formats directly via the Internet using common browsers. It will also be possible to plot the experimental points for comparison with different approximations and results of equation-of-state calculations. The user will be able to present the results of calculations in text or graphical forms and compare them with any experimental data available in the database. Our goal is to make the ISWdb a useful tool for the shock-wave community. This talk is intended to solicit your feedback and interest in submitting your experimental results to the ISWdb, as well as present an overview of the project.

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**SOUND VELOCITY IN SHOCK-COMPRESSED  
POLYTETRAFLUORETHYLENE IN STRESS RANGE  
1.5–45 GPa**

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The results of measurements of sound velocity in polytetrafluorethylene in the interval of shock compression stresses  $\sigma_{xx} \approx 1.5\text{--}45$  GPa using manganine gauges are presented. The results of measurements of longitudinal sound velocity were obtained by method of overtaking and oncoming unloading. Experimental points were split into two ranges. In each range, dependence  $C_l(u)$  was described linearly:  $C_l = 2.82 + 1.96u$ , at  $0.28 < u < 2.1$  km/s;  $C_l = 5.65 + 0.64u$ , at  $2.1 < u < 3$  km/s. Extrapolation of experimental dependence  $C_l(u)$  to zero gives much higher value  $C_l$ , than that was obtained by ultra sound method. Such behavior is typical for other polymers. Error of current measurements is assessed as 5–8% ( $2\sigma$ ).

## SHOCK COMPRESSION OF DOUBLE WALLED CARBON NANOTUBES

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Recent experiments in a diamond anvil cell (DAC) 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 shock-wave compression with the use of recovery assemblies of planar geometry. In the different shock wave experiments the maximal pressure was ramped to a certain level (14, 19, 26 and 36 GPa) with a new CNT sample but always from the same source batch. 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. Remarkably, there are indications that the largest diameter CNTs were destroyed (RBM signal disappeared) by application of the highest shock contrary to the behavior of DWNTs at comparable static pressures in DAC. The work was supported by the Swedish Institute (00906–2009) and RFBR.

## ALUMINUM–FULLERENE COMPOSITES SYNTHESIZED BY HIGH-PRESSURE TORSION

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Aluminum–fullerene composites were produced using severe plastic deformation (SPD) method through high-pressure torsion (HPT) at room temperature under pressure of 4 GPa. Al ASD-8 and C<sub>60</sub> powders were mechanically mixed and compacted prior to subjection to HPT procedure. Mass fraction of fullerene in the composites was 10–30%. In addition, sep-

arate reference specimens were made from pure Al and pure C<sub>60</sub>, only. The specimens was characterized by X-ray diffraction, scanning probe and electron microscopy and Raman spectroscopy. An apparent grain size of the Al crystals in the composites decreases with increase of the strain level during the SPD. Fullerene molecules retained their cage structure after exposure to the extreme stress during the SPD; the major fraction of the fullerene transformed into dimers coexisting with remaining C<sub>60</sub> monomers; in certain parts of the sample even an admixture of C<sub>60</sub> oligomers (short chains) was detected. The work was supported by the Swedish Institute (00906–2009) and RFBR.

## HUGONIOT ELASTIC LIMIT AND SPALL STRENGTH OF ITTRYA-DOPPED TETRAGONAL ZIRCONIA

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Specimens of the ceramic based on zirconia partially stabilized by yttrium oxide of the 97 mol % ZrO<sub>2</sub> + 3 mol % Y<sub>2</sub>O<sub>3</sub> composition were fabricated. The densities of the specimens were 5.79 and 6.01 g·cm<sup>-3</sup>. 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 in the ceramic increases. The same trend was observed in the specimens, recovered after stepwise shock compression up to 36 and 52 GPa. Recording of the profiles of the free surface velocity of the specimens during shock compression allowed us to determine the Hugoniot elastic limit ( $\sigma_{\text{HEL}}$ ), as well as spall strength of the material ( $\sigma_{\text{SP}}$ ) versus maximal shock pressure  $P_{\text{MAX}}$ . As for the high-density ceramic,  $\sigma_{\text{HEL}}$ =15.1 GPa,  $\sigma_{\text{SP}}$ =1.3 GPa (at  $P_{\text{MAX}}$ =7.9 GPa),  $\sigma_{\text{SP}}$ =0.8 GPa (at  $P_{\text{MAX}}$ =13.7 GPa),  $\sigma_{\text{SP}}$ =1.1 GPa (at  $P_{\text{MAX}}$ =20.9 GPa). As for the low-density ceramic,  $\sigma_{\text{HEL}}$ =9.1 GPa,  $\sigma_{\text{SP}}$ =1.3 GPa (at  $P_{\text{MAX}}$ =8.1 GPa),  $\sigma_{\text{SP}}$ =0.6 GPa (at  $P_{\text{MAX}}$ =14.2 GPa). The work was supported by The State Atomic Energy Corporation ROSATOM.

# WIDE-RANGE CONSTITUTIVE MODELLING OF MULTISCALE PLASTICITY AND DAMAGE-FAILURE TRANSITION UNDER SHOCK WAVE LOADING

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A physically based model in the range of strain rates  $10^3$ – $10^9$   $s^{-1}$  is desirable because the responses of metals are intimately related to the underlying microstructure. This treatment is valid for applied stresses below the mechanical threshold, which translates to rates of deformation below  $10^5$   $s^{-1}$ . Constitutive models of metals have been constructed specifically for the shock loading regime and it was assumed that all microstructural processes have saturated above a critical strain rate ( $\sim 10^5$   $s^{-1}$ ) and the effective plastic strain was used as a state variable that is somewhat unsatisfactory. Comparative analysis of PTW-models and original model allowed us to establish the link of hardening mechanisms, yield stresses under thermo-activation flow and nonlinearity of thermodynamic potential, the explanation of the singularity of transition to the self-similar (structured steady-state) and overdriven shock wave fronts. Constitutive equations with seven material parameters provided the description of material responses in the ranges of strain rates  $10^3$ – $10^{10}$   $s^{-1}$  without variation of thermodynamic potential. The model links the mechanisms of structural relaxation with the multiscale kinetics in mesodefekt, the mechanisms of plastic flow and damage-failure transitions. The definition of material parameters using the data of the SHPB test coupled with infrared technique for the estimation of dissipated and stored energy and the plate impact test coupled with VISAR pull back velocity recording and the following structural study of recovered specimens. Infrared scanning of dynamically loaded specimens revealed high variation of the part of dissipated (and consequently stored) energy depending on the metals and the load intensity. Structural study of recovered specimens subject to the plate impact test was carried out using 3D New View profilometry and AFM data to estimate the scaling properties of defect induced roughness in the bulk of specimens. The peculiarity of proposed model in the comparison with wide-range PTW model is the universality of statistically based thermodynamic potential in mentioned range of strain rates and essentially less number of material parameters. Experimental verification of wide-range constitutive model was obtained using the data of original experiments on dynamic and shock wave loading (in the recovery conditions) of poly-



crystalline vanadium and the following study of defect structure formation using New View and atomic force microscopy data.

## SPATIAL AND TEMPORAL SCALING OF BRITTLE FRAGMENTATION

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The dynamic fragmentation was studied in the impact experiments with quartz cylindrical rods [1] using a gas gun. Impact leads to the formation of fracture surfaces, which produce an intensive light emission (mechanoluminescence or fractoluminescence). Fused quartz rod samples were 10 mm diameter and 100 mm long. In order to exclude discrepancies caused by variations of contact between sample and steel flyer a buffer of the same material as sample was used. Contact surfaces of the buffer and the sample were polished. Sample was encapsulated in plastic tube 45 mm diameter. PMTs were placed on the opposing sides of the tube at the distance 50 mm from the sample end. Mechanoluminescence was in form of impulses with typical rise time 2–5 ns and fall time 5–50 ns. It was found that the impulse rate was not decreases monotonically but there was some kind of bursts or avalanches and fragmentation process time is 3–4 orders longer than acoustic time (time needed for compression wave to travel along the specimen).

We suppose that there could be some kind of temporal scaling related to the self-organized criticality (SOC) [2]. In order to check this assumption distribution of time intervals between luminescence impulses was investigated. We found that distribution of intervals is different at the beginning of fragmentation (10% of the total amount of events). At the beginning distribution is close to exponential but for the rest there is a power law distribution.

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## **FRACTURE AND HIGH-STRAIN RATE DEFORMATION OF MAGNESIUM AND ALUMINIUM ALLOYS UNDER DYNAMIC LOADINGS**

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The influence of strain rate and nano-structured surface layers on the mechanical behavior of magnesium and aluminium alloys were studied under dynamic tension and compression loads. Tests under tension at high strain rates were performed using a VHS-50/40-20 Instron servo-hydraulic machine. A drop weight testing machine and a Split Hopkinson Pressure Bar (SHPB) were used for dynamic compression tests. The nano-structured surface layers on the specimens were created by surface mechanical attrition treatment at elevated temperatures. Under quasi-static loading nano-structured surface layers increase ductility of a magnesium alloy compared to initial material. Failure of the alloys occurs by shear failure under approximately 45° of inclination. Similar failure behavior was observed under dynamic loading. Shear bands and shear crack nucleation and growth were observed by high-speed photography. Examination of fracture surfaces in the specimens show increasing of fractal dimensions under dynamic loadings. Under dynamic loading specimens of material with nano-structured layers display a notable decrease in ductility compared to the initial material, where at quasi-static loadings ductility and compressive strength increased.

## **COMPUTER SIMULATION OF DEFORMATION AND DAMAGES IN CERAMIC COMPOSITE MATERIALS UNDER PULSE LOADINGS**

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The prediction of mechanical behavior ceramic composites under pulse loadings is the complicated problem owing to insufficient knowledge about laws of structure evolution and nucleation and accumulation of damages. Computer simulation of mechanical behavior of ceramic composites at single and repeated pulse influences of submicrosecond duration are presented

in the given work. The model of the structured representative volume of ultrafine-grained ceramics composites was developed using the data of microscopic researches. Deformation and damage of structured representative volumes of some ceramic composites on meso-scale level were simulated under pulse loadings having amplitudes near several GPa. The critical fracture stress on meso-scale level depends not only on relative volumes of voids and strengthened phases, but also sizes of corresponding structure elements. It was shown that the isolated micro- and meso-scale cracks can be generated in ceramic composites at pulse amplitude less than the Hugoniot elastic limit. In the studied ceramic composites the critical failure stress in spall zone is changed nonmonotonically with growth of the volume concentration of strengthened phases.

## DEFORMATION AND FRACTURE OF CONSTRUCTIONAL STEELS WITH HVOF COVERING AT DYNAMIC LOADS

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In work influence of the shock-wave load on behavior of a steel substrate with a covering is investigated. The two-layer covering is made by a method of a high-velocity oxygene fuel thermal spray process (method HVOF). The first, external layer represents a mix of 13 percents of Co and 87 percents of alloy WC, thickness 250 microns. The second, the inside layer consists of alloy NiAl, thickness 205 microns and with maintenance 95 percents of Ni. The shock-wave loading is initiated by a steel plate and compact steel projectile with initial speed of 400 km/s.

For formation of a steady covering a powder with average diameter of particles 14 microns by means of a gas stream are transferred on a detail. Particles possess high kinetic energy which at blow about a substrate turns to the thermal. Modeling of dynamic loading is spent by a method of finite elements in three-dimensional statement. For the description of behavior of materials of coverings of a barrier it is used elastic-plastic model with the equation of a condition considering factors of a shock adiabatic curve. For the description of a material of the projectile and a substrate the equation of a condition in the form of Mi-Gruneisen is used.

# STUDY OF THE INTERACTION OF HIGH VELOCITY PROJECTILES WITH TARGETS IN A WIDE RANGE OF ANGLES OF NUTATION

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The results obtained in the experimental study and numerical simulation of high velocity interaction of rod projectiles with targets at various angles of nutation. Experiments were carried out on the ballistic stands at velocities of throwing of projectiles up to 2 km per sec. In the numerical simulation of shock interaction processes used physical and mathematical model that describes the elastically compressible plastic medium with the development and evolution of micro-damage under dynamic loads.

Nutation angle the projectile at the targets detected by X-ray pulse orthogonal shooting and was calculated from the developed techniques. We obtain spatial position of the projectile at a target in the initial moment of the collision using X-ray stand. In the experiments it was recorded depth of craters, the size of the zone of deformation and fracture in the targets, the size and shape of projectiles after the interaction. In the experiment it were used cylindrical rods of aluminum alloys, steel and tungsten alloys. Targets were plates of various alloys of aluminum and steel. Parametric studies of the depth of penetration depending on the thick steel target of varying hardness of steel for cylinders of diameter 6.7 mm and a length of 134 mm were performed.

It was performed mathematical modeling of the interaction of high velocity projectiles with targets in three-dimensional formulation. In the calculations of shock interaction model is used of damaged environments, characterized by the presence of micro cavities (pores, cracks). Modeling of damage was performed using a kinetic model of the destruction of the active type, which determines the growth of micro cracks, continuously changing the properties of the material and cause stress relaxation. The pressure in the intact material is a function of specific volume, specific internal energy, specific volume of cracks in the whole range of loading conditions was determined using the equation of state of Mi-Grüneisen.

Conducted a physical and numerical modeling of damage to targets and constructed the distribution of the temperature and specific volume of cracks in the plane of symmetry of the target. It is shown that the most significant deformation observed in a narrow range of target thickness and temperature distribution practically the same as the distribution of specific

energy of shear deformations. This work was supported by RFBR: code numbers is 10-08-00398.

## INVESTIGATION OF SHOCK WAVE EFFECTS IN TWO LAYERED TARGET UNDER IMPACT LOADING

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It is investigated a problem of the normal and nonsymmetrical contact interaction of a deformable cylinder with two layered target with regard to the changes in the development of injury in case of contact between layers. Discussed are the peculiarities of the dynamics of the process at various distances between the layers of the plate. The degree of damage is determined by medium specific volume of cracks. The system of equations describing the unsteady adiabatic motion of a compressible medium with the development and accumulation of micro damage consists of the equations of continuity, momentum, energy, changes in the specific volume of cracks. It is considered the problem of interaction between the projectile of cylindrical shape with a composite plate made of two layers of different materials, separated at the initial time interval. To solve this problem we used the method of finite elements. The paper presents the estimated timing diagram illustrating the process of punching cylinder plate made of two layers with a thickness of 5 mm each, the distance between which is 3 mm. The velocity at the beginning of the contact amounted to 2500 m per sec. Analysis shows that the destruction of the upper and the lower layer of the plate are happening to different mechanisms. For the upper layer of the plate determining factor is knocking out the disc, diameter of which only slightly exceeds the diameter of the projectile. Complete separation of the disc ends after the merger of the centers of destruction, extending from the front and rear surface of the layer. Calculations show that the ejection of the disc is accompanied by significant release of energy due to intense shearing in the upper half of the first layer of the plate, leading to local heating of the material in this area, accompanied by a decrease of the strength properties. The destruction of the second layer of the plate, which is almost through the whole process of interaction works in tension, is due to the development of cracks that occurred initially near the symmetry axis of the rear surface by penetrating particles. Therefore, the destruction of the second layer of the plate requires more energy expenditure compared to the first, which is one of the reasons for the effectiveness

of two-layer structures. It is shown that during the interaction of particles with two-layer targets kinetic energy transferred to them by the particle is less than in the case of interaction with the monolithic plate. With the growing gap between the layers in the overall energy balance of the share of the internal energy composite plates increases.

## COMPARATIVE STUDY OF THE DESTRUCTION OF POLYMETHYLMETHACRYLATE BY THE HIGH-SPEED IMPACT AND BY THE IMPULSE LASER INFLUENCE

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The comparative study of the destruction of polymethacrylate (PMMA) by the high-speed impact and by the impulse laser influence has been given.

The dependencies of the dimensionless depth of penetration,  $h/D$ , of the projectile made of polyethylene and of laser impulse into the target made of polymethacrylate are plotted in this research on the basis of the data of experimental paper [1]. The velocity of the projectile in high-speed tests varied from 0.8 to 4.8 km/s, while the energy of impulses in both types of the dynamic loading lied in ranges of 500–13200 J.

The mechanism of the destruction of PMMA in case of impulse laser irradiation has been proposed, that explains the absence of zones of axial and radial tensile stresses, even at a distance 0.5 cm from the front surface of the target and also clarifies the appearance of the rear spall, which was not found in the experiments and calculation of high-speed impacts [2].

The main conclusion of the research is following: the use of laser impulses is more effective for creating the conditions for the spall fracture in comparison with the high-speed impact, although it has been assumed that the general scheme of development of hydrodynamic processes remained the same in both cases.

So, we have shown in this study that the mechanisms of crater formation and of destruction in case of applied pulse shock destructions differ much.

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## LASER SUPPORTED DETONATION IN A CORE OF SILICA-BASED OPTICAL FIBER

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In our experiments previous work [1] a laser damage wave propagating with a velocity around 3 km/s was detected. This wave was supported by radiation of Q-switched Nd:YAG laser (1.064  $\mu\text{m}$ ). A fiber core has a diameter of several microns and consisted of silica with small addition of  $\text{GeO}_2$ . By analyzing micrographs of the phenomenon with high spatial-temporal resolution we are noticing that it is a new self-containing process localized in a fiber core and propagating more than 100 initial own diameters during laser pulse. We have referred it to laser supported (driven) detonation (LSD) wave. According to our estimation the maximum temperature in the wave was  $\sim 10^4$  K and the highest laser-heating rate of the core material  $K_T$  was  $5.4 \cdot 10^{11}$  K/s in these experiments. As a result, a pressure in the LSD wave reached  $\sim 10$  GPa. Under these conditions the core glass should be compressed and compacted by shock wave. A compaction lead to the appearance of second (slow) shock wave in flyer plate experiments just above the elastic limit [2]. It is accompanied by changes in glass network, in particular, increasing the number of overcoordinated silicon atoms. Rigid structure domains are formed around these silicon atoms. Apparently when “rigid clusters” form a rigid network (rigidity percolation) breaking and rebounding of chemical bonds dramatically increase [3]. After the onset of LSD we observed a threefold decrease of laser plasma brightness. This may be explained due to self-trapped exciton (STE) absorption of visible radiation from the laser plasma because of energy states of STE changed under relaxation of Si-O bond [4]. Therefore STEs would be excited in  $T_1$  state in the shock wave front. And a subsequent ionization of the exited STEs apparently is necessary to generate of free electrons, which are responsible for laser heating of  $\text{SiO}_2$  at 1.064  $\mu\text{m}$  [5].

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## QUANTUM PHENOMENA IN INITIATION OF DETONATION WAVES OF CONDENSATION

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A new physical phenomenon, namely, the initiation of a detonation wave in the case of the release of the carbon vapor condensation energy was recently discovered in [1–3]. A necessary condition of the appearance of this detonation wave is that supersaturated vapor is formed immediately behind the shock wave front as a result of the fast decay of volatile carbon containing molecules. The features of the kinetics of the initiation of detonation condensation waves in carbon suboxide and acetylene have been experimentally studied at high pressures near the low temperature limits. It was shown that at temperature decrease below 1700–1600 K Arrhenius dependence of induction time of detonation formation flattens, defining essential decrease in effective energy of activation of the given process. The role of quantum effects in the observed phenomenon and corresponding expansion of detonation limits has been analyzed. Quantum corrections to the endothermic reaction rates, which are caused by an increase in the high energy tails of the momentum distribution functions at high pressures due to the manifestation of the uncertainty principle for the energy of colliding particles at a high collision frequency, have been quantitatively estimated. It has been shown that experimentally observed deviations in Arrhenius dependences of the induction time of the initiation of detonation condensation waves are well described by the proposed quantum corrections.

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## DETONATION CHARACTERISTICS OF BTF

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Recent advances in the equipment of elementary particle accelerator have resulted in new contactless techniques for investigation into the explosion processes. These techniques are based on dynamic transillumination of objects with high-energy beams of various nature. Due to the large penetrability of the applied radiation and high spatial and time resolution it is possible to produce high-quality shadowgraphs of flow under study, restore the inner distribution of parameters of objects by means of tomographic methods and measure diffraction (small-angle) distribution. Relying on the X-ray measurements, we have determined the detonation flow parameters for Benzotrifuroxan (BTF) charges. We have derived the parametric equation of state for explosion products in the density range of 500 to 2500 kg/m<sup>3</sup>. Measurement of small-angle SR scattering has allowed us to determine the dynamics of condensed carbon nanoparticle sizes at detonation of BTF.

## RESEARCH OF RDX DETONATION IN A NONIDEAL REGIME

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Velocity of a detonation of high explosive (HE) charge in a ideal regime  $D_{as}$  can be expressed as a function of a velocity of detonation with bulk density  $D_{bp}$ , of a charge density  $\rho$  and of some factor  $M_{as}$ :  $D_{as}(\rho) = D_{bp} + M_{as}(\rho - 1)$ . Velocity of a detonation of HE charge in a nonideal regime can be expressed as a function of the velocity at ideal detonation regime  $D_{as}$ , of charge diameter  $d$  and of some factor  $K$ :  $D(d) = D_{as}(1 - K/d)$ . On the basis of our experimental data we have constructed dependences of velocity of a detonation versus RDX density  $D = D(\rho)$  for charges with different diameters and have determined empirical dependence of factors  $M$  and  $K$  from the diameter and from the density of HE charge, accordingly. These dependences have linear form and are characterized by different derivatives

$M(d_i) = \Delta D(d_i)/\Delta\rho$ . Dependences with the greater derivative ( $M2 > M1$ ) is connected with charges which have biggest diameters ( $d2 > d1$ ). These dependences allowed us to study three data types. The first type gives that a detonation velocity at the bulk RDX density of a charge does not depend on its diameter:  $D(1 \text{ g/cm}^3) \neq D(d)$  at  $d > 10$  mm. On the basis of the data of the second type we have found dependence  $D(d)$  in form  $D(d) = D_{as}(1 - K/d)$  in which we have determined values of velocity of ideal detonation  $D_{as}$  for any RDX density. Besides we have found, that the factor K (mm) depends on RDX density as  $K = 3.1(1 - 1/\rho)$ . The resulting dependence of velocity of nonideal detonation vs the diameter and the RDX density of a charge has a form  $D(\rho, d) = D_{as}(1 - 3.1(1 - 1/\rho)/d)$ . On the basis of the data of the third type we have found dependence  $M(d)$  in a form  $M = M_{as}(1 - A/d)$  in which we have determined that a velocity derivative  $M_{as}$  has value  $3.9 \text{ (km/s)/(g/cm}^3\text{)}$  in dependence of velocity of ideal detonation versus RDX density. Besides, we have found that the factor A has value 4.2 mm. The resulting dependence of velocity of nonideal detonation vs diameter and RDX density of the charge has a form  $D(\rho, d) = 6.08 + 3.9(1 - 4.2/d)(\rho - 1)$ . This dependence is valid for the charges with the densities of  $1 \text{ g/cm}^3$  and more and with the diameters of 10 mm and more. 3D-dimensional graphic constructions of both variants of dependence  $D = D(\rho, d)$  have shown their full mutual identity and similarity with the experimental data.

## EXPERIMENTAL STUDY OF THE STRUCTURE OF MILLED DIAMOND-CONTAINING PARTICLES OBTAINED BY THE DETONATION METHOD

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The detonation-produced diamond-containing material (DCM) was mechanically milled using KM-1 and AGO-2S mills. Experimental spectra of infrared (IR) absorption, Raman-scattering, and X-Ray diffraction patterns (XRD) were obtained for the treated DCM samples. Comparison of the Raman and IR spectra for the KM-1 milled samples led us to conclude that the surface of DCM particles was not uniform. Mechanical milling in AGO-2S destroyed the particles. Experiments showed that the mechanical force destroyed the non-diamond part and initiated some irreversible physical and chemical changes in the particles. The destruction

of diamond grains was the consequence of these irreversible changes. The dipole momentum of the DCM particle, as follows from the experiments, was caused by the presence of polar fragments of molecules. The constant dipole momentum of the particles facilitated the aggregation. A model of a structurally inhomogeneous DCM particle was proposed.

## ON INSTABILITY OF CONVERGING SHOCK WAVES OF POLYGONAL FORM

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The effectiveness of converging shock waves as a means of creating high energy density near the focus, among other factors depends on the development of hydrodynamic instability of the shock wave, leading to limitation of cumulation. Two factors that affect the development of hydrodynamic instability of a converging shock wave are the subject of the present study: the influence of strong symmetric perturbations and influence of the thermodynamic properties of matter. In literature it was suggested that converging process becomes more stable if the shock wave is subjected to strong symmetric perturbations. The perturbations results in formation of symmetric polygonal shock which reshapes repeatedly in the process of collapse. It was shown previously [1] that the shock waves of symmetric polygonal form provide unlimited cumulation with characteristics that correspond to cumulation in a cylindrical shock wave. The converging shock waves of this kind were proposed to be stable with respect to small violations of symmetry [2]. In the present work this problem is treated numerically. The technique of integration of the 2D Euler equations on moving (contracting) grid is used. The polygonal shock waves are found to be unstable with respect to symmetry perturbations of special form with an angular period  $\pi$ . Transition to regular reflections and termination of the pressure growth at finite distances from the focus was observed. With the use of hard-sphere model (equation of state of Carnahan-Starling) it is shown that the thermodynamic non-ideality associated with the repulsion of particles (hard spheres) leads to a significant increase in the degree of cumulation achieved. Conclusion is based on calculations of the instability for different values of packing fraction  $\eta$  in the initial (pre-shock) state in the range  $0 < \eta < 1/3$ .

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**ANALYTICAL DETERMINATION OF BOUNDARIES  
OF EXISTENCE OF TRIPLE SHOCK WAVE  
CONFIGURATION WITH A NEGATIVE ANGLE  
OF REFLECTION IN STEADY SUPERSONIC FLOW**

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This work is a continuation of the investigation of intersection of shock waves [1], which predicted the existence of a new kind of reflection in a supersonic flow—the irregular reflection with a negative reflected angle, in addition to the known types of reflection: the regular and the irregular reflection with positive reflection angle. In all papers and textbooks three shock configuration is represented only with a positive angle of reflection [2]. However one can expect a new type of configuration with a negative angle of reflection for real gases, when physic-chemical transformations arise behind strong shock waves, the adiabatic index  $\gamma$  decreases, and the compressibility of gas greatly increases.

The boundaries of regions with negative angle of reflection have been defined in this paper. A series of calculations have been performed using the analytical method of shock polars. The freestream Mach number range from 3 to 15, ratio of specific heats  $\gamma$  varied from 1.05 to 1.66, angles of incidence of the shock wave  $\omega_1$  range from 0 to 90°. Calculations have been made for the effective values of the adiabatic index, which describes the full range of possible parameters of the gas.

It has been shown that the adiabatic index  $\gamma \geq 1.4$ , there are only two kinds of reflection: the regular and irregular with a positive angle of reflection. We have found that at high Mach numbers and low values of the adiabatic index, the reflected wave must settle beneath of the line of flow, ie in a steady stream, except for certain configurations (regular and irregular reflection) there must be a new—an irregular configuration with a negative angle of reflection.

Flow parameters: the angle of incidence  $\omega_1$ , Mach number and ratio of specific heats  $\gamma$ , where the reflection angle becomes negative have been given.

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## NUMERICAL INVESTIGATIONS OF DEVELOPING OF SHOCK WAVES IN A SHOCK TUBE WITH A FINITE TIME OF DIAPHRAGM OPENING

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One of the key issues in nuclear power is the definition of the ignition delays of mixtures of hydrogen with air. They are calculated theoretically and determined experimentally in shock tubes. It turns out that in some areas the temperature difference between the experimental values from theoretical are extremely high and up to several orders of magnitude [1]. There is an assumption that these deviations are due to the fact that in experiments temperature behind the shock wave is not correctly determined. Due to the finite time of diaphragm opening the stationary shock wave is formed not immediately, but at a distance. Moreover, the temperature behind the shock wave is not constant along the length of the heated region. The formation of a shock wave in a shock tube with a gradual disclosure (opening) of the diaphragm is investigated numerically in the present work. A one-dimensional calculation is performed on a Lagrangian grid for implicit numerical scheme, using three iterations at each time step. To stabilize the numerical solution of artificial viscosity is used, which consisted of a combination of linear and quadratic viscosity. To account for the variable of the pipe and valve opening process, the homogeneous difference scheme is modified in three coordinates that contain these features, where the changes were introduced to the equations of flows of gas-dynamic parameters. The area of the valve opening time is varied linearly. Such the law is taken on the basis of experimental studies of high-speed valve for shock tube [2]. These studies are conducted in a tube, where the high and low pressure chambers camera have the same cross section, as well as in the case of different sections.

As a result of the calculation systematic data have been obtained on the location of shock waves and profiles behind them for the testing in a

shock tube, when there is hydrogen in the high-pressure chamber and air in the low pressure chamber in dependence on the pressure drop across the diaphragm and the ratio of a cross-section high and low pressure chambers.

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## A NEW TYPE OF TRIPLE CONFIGURATION IN A STEADY SUPERSONIC FLOW

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This work is a continuation of research which identified the boundaries of existence of a new kind of triple configuration with negative angle of reflection [1]. The new type of reflection has been obtained in this paper with numerical studies.

The software STAR-CCM v. 5.02 has been used for the study, designed for the numerical solution of problems in continuum mechanics. The program incorporated the method of averaging the Navier-Stokes equations (RANS—Reynolds-averaged Navier-Stokes equations) [2]. To close the system of equations Spalart–Allmaras turbulence model [3] is applied for the emergence of new functions that characterize the turbulent stresses.

The reflection from a plane of symmetry of shock waves generated by the two wedges placed in a supersonic flow was used as an adopted model. Calculation has been carried out for verification of program, which received a good agreement with experiment.

The main attention has been paid to the calculation of the existence of a negative angle of reflection. Research in this area is greatly complicated because of the effect on the wave flow the pattern and geometric characteristics of the environment downstream. Numerical experiments have shown that if the calculations are carried out, for example, for the flow parameters  $M = 10$  and  $\gamma = 1.3$ , then because of the impact of rarefaction fan at the rear edge of the wedge with the incident wave, it becomes curved, and its reflection occurs in a regular manner, three shock configuration does not arise at all. This shows that one must specifically select the geometry of the flow, in

order to get the new configuration with a negative angle of reflection.

The authors have suggested including to the geometrical system two small wedges downstream. As a result the height of the Mach wave increased. With the above-described method the new configuration of the irregular reflection with a negative angle has been obtained.

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## **TURBULENCE DIAGNOSTICS IN FLOWS WITH SHOCKS BY DIGITAL BOS, SPECKLE AND TALBOT TECHNIQUES**

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Modern optical techniques based on computer-aided image pattern analysis extends the methods of flow visualization and diagnostics and allows the quantitative derivation of a two dimensional map of deflection angle experienced by light passing through a flowfield under study [1]. Such line-in-sight diagnostics with the use of digital images analyses becomes especially attractive when turning to the statistical analysis of the complex flow pattern in turbulent flows with shock waves [2].

In present paper three optical line-in-sight methods, namely, Background Oriented Schlieren, BOS, Laser Speckle Photography, LSP, and, Talbot interferometry, TI, have been applied to on-line turbulence structure monitoring.

It has been shown that digital versions of BOS, LSP, and TI are effective methods for monitoring and quantitative visualization of temporal and spatial changes in the correlation scales of turbid media variations.

Abel, Radon and Erbeck-Merzkirch integral transforms have been used for local microstructure scales evaluation [3]. The use of Erbeck-Merzkirch integral transform allows to perform tomography reconstruction and to determine 2D maps of micro- and macroscales of turbulence.

The results obtained point to a high spatial and temporal resolution of the methods and to the possibility of real-time operation mode realiza-

tion. It has been shown that noise filtering is an important part of the images processing. Sensitivity, temporal and spatial resolution of these three methods are analysed and compared.

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## **THE APPLICATION OF THE TALBOT EFFECT FOR THE MEASUREMENTS OF DISPERSION CHARACTERISTIC OF REFRACTIVE INDEX IN AXISYMMETRIC METHANE JET FLAME**

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In the recent years, the possibilities of the numerical modeling in the field of the turbulent combustion have increased significantly. However, there are a lot of processes which have a direct relation to practical systems, and are required to further verification of simulation models. Today the main working tools for experimental studies of combustion processes are optical diagnostic methods. The major comparison of modeling and experiments are based on the time-averaged statistics of velocity, temperature and concentration of the mixture components.

The aim of this work is adaptation of the method based on the Talbot effect for the diagnostic of turbulent combustion processes with high-frequency fluctuations and small-scale structures.

The paper describes the experimental system based on the Talbot effect which is used for measurements of average concentrations of major species in a methane-air reacting axisymmetric jet. In the paper the principles of Talbot effect based technique for analysis of optical inhomogenities are discussed and the optical scheme for the technique is represented. The relations between experimental Talbot images and characteristics of the investigated flow are indicated. The possibility of using the dispersion



characteristics of the refractive index for calculation of major species concentration in methane-air mixture is shown. It is shown that the method of time-averaged Talbot images provides measurements with high spatial resolution of the dispersion characteristics of the refractive index in the flow field of an axisymmetric jet of methane. On the bases of these data, the concentrations of the major components of reacting methane-air mixture can be calculated. The results of diagnostic of reacting methane-air jet by means of averaged Talbot images at 6 wavelengths are presented.

## DDT IN SUBCRITICAL DIAMETER CHANNEL ATTAINABILITY CRITERION

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It is well known, that the distance of detonation wave formation from the flame front in gaseous mixture in channel strongly depends on channel diameter. To reduce the run-up distance it is reasonable to initiate DDT process in narrow channel of about or sub critical diameter.

It is well known that stationary detonation in channel is impossible when the channel diameter less than critical value equal to  $L/3$ , where  $L$  is detonation cell. Critical value of deflagration to detonation transition in straight cylindrical channel occurs to be bigger than one for stationary detonation. The main reason that prevents deflagration to detonation transition in narrow channel is high heat losses into channel walls comparatively to energy of burning [1] at the initial stage of flame propagation. Due to this stationary regime of slow flame propagation establishes and transition to detonation becomes impossible.

In present work deflagration to detonation transition in subcritical channel was achieved because of using for-chamber placed at the entrance of detonation channel. Influence of for-chamber parameters on DDT process in channel with subcritical diameter was investigated experimentally for hydrogen-air and methane-oxygen mixtures in terms of additional energy emitting in for-chamber as a result of additional mixture burning. Mechanisms of for-chamber influence on DDT process was investigated experimentally.

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**EXPERIMENTAL STUDY OF THE VISCOUS  
ENTRAINMENT MECHANISM IN TURBULENT JETS  
WITH TOMO-PIV**

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We test experimentally predictions, arising from the entrainment mechanism due to the small-scale nibbling process, in a turbulent round submerged liquid jet. The model postulates the existence of a thin shear layer at the turbulent/non-turbulent interface and relates its propagation velocity with the mean flow properties across the interface. This is an extension of several previous works. The first difference is that we detect the turbulent/non-turbulent interface directly from the vorticity field. Secondly, we present results for a range of Reynolds numbers  $Re = (3.5-15) \cdot 10^3$ . For that, we set up a careful experiment, zooming in at the fluctuating boundary of the jet. With the Tomographic Particle Image Velocimetry (Tomo-PIV), we measure the full velocity gradient tensor in multiple points inside the flow with a sufficient spatial resolution. We confirm the predictions from conditional flow statistics across the interface.

**ACOUSTIC INFLUENCE  
ON METHANE DIFFUSION FLAME**

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One of the major scientific and technological problems associated with the combustion process is the study of the flame acceleration or deceleration effects. These effects can be used to control of combustion speed and toxic combustion products in many applications. The main effect caused by combustion zone turbulization is an increase of the flame area surface. That leads to intensification in thermal conductivity and diffusion processes which is the main combustion processes. In turn this leads to enhancement of nonlinear processes in the combustion front, the further

development of turbulence and a significant acceleration of the flame. One of the natural ways of the hydrodynamic effect on the flame region is the acoustic field influence.

In the case of diffusion combustion, when the fuel gas expires in ambient air, the sound waves interact with fire both directly and implicitly. Indirect interaction occurs in the not yet reacted gas flow region regardless of the flame characteristics and may affect the flow stability [1]. The result of acoustic influence on the diffusion flame is many effects, such as soot suppression [2] and reduction of the nitrogen oxides concentration [3] in the combustion products, the increase in fuel efficiency [4]. All the above phenomena are resonant, that is occurring at certain frequencies of acoustic field. Response to determination of resonant frequency requires a greater amount of experimental data.

In this paper the acoustic disturbances influence on the diffusion flame was experimentally studied. The frequency dependence of nitrogen oxides and soot concentrations in combustion products was obtained. The bifurcating phenomenon in lifted diffusion flame was observed.

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## **AUTO-IGNITION OF HYDROGEN-AIR MIXTURES AT INTERMEDIATE TEMPERATURES IN RAPID COMPRESSION MACHINE**

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Hydrogen auto-ignition has been extensively studied during last 50 years in shock tubes under conditions of relatively low pressures and high temperatures. These data are in good coincidence between different investigators and with the homogeneous gas phase kinetic predictions. But at intermediate temperatures (below 1100 K) the so-called strong ignition process, changes on a mild ignition. Experiments show that induction times in this regime are very sensitive to different kind perturbations by the presence of contaminants, fluid dynamic effects and catalysis from

particles or surface materials. It can lead to significant reductions of measured induction times in the mild ignition regime by as much as several orders of magnitude. Therefore, experimental data at these conditions are rather discrepant and differ from model predictions that do not account for these perturbations. It is clear that these data can not be directly used for kinetics mechanism validation and updating. Additional knowledge is needed to correct experimental data interpretation and to make adequate assumptions. In order to get deeper understanding of mild hydrogen auto-ignition phenomenon the present study was conducted by means of rapid compression machine. New data were compared with previously obtained shock tube data for the same mixture compounds and densities. High-speed digital image has been additionally used to investigate the effect of different perturbations on induction time. The narrow tracks, probably produced by burning particles, were registered on images. It can explain a big scattering of obtained new experimental data if assume that these particles initiate auto-ignition of hydrogen-air mixture.

**AN EXPERIMENTAL INVESTIGATION  
OF SELF-IGNITION OF HYDROGEN IMPULSE JET  
DISCHARGED UNDER HIGH PRESSURE INTO AIR**

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The ignition of gas mixture occurs not only in preliminary mixed mixtures: the ignition of gases is possible at the contact surface of fuel and oxidizer [1]. A necessary concentration ratio between the components is ensured due to the diffusion and intermixing [2]. In this case the ignition of gases are determined not only by the thermodynamic parameters of components, but also by the rate of mixing, by rate of the expansion of contact surface, and consequently, by the rate of the achievement of the concentration limits of ignition [3].

One of such cases is self-ignition of hydrogen or another combustible gas at a pulse discharge from a vessel under high pressure into air. Required temperatures for self-ignition were reached due to heating the air by a shock wave which appears as a result of the non-stationary discharge of hydrogen from the high pressure vessel.

The aim in the present work was an experimental investigation of influence of hydrogen jet formation on self-ignition of hydrogen at pulse discharged from a high pressure chamber into an open channel of low pres-

sure. Initial pressure of hydrogen was varied from 3 to 14 MPa.

Formation of a shock wave flow structure at the pulse discharge of compressed hydrogen was studied, and ignition delays of hydrogen were determined. It was shown that intermixing of hydrogen jetted into channel with air has turbulent character and can not be neglected at the process of ignition. Ignition delays for non-premixed hydrogen with air were compared with preliminary mixed ones.

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## TRANSDETONATION REGIMES OF COMBUSTION IN MOVING METHANE-AIR MIXTURES

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One of the most popular fuel is methane or nature gas. In spite of the mixture of natural gas with air is characterized by the greatest detonation cell size among the hydrocarbons (270–350 mm [1]) and energy of direct initiation 9–88 MJ [2] a detonation regime of combustion can be used in a perspective detonation engine and combustion device. On the other hand, for using the detonation of natural gas in the devices of crushing, stamping or combustion of withdrawals it is necessary for the energy of ignition to be not more then several joules.

The presence of flow in the mixture can substantially accelerate a flame front [3]. The decrease of predetonation distance and the deflagration-to-detonation transition can prove to be possible with the energies, much smaller energies of direct initiation.

Another essential factor, which is capable to considerably reduce predetonation distance, is the presence of obstacles in the channel [4].

The goal of the investigation was the decrease of pre-detonation distance in methane-air mixtures with using of ring obstacles during inter-chamber mixing of components in the flow with the speed of 30–40 m/s.

Narrow channel with a parameter of  $\lambda/D = 3$  was used, where  $\lambda$  – width of detonation cell, and  $D$  – chamber diameter.

The separate supply of methane and air into the combustion chamber and the chamber mixing of gases were used. The optimal arrangement of ring obstacles along the axis of the detonation combustion chamber was determined. Diameters of obstacle orifices, its quantity and locations were determined, at which maximum of the speed of flame front was reached.

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## ON CHARACTERISTICS OF HYDROGEN AND HYDROGEN-METHANE MIXTURES SELF-IGNITION AT PULSE DISCHARGE INTO CHANNEL

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Characteristics of the diffusion ignition of hydrogen were experimentally studied at a pulse discharge into a channel, filled with air. The ignition of hydrogen occurred on the contact surface of hydrogen discharged into air. The necessary temperature of self-ignition was reached due to heating of air by the shock wave, which appears as a result of the pulse discharge of hydrogen from the high pressure chamber [1]. However, the duration of diaphragm rupture may have the critical effect on the ignition of hydrogen [2], since in this case a system of shock waves appears and regions with thermodynamic parameters exceeding the one-dimensional calculation can be formed [3].

In this work was studied the influence of diaphragm rupture duration on ignition delay of hydrogen. For 5 mm diameter channel were meshured rupture durations of the diaphragms ranged from 10 to 100  $\mu\text{s}$  depending on the material of diaphragm (copper, brass, steel and aluminum), width of channel and initial pressure. After all it was investigated influence of additive (methane) on ignition delay.

For rectangular  $10 \times 10$  mm channel high speed visualisation of appearance and propagation processes of diffusion flame in channel and its discharge into opened area. The way of diaphragm rupture influence on position of original ignition hearth, and so on subsequent propagation of contact surface and flame front. It was experimentally defined position of original ignition hearth in a number of experiments [4].

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## **SPECIFIC IMPULSE OF NOZZLE OF THE PULSE ENGINE**

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In the last century it was proved that continuous stationary detonation combustion is impossible to achieve. The fact necessitates that for an energy converter pulsed operation mode should be used. It leads to the concept of a Pulse Detonation Engine (PDE) [1].

Operation of a PDE relies on pressure-rise detonation combustion rather than constant-pressure deflagration currently used in conventional engines, for instance, piston engines, gas turbine engines, and scramjets. High thermal efficiency of PDE attracts researchers to apply it as a new technology for aerospace propulsion.

The possibility of using of nozzle for increase of a thrust of a pulse detonation engine and influence of its geometrical parameters were investigated by experimentally and numerically [2]. The influence of nozzle configuration on the thrust was studied experimentally in present work in a periodic regime. In present work thrust was created due to the periodic

combustion of stoichiometric hydrogen-air mixture. The main problem was to define specific impulse. It was determined experimentally.

Then it was determined by theoretic methods and matching with results of other researchers. Analysis has shown, that experiment gave single-order smaller impulse than theoretical calculation.

It was shown that dependence of specific impulse on diameter of the nozzle has extreme.

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## **SHOCK WAVE REFLECTION FROM OBSTACLE MADE OF EASILY DESTRUCTIBLE GRANULAR MATERIAL**

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Nowadays explosions pose a serious risk. It is known that one of the most damaging factors of an explosion is shock wave. Therefore, the weakening of the shock wave is an actual problem, aimed at protecting people from terrorist attacks and industrial explosions. Especially dangerous are reflected shock waves, as they have a higher intensity.

There are several approaches to the creation of the material, which reduces the intensity of the shock wave. In different works it was 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 [4].

In this paper the shock wave reflection from obstacle made of easily destructible granular material was investigated. The technique of studying of shock wave attenuation after reflection from easily destructible obstacle was developed. The dependence of the attenuation of the shock wave on the thickness of the barriers and the distance from the wall to the obstacle was determined. Also dependence of the attenuation of the shock wave from her profile was studied.



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## SHOCK WAVE INTERACTION IN GAS WITH SOLID BODIES

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Supersonic movement of airspace apparatus can take place at conditions of presence of particles in atmosphere. The work purpose is to estimate thermal and mechanical action of shock waves on bodies of the various forms. The retarding force acting reverse to stream velocity on bodies of various form, is defined by the characteristic area of the body, density of the fluid and a square of speed of the object relative to the fluid. The proportionality factor connecting the drag force and above-noted values is dimensionless and is called drag coefficient  $k$ . It is known that  $k$  is determined by the similarity law. The similarity law claims that the drag coefficients of two geometrically similar bodies equally placed in the stream will be identical, if Reynolds's numbers of these two bodies are equal.

It is carried out two-dimensional hydrodynamic modeling of the shock wave flow in a pipe around of bodies of various forms in the range of Reynolds's numbers  $3.5 \cdot 10^3 - 3.0 \cdot 10^5$ . In our calculations it is shown only the moments of time, which exceed relaxation time. Shock wave was caused by instant remove of the diaphragm that had separated the gas with different pressures. Gas was considered as ideal. The body was located on such removal from a diaphragm, that it was generated the area of a constant current, in which pressure was almost constant behind the shock wave front. Besides, the body was far from the front of the shock wave to avoid non-stationary perturbations of the stream. Pipe and body walls were adiabatic. The pipe diameter was much larger then diameters of bodies in order to walls of the pipe do not influence a settling down of a stationary flow. It was modeled the flow around

bodies of cylindrical, conic and spherical form. The body axes were parallel to the stream. Tops of cones were oriented both in the stream direction, and against the stream direction. It was studied interaction of a shock wave with the bodies of the specified forms. It was used the stress tensor written in cylindrical system of coordinates [1] in order to calculate the drag force effecting from the shock wave on bodies. Calculated values are analyzed with respect to matching to the law of similarity [2].

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## **A CONCEPTUAL MODEL FOR CARBON NANOPARTICLE FORMATION IN SHOCK WAVE PYROLYSIS PROCESSES**

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A great number of works is devoted to investigation of processes of formation of the condensed carbon from a gas phase in shock waves. An extensive review of this information is presented in [1]. The accepted notions about the regularities of growth of carbon nanoparticles are that temperature dependence of volume fraction of the condensed phase has the bell-shaped form with a maximum around 1600–1800 K, and the rate of particle formation exponentially increases with temperature. Hereby the questions: (1) Why the quantity of the condensed carbon decreases at  $T > 1800$  K, in spite of fall of stability of all hydrocarbons, while a carbon should be in the condensed state up to 3000–3500 K? And (2) why the rate of condensation grows sharply, though this process has no energy of activation? – remain without the answer.

In the given work a new conceptual model of formation of carbon nanoparticles in the shock waves, based on the last data about temperature dependence of the final size of formed particles [1] and the sharp rise of their refractive index at the change of particle size from 2–5 nm to 10–15 nm [2] is proposed. These results have allowed to base the model on two new, physically grounded statements – the volume fraction of the condensed carbon remains constant from the temperatures of complete decomposition of initial molecules (1600–1800 K) up to the temperatures of evaporation of carbon nanoparticles (3000–

3500 K), and the rate of surface growth of nanoparticles is determined by frequency of vapor–particles collisions, i.e. slightly grows with the temperature as  $T^{1/2}$ . Thus, the number density of nuclei of condensation, defined by a ratio of the rate of formation of active carbon-bearing radicals to the rate of quenching of non-stable particles, exponentially grows with temperature, reflecting the rise of the rate of dissociation of initial molecules.

The proposed physically transparent model allows explaining all observable regularities of carbon particles growth, including reduction of the final particle size with the temperature rise and corresponding decrease of time of particle formation.

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## **SINGULARITY OF CHARGING OF FORMING CARBON NANOPARTICLE IN SHOCK-HEATED PLASMA IN THE PRESENCE OF CHLORINE ATOMS**

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In the present paper we continue the study of charged carbon nanoparticles formed at pyrolysis of various carbon-containing substances behind shock waves [1, 2]. In this paper we have presented experimental results and computer simulation of the electrical charging of carbon nanoparticles produced during the pyrolysis of  $\text{CCl}_4$  in shock waves. To account for the influence of free chlorine on electron concentration several series of experiments in a mixture containing 1%  $\text{Cl}_2$  in argon were carried out. It was shown that the excess of chlorine atoms in the mixture leads to a significant decrease in the concentration of electrons in the gas-particle systems, and to reduction of the concentration of charged nanoparticles. In the presence of condensed carbon nanoparticles produced during the pyrolysis  $\text{CCl}_4$ , for about 10 microseconds after the arrival of the front of the reflected shock wave free electron concentration is reduced by two orders of magnitude, while the concentration of positive ions changes slightly. The equilibrium concentration of free electrons in the presence of particles in the mixture is much smaller than in the same gas without particles. The time required for

the equilibrium charge distribution in a gas-carbon nanoparticles mixture at pressures of 6–30 bar decreases from 400 to 100 ms when the temperature rises from 2000 to 3600 K. 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.

This work is supported by Russian Academy of Sciences and RFBR (Project N 11–08–00873–a).

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## **TEMPERATURE AND SIZE MEASUREMENTS OF CARBON PARTICLES FORMED IN BENZENE AND ACETYLENE PYROLYSIS BEHIND SHOCK WAVES**

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The temperature of reactive mixture may change in pyrolysis of various hydrocarbons due to heat loss at the initial molecules decomposition and the heat release of condensed carbon particles formation [1]. The heat balance of the pyrolysis of various hydrocarbons is crucial for many applications such as initiation or inhibition of ignition, combustion and detonation as well as for the calculation of heat transfer in real combustors. This work is devoted to the measurements of temperature, particle size and volume fraction of condensed phase formed in benzene and acetylene pyrolysis to get the data for kinetic modeling of carbon particles formation. Several series of experiments with the mixtures of 3% C<sub>2</sub>H<sub>2</sub> and 2% C<sub>6</sub>H<sub>6</sub> diluted in Ar in the temperature range of 1800–2400 K and pressure range of 6–8.5 bar were carried out behind reflected shock waves in a conventional diaphragm-type shock tube with the inner diameter of 50 mm. Laser light extinction and laser-induced incandescence were applied simultaneously for observation of optical density of condensed phase and carbon particle sizes. At the same time the temperature time profiles were measured by emission-absorption spectroscopy method in visible range at the wavelength of 589 nm. Considerable temperature drop relatively to initial temperature behind the shock wave front was observed during benzene py-

rolysis. The reasonable explanation of this effect is excess energy required to break bonds of benzene molecules over the energy released during the condensed particle formation on this stage of the process. No significant deviation from calculated temperature behind reflected shock wave was observed during acetylene pyrolysis. Seemingly energy release by carbon particle formation compensates heat loss by acetylene molecules decomposition under investigated conditions. The results of kinetic modeling of initial stages of benzene and acetylene pyrolysis are discussed.

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## **STATISTICAL ANALYSIS OF LASER-INDUCED INCANDESCENCE MEASUREMENTS OF CARBON PARTICLE PROPERTIES IN PYROLYSIS FLAMES**

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The method of laser-induced incandescence (LII) is one of the most modern methods of diagnosis of nanoparticles formed in the gas phase. The method is based on a pulsed laser heating of nanoparticles and the registration of the time profile of the emerging radiation. Typically, measurements of particle radiation are 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.

The method of LII is widely used for the diagnostics of soot particles formed in combustion processes [1]. Under these conditions, particles are formed very quickly and method allows registering the soot with the well-known properties, which makes the problem of analyzing and interpreting the data quite easy.

In our study, the method of LII was first applied to study the process of particle formation in pyrolysis flames, where the growth of particles can be well resolved along the height of the flame [2]. Such arrangement of experiments presents the new opportunities to study the young carbon particles with poorly known properties. For the other hand, the serious problems with the analysis of the data due to a sharp decrease in the intensity of the LII signal and a significant increase in the scatter of the recorded signals have to be solved. Therefore, 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.

This paper presents the results of LII measurements of the size and volume fraction of carbon particles in pyrolysis flames of  $C_2H_2$  and  $C_3O_2$  obtained with the developed programs.

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## HIGH TEMPERATURE DECAY OF HYDROCARBONS BEHIND THE REFLECTED SHOCK WAVES AND DYNAMICS OF SOOT FORMATION

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The soot is one of the main products formed due to pyrolysis of hydrocarbons. That is why the carbon particles formation problem attracts great interest of researchers worldwide both numerically [1, 2] and experimentally [2, 3]. The goal of the present study was to investigate the soot formation, structure and yield at the pyrolysis of acetylene, propane and methane within a wide range of post-shock temperatures and moderate pressures.

Shock tubes are frequently used for pyrolysis studies. The  $50 \times 50$  mm square diaphragmless shock tube of 4.8 m long was applied for this investigation. Hydrocarbon gaseous mixtures such as 2%  $C_2H_2$  + 98% Ar, 4%  $C_3H_8$  + 96% Ar and 4%  $CH_4$  + 96% Ar were used in these studies.

The gas emission was registered at two wavelengths and recorded by photomultipliers. A He-Ne laser and a fast Si-photodiode were used for extinction measurements. Soot carbonaceous particles that deposited on the end wall of the shock tube were explored by electron microscope.

It was shown that the induction time  $\tau$  of soot condensation reduced with temperature increase according to Arrhenius law  $1/\tau \sim \exp(-E_{ind}/RT)$ . The dependence of soot yield vs. temperature behind

the reflected shock wave for  $C_2H_2/Ar$  mixture has a typical “bell-shaped” form with a maximum in a range of temperatures 1900–2200 K as in [3]. However the soot yield curve for the propane-argon mixture has a maximum at 2400–2800 K and unlike acetylene its profile is essentially broadened. Analysis of soot microphotos and electron photographs has not revealed the presence of fullerenes and nanotubes in sample materials. It was found that for all investigated ranges of temperatures and pressures the fine-dispersed graphite is the main component of the soot structure.

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## **EXPERIMENTAL AND NUMERICAL STUDY OF ENERGY EXCHANGE OF HEAVY AND LIGHT MOLECULES NEAR THE SHOCK WAVE DENSITY GRADIENT**

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The work is carried out in the context of study of physical-chemical processes within the zone of translational relaxation of shock wave, propagating in gas mixture of molecules with high ratio of molecular masses. The experimental study of shock wave propagation in light gas with small admixture of heavy gas with mass ratio about 30 is carried out. Near the shock wave density gradient, the layer of charged particles is revealed. The concentration of charged particles and the cross-section of inelastic process resulting in ionization, are evaluated.

Using the direct simulation Monte Carlo method, the influence of cross-section value of collisions between heavy molecules on the distribution function of energy of pare collisions in the shock wave front is studied. It is revealed, that beginning from the certain threshold value, the increase of that cross-section by the factor of two results in the two-order of magnitude increase of the frequency of high-energy collisions near the density gradient. In this case the layer, where these high-energy collisions occure with the maximal probability, shifts towards the density gradient.

**SUPPRESSION OF COMBUSTION AND EXPLOSION  
OF HYDROGEN-AIR MIXTURES IN A LARGE VOLUME  
BY USING OF AKAM INHIBITOR**

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AKAM inhibitor is a mixture of three gases: propane, butane and propylene. It had been shown [1] that it is effective in suppression of explosions of hydrogen-air mixtures inside of cumulation devices. Inhibitor is added to the stoichiometric hydrogen-air mixture in amounts of 1.5–6%. Experiments were conducted with spherical gas charges 7 m<sup>3</sup> in size that initially had been bounded by compliant envelope. The mixture is initiated by energy 1–14500 J. The measurements of pressure in blast waves (waves with a short positive phase) at different distances from the point of initiation along the bar, at which the detection elements of diagnostic equipment were placed, were taken. Recorded was the glow of the gas inside the rubber envelope as well as after its destruction at the stage of the process evolution in a large explosion chamber 13Ya3, in which the reaction volume was placed. The conducted studies and calculations of detonation limits of gas mixtures by the rule of Le Chatelier showed that the AKAM inhibitor more effectively suppresses detonation and explosion of stoichiometric hydrogen-air mixtures than their ignition.

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**REGIMES OF CHEMICAL REACTION WAVE  
PROPAGATION INITIATED BY TEMPERATURE  
NON-UNIFORMITY FOR CHAIN-BRANCHING KINETICS**

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The paper discusses a classification of the propagation regimes of chemical reaction initiated by initial temperature non-uniformity for mixtures whose chemistry is governed by chain-branching kinetics. The purpose is to generalize the classical results of the paper [1], where the classification



of combustion regimes initiated by the temperature gradient has been obtained for a single-step kinetic model. The problem setup is a uniform initial conditions apart from a linear temperature gradient similar to that used in the previous studies for one-step reactions. To achieve comprehensive examination of such complex processes, that in addition are stiff dependent on initial conditions one has to use numerical approaches based on detailed mathematical models. In this paper we used full gasdynamic model with equations of state for real multicomponent mixture and detailed chemical kinetics scheme of nine equations were used. Different regimes of the reaction wave propagation are identified for the  $\text{H}_2/\text{O}_2$  and  $\text{H}_2$ -Air mixtures in wide range of initial pressures and temperatures depending on the steepness of the linear temperature gradient. The limits of the regimes depend upon the values of spontaneous wave speed and the characteristic velocities of the problem. Because of the difference in the induction time and time when the exothermic reaction starts the velocity of spontaneous wave in the early stage of the adiabatic explosion development for the chain-branching reaction is much less compared to the values obtained for a one-step model. This difference significantly affects the ignition and evolution of spontaneous combustion wave, especially below "crossover" temperatures. Because of this the regimes with the formation of shock waves and detonation wave occur for much shallower temperature gradients than predicted by a one-step model. The difference between a one-step model and a detailed chemical model is particularly large at lower pressures and for slowly reacting mixtures. Features of the chemical kinetics for other slow reactive mixtures, such as hydrocarbon-oxygen mixture may be qualitatively different. For example, kinetic model for isooctane and n-heptane includes cool flames so that the exothermic reaction can start at low temperatures during the induction phase.

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## TRANSIENT COMBUSTION IN CLOSED CHANNELS

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The flame acceleration in channels of different geometry, shock wave formation in the upstream flow, and transition from deflagration to detonation (DDT) in hydrogen-oxygen mixture are studied using two-dimensional high resolution simulations with a detailed chemical kinetic model. Re-

cently it was shown [1] that DDT occurs as a consequence of pressure increase in the reaction zone connected with the features of flame acceleration in channels with non-slip walls. Depending on the channel width and length the dynamics of flame acceleration and DDT can be different. For example, in thin channels [2] the exponential increase in flame speed is not bounded in time till DDT. For “short” channels the flame propagates in conditions of upwind flows generated behind compression waves and weak shocks generated by the flame and then reflected from the end-wall. Influence of the acoustic perturbations changes the evolution of the flame front propagating through the channel. In this case the perturbations begin affect the flame dynamics on the first stages and can even prevent sufficient flame acceleration and detonation formation. On the other hand there is approximately no sufficient impact on the flame dynamics in case when the perturbations begin affect the flame on the very final stage when the pressure pulse is already localized in the reaction zone. In the channels of moderate lengths the influence takes place on the stage when the pressure pulse is already emerges but it is not yet localized in the reaction zone. In such conditions the counter running perturbations can flow the pressure pulse out from the reaction zone and prevent detonation formation. However the stronger wave interacts with the flame after reflection from the back end-wall. Such interaction can trigger a new regime of flame acceleration and transition to detonation. One frequently uses channel with antechamber to study DDT. In this case combustion in the antechamber may become a source of compression waves affecting the flame front propagating in the channel. These waves may flow the pressure pulse out from the reaction zone, decelerate the flame front in the reflected flow and make it possible to ignite volumetric explosion ahead the flame front in the compressed and heated mixture.

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**PHENOMENON OF REDUCTION OF THE ENERGETIC  
MATERIAL BURNING RATE IN THE ELECTRIC FIELD:  
LEARNING TO SEE THE INVISIBLE**

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Propulsion are key point in the miniaturization of micro-satellites because such satellites would need very small and very accurate force to realize the stabilization and the large angle attitude maneuver. The level of thrust and the impulse precision required for micro-satellites maneuver cannot be reached with conventional propulsion systems. Improvement of representations regarding the combustion mechanisms of the energetic materials gives possibilities for development of new means and technologies for effective control by the parameters of the ignition and combustion processes. The lack of restart ability of the micro solid propellant thruster can be overcome by electro-thermal supporting of the temperature and electric conductivity of the liquid-viscous layer of the solid propellant. Recent experimental research, connected with study of burning of the composite solid propellants in the electric field, show that at level of pressure more than 3 MPa is observed reduction of the burning rate. For explanation of this phenomenon in the paper suggested new concept, connected with interaction of the electric field micro-structures in the burning zone. The electric field micro-structures generated in the heated-up liquid-viscous layer of burning energetic material gives the program for formation of the cellular-pulsating micro-structures in this layer, on the burning surface and over the burning surface of the energetic material. As show the experimental data, over the burning surface there are electric field micro-structures. In accordance with suggested concept, during interaction of the electromagnetic fields excited in the liquid-viscous layer and electro-magnetic fields of toroidal vortex micro-structures over the burning surface occurs displacement of burning zone from the burning surface. With increase of the pressure, the sizes of micro-structures in the liquid-viscous layer decrease and also the scale of vortex micro-structures over the burning surface decrease. Accordingly, with increase of the pressure the stability of the vortex micro-structures will be decreased. At destruction of the vortex micro-structures, occurs decrease of the heat flow onto the burning surface and the burning rate decrease. Actually, this phenomenon has some analogy with phenomenon of negative erosion. Also the role of the phenomenon of self-synchronization of the torch micro-structures pulsa-

tions and the electro-magnetic field micro-structures in reaction zones is discussed.

## **2-D TEMPERATURE FIELDS MEASURING SYSTEMS FOR SCIENTIFIC AND INDUSTRIAL APPLICATIONS**

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It is difficult to mention the area of technology or technical physics where it was not required to measure the temperature of solid, fluid or gaseous substances. In particular, the modern experimental thermophysics investigates various processes of thermal effects and consequently measuring of temperature in these experiments plays a vital part. In the modern industry and power engineering a plenty of new thermal processes proceeding at extreme state and at high temperatures also is implanted, e.g.: combustion of hydrocarbon fuel in aviation engines, heat exchange in nuclear reactors, thermal plasma spraying, rapid laser prototyping, laser welding, laser cutting, etc. It is obvious, that all these processes are characterized by three-dimensional temperature distribution which determines existent thermal processes and the concerned with them quantities (thermal tension, dimension change, etc.). Therefore in the specified applications a necessity for measuring temperature fields (instead of measuring in one point) occurs. For example, in microelectronics, at the control of thermal resistances of integrated circuits it is necessary to measure 2-D temperature fields for definition of the most heated area and for calculation of their thermal characteristics.

It is essential to note especially, that today there is a critical necessity for creation of the pyrometric system allowing investigating the dynamic processes of burning and mechanisms of formation  $\text{NO}_X$ , CO, a smoke on an outlet of aviation combustion engines by a non-invasive method. It is necessary for verification of models of the existent physicochemical processes in combustors and for optimization of designed new generation engines. One of the key problems is the registration of 2-D temperature fields by the non-invasive method in the given section on an outlet of a combustor.

Two systems for measuring temperature fields designed by authors are described, first is intended for measuring 2-D temperature fields in microelectronics. The second high-speed diagnostic system allows registering 2-D particles temperature fields in high-temperature heterogeneous jets

at thermal plasma spraying and at diagnostics of existent processes in combustors of aviation engines. The system allows to measure brightness temperature of the particles in one projection in real time. Designed systems demonstrate an opportunity of temperature fields measuring in high-temperature heterogeneous plasma jets and in microelectronics. Work was performed with the support of the RFFR (project 11-08-12117-ofi-m-2011).

**LASER WAKEFIELD ELECTRON ACCELERATION:  
ACHIEVEMENTS AND PERSPECTIVES**

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One of the promising applications of short intense laser pulses is the Laser Wake Field Accelerator (LWFA) of electrons. The idea to use the plasma wave excited by the laser for the electron acceleration was suggested by Tajima and Dawson more than thirty years ago, but real successful experiments on quasi-mono-energetic acceleration of electron bunches to GeV energies were realized during last few years only. The electric field strength in the relativistic plasma wave (with phase velocity close to the speed of light) can achieve huge values, a few orders of magnitude higher than that in conventional radio-frequency accelerators. The proof-of-principal experiments show that an ultra-high accelerating wakefield can be generated by available lasers in plasma and that this plasma wave can accelerate electrons to relativistic energies. It is shown that a long distance propagation of intense laser pulses and wakefield generation over many Rayleigh lengths (that is necessary for the regular electron acceleration to ultra-relativistic energies) are possible in preformed plasma channels and gas-filled capillary tubes. The progress and use of laser-plasma accelerators in many applications depends substantially on the possibility to provide extended quasi-monoenergetic acceleration of short electron bunches to high energies (see e.g. Ref. [1] and reference therein). One of the possible approaches to produce stable and controllable acceleration of electrons is based on the external injection of electron bunches into the wakefield generated in a moderately nonlinear regime by a short intense laser pulse propagating in guiding structures [2, 3]. Different schemes of the electron bunch injection into the LWFA and possible applications of the accelerated electron bunches are discussed.

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## IMPROVEMENT OF LASER CONTRAST IN EXPERIMENTS WITH HIGH-INTENSITY BEAMS

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Laser contrast is a crucial parameter in experiments with high-intensity high-energy pulses. For high intensities of the main pulse  $\gtrsim 10^{19}$  W/cm<sup>2</sup>, even high-contrast beams can produce plasma on the target surface and result in undesirable early smearing of the target due to long nanosecond prepulse action. In particular, dynamics of thin foils under the prepulse action is especially important for the laser ion acceleration technique and the promising target design. At the same time, a thin foil can be placed ahead of the target to shield it from the long laser prepulse. To analyze the multi-stage foil dynamics we use a wide-range two-temperature hydrodynamic model, which correctly describes the foil expansion starting from the normal solid density at room temperature. Simulations show that varying the foil thickness one can diminish the prepulse transmission through the foil material in several orders of magnitude and at the same time provide the total transparency of the foil plasma by the moment of the main high-intensity ultra-short laser pulse arrival. However the prepulse energy re-emission by the shielding foil can be sizable and result in undesirable early heating of the target placed behind the foil.

## THERMAL CONDUCTIVITY DUE TO s-s AND s-d ELECTRON INTERACTION IN NICKEL AT HIGH ELECTRON TEMPERATURES

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The essential feature of warm dense matter arising when ultrashort laser pulse acts on a metal target is a two-temperature state with hot electrons and cold crystalline lattice. Laser irradiation absorbed by a target

initially heats a target within thin irradiation attenuation depth. Then heat propagates into the bulk target dominantly via the electron thermal conductivity being accompanied by the electron-ion energy exchange. In such a manner a target heated layer is produced. Because of ultrashort laser pulse duration and high speed of electron heat transfer the heated layer is formed with practically unchanged volume of a target. Depth of this heated layer and later dynamics of a target expansion up to its ablation essentially depends upon the magnitude of electron thermal conductivity. For simple metals such as aluminum electron thermal conductivity coefficient was calculated in [1]. In transition metals (nickel as an example) there are two groups of electrons which affects the thermal conductivity caused by electrons. First of them are s-electrons with small effective mass, they have a high mobility and mainly contribute to the electron heat transfer. And the other group is d-electrons with much larger effective mass and as a consequence their mobility and contribution to the heat flow is much smaller than for s-electrons. But d-electrons cause effective scattering of s-electrons in addition to s-s-scattering. We calculate the electron thermal conductivity coefficient and effective frequencies of s-s and s-d interactions in nickel at the wide range of electron temperatures when the thermal excitation of both s- and d-electrons is significant.

The work is supported by the RAS program “Thermophysics and mechanics of extreme energy action and physics of highly compressed matter” and Russian Foundation for Basic Research, project 11–08–01116–a.

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## COMBINED MOLECULAR AND HYDRODYNAMIC MODELLING OF METALS IRRADIATED BY ULTRASHORT LASER PULSES

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A numerical modelling of interaction of femtosecond laser pulses with metals is performed. Two methods are used: (i) a two-temperature one-velocity hydrodynamic model [1] and (ii) a combined model, which is based on the molecular-dynamics simulation for ions and on the heat conduction equation solution for electrons (TTM-MD) [2]. These two models take into account electron-phonon coupling and electronic heat conductivity. Multi-



phase two-temperature equation of state of metals is used in both models, and the substance properties are described by EAM-potential in combined model. On one hand, the hydrodynamic model describes correctly laser absorption and the evolution of both electronic and ionic subsystems, but represents rather roughly substance disintegration processes. On the other hand, the combined TTM-MD model does not take into account electronic energy, but describes fragmentation accurately.

An improved model found on combined model is offered. This model takes to account laser absorption according to Helmholtz equation and electron heat transfer and electron-ion coupling dependence on density and temperature.

Results obtained by these different methods are being analysed here for nickel and aluminium.

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## MELTING OF METALS UNDER ULTRAFAST HEATING BY A FEMTOSECOND LASER PULSE

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Commonly, in order to solve the problem of heat transfer, the Stefan problem is used. The melting area is supposed to be infinitely thin. In the present work, we analyze the melting under ultrafast femtosecond laser pulse action on metals. Our computational model is based on the electron heat-transfer equation considering the electron-ion exchange and a multi-phase equation of state. We consider 3 variants: the Stefan problem with realistic heat capacity and heat of melting, the equilibrium melting with the finite melting zone, and the non-equilibrium melting with kinetics. The results of numerical simulations show that accounting of the melting kinetics diminishes the melting region in comparison with the equilibrium melting, but the melting zone width is non-negligible.

**PARTICULARITIES OF PROPERTIES OF MATTER  
IN THE FIELD OF NEGATIVE PRESSURES CREATED  
BY MEANS OF PICOSECOND LASER PULSE**

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The experimental studies of dynamic mechanical durability of aluminum, alloy AMg6M and polymethylmethacrilat at the influence on them of laser pulse with duration 70 ps are presented. In preceding experiences of authors duration of laser pulse was 2.5 ns. Using of more short pulses has allowed to realize in this study of strain rate above  $10^7$  1/s. Results of experiments have shown that, when increasing a strain rate spall strength of matter under investigation tend to their essential reducing with respect to the theoretical limit of toughness. It was established that behavior of matter in the field of negative pressures when using the laser influence depends in big degrees from history of dynamic pressure, comprising of itself much factors, amongst which vital importance has both amplitude, and shock wave pulse duration influencing on target.

**EXPERIMENTAL INVESTIGATION OF A QUANTUM  
YIELD OF A CHARACTERISTIC X-RAY RADIATION  
AT INTERACTION OF FEMTOSECOND S-POLARIZED  
LASER PULSES WITH NANOSTRUCTURED Cu TARGETS**

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The goal of experimental investigations was to measure an absolute yield of a characteristic X-ray radiation when the femtosecond s-polarized laser pulses with intensity  $\sim 10^{17}$  W/cm<sup>2</sup> interact with nanostructured Cu target and Cu foil without nanostructure on the surface.

Experiments were carried out at the multiterawatt femtosecond titan-sapphire laser system consisting of the seed oscillator, the stretcher, the regenerative and multipass amplifiers and the compressor. Laser system

generated pulses at the wavelength of 800 nm. The pulses had duration  $40 \pm 5$  fs, energy up to 250 mJ and repetition rate 10 Hz.

X-ray von Hamos spectrometer with the focusing mica crystal was used for registration of X-ray spectra radiation. As the detector of X-ray radiation CCD array (TCD 1304AP) was applied.

An absolute yield of X-ray characteristic  $K_{\alpha}$ -radiation for  $s$ -polarized laser pulses was investigated experimentally, depending on type of a target. There were two types of targets used for carrying out the experiments: Cu foils 8  $\mu\text{m}$  thick and a target with Cu nano-rods, consisting of about  $10^8$  rods/ $\text{cm}^2$ ; each rod was of 400–500 nm in diameter and approximately 1  $\mu\text{m}$  in height.

The experimental results indicated that the nanostructured targets can be used to increase the yield of characteristic X-ray radiation under action of high contrast femtosecond laser pulses at moderate intensities.

## **FAST RESPONSE TIME TEMPERATURE MEASUREMENTS AT PULSED LASER IRRADIATION OF DIFFERENT MATERIALS**

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Fast response of different materials to the heating by millisecond laser pulses has been studied by photoemission methods. Temperature measurements were carried out with time resolution 1  $\mu\text{s}$  in the range of 1200–2800 K under heating graphite, W, Si wafers and  $\text{SiO}_2/\text{Si}$  films.

Temperature measurement by the spectrometry of photoelectrons (photoemission method) is based on the dependence of the distribution of photoelectron energy due to extrinsic photoeffect on the energy distribution in the radiation spectrum. A thermometric substance is a photoelectron gas nearby the emitting surface. Temperature can be determined from cutoff voltage of current voltage (I-V) diagrams of photoelectron devices. We can use photomultiplier for photocurrent-normalized light flux [1] or measure photoelectron energy distribution in dependence on temperature [2].

The temperature measurements are based on the registration of a two-level oscillogram  $U(t)$  under modulation of the electron flux by negative relative to photocathode rectangular pulses. In each period of modulated signal the dependence  $k(t)$  is calculated from the level of this signal. In the processes under consideration temperature dynamics  $T(t)$  is determined by means of the calibration of  $T(k)$  realized with standard temperature radia-

tor. Modulation of photoelectron flux in near-cathode region of photomultiplier with frequency 1 mHz, allows us to carry out such measurements with time resolution 1  $\mu$ s.

The samples were irradiated by a Nd:glass quasinonspiking laser, generating 0.6 millisecond (FWHM) single pulses of radiation with  $\lambda = 1.06 \mu\text{m}$  at high homogeneity of the laser beam about 1 cm in diameter,

Our investigations have shown experimental possibilities of the photoemission method in diagnostics of laser-induced thermal processes. The data obtained characterize the heat action of millisecond laser pulses on some metals under irradiation in different conditions.

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## MATHEMATICAL MODELING OF THE FAST IGNITION OF THE ICF TARGETS

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The classic approach to initiate the fusion processes in the laser targets consists in the so called the “Spark Ignition”. But, we well know, that more effective way is an approach, connected with the “Fast Ignition”. In present work we consider the some examples of such a way, concluded in a “impact fusion” method. We analyzed the possibilities of the thermonuclear fuel ignition by the impact of a micro particle. The numerical investigations have determined the parameters of a target. The processes of an ignition origin are analyzed also.

## AB INITIO CALCULATIONS OF THE PARAMETERS OF THE ELECTRON-PHONON RELAXATION IN METALS WITH EXCITED ELECTRON SUBSYSTEM

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In the work we consider warm dense matter—the state between heated condensed matter and plasma. It may be generated in different ways: by strong short laser irradiation of metal, during the electrical explosion

of conductors, in the matter of cathode during heavy-current pulse discharge etc. For all general mechanisms of warm dense matter formation it is common that the two-temperature state is formed right after initial energy deposit. In this state the temperature of electron subsystem is significantly higher than the one of the ions. Actually, we can consider such systems as if all the energy absorbed during excitation was absorbed by the electron subsystem while lattice remained practically unaffected. The evolution of such states after energy deposit is determined by the rate of electron-phonon energy exchange and the electron and lattice heat capacities. Theoretical approaches, initially developed in the superconductivity physics, allow calculating these quantities using basic microscopic characteristics of matter such as electron and phonon densities of states.

We calculate the dependencies of densities of states and the electron-phonon coupling constant for Al, Ag, Au, Pt and W on the electron temperature in the range from 0 to 4 eV. It gives the values of the electron-phonon coupling factor, electron and lattice heat capacity in the same range of electronic temperatures. The electron DOS is calculated using VASP package [1], phonon DOS—using PHON utility [2] and the electron-phonon coupling constant is calculated with Quantum espresso distribution [3]. Obtained values are compared with the ones from the work [4] in which changes in densities of states weren't taken into account. The results show that for the electron temperatures higher than 1 eV considered quantities may change significantly and their values for ground state can not be applied to the description of the system with strongly superheated electrons. It is also shown that relaxation times for the two-temperature state may differ for an order of magnitude for different metals depending on their electronic structure and lattice properties.

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

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The interaction of ultra-short laser with metal result in the two-temperature ( $2T$ ) 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 coefficient. 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  $T_e$  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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1. Inogamov N. A., Petrov Yu. V. // JETP 2010. V.110. No. 3. P. 446.

## SPATIALLY RESOLVED RECONSTRUCTION OF LASER RADIATION SPECTRAL PROFILE BY NUMERICAL SIMULATION OF A DIFFRACTION PATTERNS

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The work is aimed to the development of diagnostic methods providing the parameters of intense laser radiation penetrating as in vacuum as in transparent but strongly non-linear media. In order to determine spectral parameters of a laser pulse it is suggested to analyze the diffraction patterns obtained in the interaction of investigated laser pulse with a

test object of well-known geometry. The code for numerical simulation of diffraction pattern is developed based on solving Helmholtz equation for set of weakly divergent flat waves. Aim is to find complex amplitude  $\bar{A}$  in plane  $z + \Delta z$  using known amplitude  $A$  in plane  $z$ . Solving is

$$\bar{A} = F \left[ F^{-1} [A] \exp \left( i \frac{k_x^2 + k_y^2}{2k} \Delta z \right) \right]. \quad (1)$$

where  $F[A]$  is Fourier transform Numerical simulation needs grid with steps  $\Delta x, \Delta y$  and coordinates  $i, j$ . Number of steps is  $N_x, N_y$ . In simulations the laser pulse was introduced as a plane wave with Gaussian time profile. The correspondence between experimental and modeled diffraction pattern has been achieved including the following parameters: number, period and visibility of diffraction fringes, related intensities of diffraction minimums and maximums, the position of the first diffraction fringe. The developing method was applied to analyze the patterns of femtosecond Ti:Sapph laser pulse diffracted at metal and plastic wires of 200 and 300 um diameter, respectively. The patterns were registered by LiF detector due to excitation of color F-centers. As a first result, the method demonstrated very high sensitivity to determine spectral width and central wavelength of the laser pulse. Also, it was proven the F-centers in LiF created due to single-photon (not multiphoton) excitation regime. The function of nonlinear response of LiF detector to the intensity of incident laser radiation was determined. Due to registered diffraction patterns have submicron spatial resolution, the proposed method provides the reconstruction of laser radiation parameters simultaneously in different areas of the laser beam.

## INTENSE X-RAY RADIATION OF Al HOLLOW ATOMS EXCITED BY PW LASER PULSES

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Laser pulses of Vulcan Petawatt facility of very high contrast and hundreds J of energy allowed interaction studies between the laser field and solid state at  $10^{20}$  W/cm<sup>2</sup>. The use of spherically bent crystal spectrometers provided the data in the spectral range from H-like Al Ly $\alpha$  to neutral Al K $\alpha$  lines with very high spectral resolution.

Intense emission of exotic spectral lines related to the transitions in Al hollow atoms were observed from Al targets. Specifically for 1.5  $\mu\text{m}$  thin foil target the hollow atom yield dominated the resonance line emission. It is suggested that the hollow atoms were predominantly excited by the impact of keV X-ray photons generated on the front surface of the target.

On the contrary, the spectra of aluminum foils buried in several microns of CH demonstrated lower K-shell emission and contained much weaker yield of hollow-atom lines. In this case the laser did not interact directly with aluminum matter, so most probably hollow atoms excited by fast electrons penetrating the target.

The mechanism of hollow atom excitation is still far from clear understanding. The obtained X-ray spectroscopic data evidently demands further studies and interpretation supported with plasma and atomic kinetics simulations.

## **LASER WAKE FIELD ACCELERATION OF AN ELECTRON BUNCH INJECTED IN FRONT OF A LASER PULSE GENERATING WAKE WAVE**

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A study is made of a promising method for injecting an electron bunch into an accelerating laser plasma system [1]. A bunch is injected ahead of the front of a laser pulse generating a wake wave and has a velocity lower than the pulse group velocity. It has been shown, that the effect of the initial energy spread of the injected bunch on its length and energy spread in the acceleration stage can be far more significant than the effect of its initial length. Nevertheless, wake waves, in which the region of overlap of the accelerating and focusing phases is large, can provide such trapping conditions for the bunch electrons, under which on a certain acceleration distance the effect of the initial nonmonoenergetic character of the bunch becomes very small. The energy spread of the electron bunch on optimal acceleration distance is minimized due to the fact that the portrait of the bunch in the phase plane rotates so that its projection onto the pulse axis becomes minimum [2]. It is found, that in such a way it is possible to receive compact electron bunches accelerated to energies in some GeV's, with a energy spread less of 1%.

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## **GENERATION OF STRONG MAGNETIC FIELDS BY COUNTERPROPAGATING MODERATE-INTENSITY LASER PULSES IN A LOW-DENSITY PLASMA**

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The generation of strong magnetic fields by counterpropagating moderate intensity laser pulses of different frequencies in a low-density plasma has been investigated. The generation of long-lived strong magnetic fields is attributed to small-scale plasma waves that are excited in the overlap region of the pulses under the action of their ponderomotive force at the difference frequency. It has been shown that the strongest magnetic fields are generated under resonance conditions such that the frequency difference between the laser pulses coincides with the plasma frequency. In this case, because of the frequency difference between the pulses, the magnetic field generated by them is more stronger than that generated in the interaction between two pulses of the same frequency but of different durations. The spatiotemporal distribution of quasistatic magnetic fields has been investigated, and it has been shown that the spatial scales on which the magnetic field strength decreases from its maximum value to zero are comparable to the sizes of the localization region of small-scale plasma waves. The pattern of the contour lines of the constant electric current has been calculated.

## **3D PIC SIMULATION OF INTERACTION OF ULTRASHORT LASER PULSES WITH SOLID TARGETS**

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Short high-intensity laser pulses are used in many applications, including generation of hot electrons from solid targets and subsequent X-rays generation. In particular, such experiments are carried out at GSI laser

facility PHELIX with solid metal targets. In the present work the acceleration of electrons is investigated by means of 1D and 3D Particle-in-cell code VLPL. Dynamics of the electron spectra, plasma density and electromagnetic fields in the process of laser-matter interaction is presented and analyzed. Obtained results will be used for the interpretation of real experiments.

## **ABSORPTION OF LASER RADIATION BY SOLUTION OF MAXWELL EQUATIONS FOR THE ENVELOPE OF ELECTROMAGNETIC WAVE**

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In applications dealing with the propagation and absorption of monochromatic electromagnetic radiation in inhomogeneous media, the following approach seems to be effective. It is based upon the solution of the Maxwell equations in a simplified form, stated for the envelope of an electromagnetic wave; the rapidly oscillating factor is neglected. In the present work the numerical solution of these equations is found similar the well-known finite-difference time domain (FDTD) procedure. The medium properties are described by density- and temperature-dependent complex dielectric permittivity, thus taking into account the dielectric or metallic character and inhomogeneity of matter. We consider 2- and 3-dimensional cases and present an algorithm for calculation of the laser energy absorption. We intend to apply this approach for 2 and 3-dimensional hydrodynamic simulation of laser-matter interaction.

## **STRONG FIELD MULTI PHONON EFFECTS IN INTERACTION OF HIGH ENERGY ELECTRONS WITH ORIENTED CRYSTALS**

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Oriented crystals provide strong electrostatic fields which can exceed the Schwinger critical field during the process of penetration of super relativistic electrons through such crystals being measured in the rest frame of

the electron [1]. The value of invariant Schwinger parameter  $\chi$  depends on the type of the crystal and on the electron energy such that at energies of about 150 GeV it becomes  $\chi \sim 1$  and electromagnetic strong field effects become significant [2–5].

Intense hard photon radiation process in interaction of ultra relativistic electrons with energies up to few TeV with silicon, germanium and diamond single crystals oriented along  $[110]_c$  direction to electron beam has been studied by the method of cascade equations. Analytical solutions has been presented for the distribution function of electrons over their energy losses. Special attention is paid to multiphoton processes of emission of relativistic electrons in amorphous media and in oriented crystals.

Another aspect of the problem is the study of the multiphoton nature of radiation. Since all photons emitted by an electron arrive at a detector almost simultaneously and are indistinguishable, information on the initial one-photon radiation cross sections cannot be obtained from direct measurements. Nevertheless, we show that the probabilities of processes and distribution functions for measurable quantities can be calculated.

The experimental data for 150-GeV electrons in oriented crystals are thoroughly analyzed.

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## **APPLICATION OF OPTICAL PYROMETERS FOR INVESTIGATION OF GAS-ASSISTED LASER CUTTING**

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Investigations of the dynamics of the melt in the gasjet-assisted CO<sub>2</sub> laser cutting by pyrometer have been performed. Cutting trials were carried out with CO<sub>2</sub> laser (10.6 mkm, 1200 W) and ytterbium-doped fiber laser (1.07 mkm, 1800 W). The bar was used that consists of 4 two-color photo-diodes coupled by fiber-optic cables with lens optics for this purpose. Local brightness of metal melt has been measured precisely with

long dimension resolution about 0.1 mm and with time resolution as short as 0.03 ms. The results of data processing for steel plate 3, 6 mm and 10 mm thick are reported for different values of cutting speed and assisted gas pressure. The measurements brightness temperature and fluctuations of local brightness were conducted. Special attention in this project was given to frequency range of temperature fluctuation above frequency of melt overflight aiming on-line monitoring applications. It is shown early, that local fluctuations of  $T$  are related to local melt surface deformations due to unequal radiation absorption. Both region of turbulent pulsations, hydrodynamical turbulence and capillary-wave turbulence, were selected in measurements, thus noise spectrum of  $T$  fluctuations reflects turbulent surface deformation, caused by gas jet and capillary waves. It is shown that the method allows obtaining the data on melt movements in the process of laser cutting.

**INVESTIGATION OF AlO MOLECULES EMISSION  
FORMATION OBTAINED BY Al TARGET VAPORIZATION  
BY RADIATION OF PULSED CO<sub>2</sub>-LASER**

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Some target with Al (sapphire, pure Al plate, pressed Al powder) were vaporized by radiation of pulsed CO<sub>2</sub>-laser in various gaseous medium. The cloud of electron-excited AlO molecules formation dynamics was experimentally researched. It was found that AlO molecules emission ( $B^2\Sigma^+$  -  $X^2\Sigma^+$  transition) appears in two areas of space. It was showed that AlO molecules formation reasons are different. Also the space-time distribution of AlO cloud vibration temperature was derived.

# MECHANISM OF BREAKDOWN OF OPTICALLY TRANSPARENT DIELECTRICS BY LASER BEAMS

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Laser radiation of high intensity can lead to radiation breakdown of transparent solids. Destruction occurring in such environments by laser pulses, the most convenient to divide the devastation occurring in a perfectly clean environment, and the destruction caused by impurities [1]. Under this approach, we differentiate the improper threshold laser breakdown due to the destruction of the defects, impurities, inclusions, and the threshold of his own breakdown, defined extreme radiation resistance of a pure substance.

For beam breakdown of transparent solids by short laser pulses is a certain threshold of radiation damage dependence on pulse duration. Study of the nature of this dependence, helps to understand the mechanisms and patterns of laser breakdown.

This approach has been applied by us and for the analysis of the mechanisms of breakdown of ionic crystals in strong electric fields. Data on the breakdown threshold of nanosecond electrical pulses were taken from [2], the breakdown thresholds nanosecond and picosecond laser pulses— from [3], the thresholds of radiation damage by femtosecond laser pulses— from [4]. As shown by our experiments, the radiation resistance of alkali metal chlorides under the action of nanosecond laser pulses in good agreement with the breakdown threshold of the same crystals when exposed to short electrical pulses of nanosecond duration. Each section of the dependence of the damage threshold of transparent dielectrics by a laser or electrical pulse can give information about the dominant mechanism of destruction, running at a given pulse duration. In the first section of the characteristic dependence of this may be the mechanism of thermal explosion of inclusions, in the last section—ablation.

Thus, the mechanism of its own breakdown of transparent solids by laser beams ultrashort duration is not constant, but is determined largely the laser pulse duration.

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# THE REFLECTION ENERGY FACTOR ANALYTICAL STUDIES FOR THE NANOFILMS OF THE DIFFERENT COMPOSITION

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The thin films optical and geometrical parameters determination from the experimental data demands enough difficult computer calculations [1–4]. But it is often need to have the equations for the experimental results analysis. The ratio between the optical sizes and scattering parameters of the film can be written down in the compact mathematical form [1]. However the working analytic expressions are necessary for the final data analysis as in [2]. These formulas frequently depend on the optical constants measuring methods. The combination of the wave and geometrical optics methods is frequently allows to reduce this way to the description of the monochromatic wave distribution in the linear isotropic medium without of a spatial dispersion. The films optical constants measurements are very critical to its chemical composition and their manufacturing conditions. In our experiments the films parameters were measured by the spectrophotometer by the comparison of the energy values in the falling and reflected waves and then calculated as in [1, 3]. But our studies plan demands to calculate the optical parameters of the multilayer films as the system of the different mediums. For this purpose the energy factors of reflection and refraction have been deduced as the next equations:  $A = a_{01} + f_1 b_{10} d_{12} d_{01} + b_{10} \sum_{i=2}^{\eta-1} d_{i+1, i+2} \prod_{k=1}^{i+1} (f_k) \prod_{k=1}^{i+1} (d_{k-1, k}) \prod_{i=1}^{j-1} (f'_j \prod_{i=1}^{j-1} (d'_{j+1j}))$ ,  $B = b_{\eta-1\eta} \prod_{i=1}^{\eta-1} (f_i) \prod_{i=1}^{\eta-1} (d_{i-1, i})$ , where  $a_{i-1j}$  is the reflection factor,  $b_{i-1}$  is the refraction factor and  $d_{i-1i}$  is connected with the wave absorption in the according mediums and their boundaries,  $f_i$  and  $f_j^k$  are the mathematical factors connected with repeated light reflection and refraction in each medium.

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# DESTRUCTION OF FRACTAL SOLID STATES UNDER THE ACTION OF PULSED LASER RADIATION

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In this paper we consider the mechanism of thermal destruction of fractal solid under the action of pulsed radiation. In the simulation of heating are taken into account the following processes: 1) the absorption of laser radiation, 2) reflection of the laser radiation from the surface, and 3) thermal radiation from the heated sample. Convective heat from the space surrounding us in this problem is disregarded. This is a true if the irradiation of the material is carried out in vacuum conditions. The one-dimensional heat conduction equation takes the form:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial z^2} + \frac{\alpha \exp(-\beta z) \Phi(t_0 - t) - \gamma u^m + 1}{G(u)}, \quad (1)$$

$G(u) = D^2 u^D \int_0^{1/u} \frac{x^{D+1} \exp(x) dx}{(\exp(x)-1)^2}$ , where  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $m$ ,  $D$  are the positive dimensionless parameters,  $u = u(z, t)$  is the dimensionless (divided by the Debye temperature) the temperature,  $t$  and  $z$  are the dimensionless time and coordinate,  $\Phi(t_0 - t)$  is the Heaviside function, which simulates the laser pulse duration. We assume that the same temperature is maintained at the ends of the irradiated sample, which is equal to the ambient temperature:  $u(z, 0) = u(0, t) = u(l, t) = u_0$ ,  $t \in [0, t_c]$ ,  $z \in [0, l]$ , where  $u_0$  and  $l$  are the determine the ambient temperature and the linear size of the sample respectively,  $t_c$  is the calculation time. To be of interest to consider two cases separately at numerical modeling:  $t_c \leq t_o$  and  $t_c > t_o$ . The condition of the laser breakdown:  $u(z, t) \geq u_m$ , where  $u_m$  is the dimensionless (divided by the Debye temperature), melting temperature of the sample. To evaluate  $u_m$  the use of a result in [1], which in this case is written as:  $u_m = 1.75 \cdot 10^{-5} (2n^2 + 1)^2 \theta$ , where  $\theta$  is the Debye temperature of the sample,  $n$  is the principal quantum number.

The numerical solution of the heat equation show, that the fractal properties of the sample can significantly affect the heating process.

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## LASER DOPING OF CdTe BY In

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The effect of fast diffusion caused by the high mobility of atoms in crystals at pulsed laser irradiation (PLI), allows the realization of the solid-phase and liquid-phase doping of the submicron layers of the semiconductor crystals by pulsed irradiation of the metal–semiconductor system. This method of the doping of semiconductor crystal surface layers is very efficient for forming of the sharp p-n junctions at the small depth. At the same time the mechanisms of the fast diffusion in metal–semiconductor structures at PLI are not clearly understood. The elucidation of these mechanisms is important for the forecast and controlled changes in physical, electric, photo-electric properties of semiconductor structures. The object of the work is the determination of the dominating mechanisms of the fast diffusion of indium in CdTe at PLI of the thin-film In/CdTe system.

The In/CdTe structures were irradiated from the side of indium film by ruby laser pulses (wavelength  $\lambda = 694$  nm, pulse durations  $\tau_p = 20$  ns or 80 ns). The samples were also irradiated by the pulses of the Nd:YAG laser ( $\lambda = 532$  nm,  $\tau_p = 7$  ns) and the pulses of the KrF excimer laser ( $\lambda = 248$  nm,  $\tau_p = 20$  ns). The measurements of In distribution in CdTe after laser treatment were carried out using the Auger electron spectroscopy after layer-by-layer etching CdTe:In by the beam of argon ions.

The different mechanisms the laser-stimulated diffusion of indium in CdTe (concentration diffusion, thermal diffusion, baro-diffusion, shock wave stimulated diffusion, diffusion in liquid phase) are analyzed.

It is established that the dominating diffusion mechanism at the laser solid-phase (before the melting of the CdTe substrate) doping the CdTe crystal with indium is baro-diffusion. The deep and fast penetration of indium atoms into CdTe is caused by significant gradients of the elastic stresses arising due to the fast processes of heating and melting.



## NANOPULSED LASER ACTION ON $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ LAYERS

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The action of pulsed radiation (80 ns) of a ruby laser on epitaxial  $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$  layers (10  $\mu\text{m}$ ) on GaAs substrates has been studied (in situ) by time-resolved reflectivity measurements (TRR) at  $\lambda = 0.53/1.06 \mu\text{m}$  and (ex situ) by Raman spectroscopy. Raman spectra were recorded using Spectra Pro 500i spectrometer (Acton, USA) at an angle between the excitation beam and the recorded scattering signal of  $180^\circ$ . A Nd:YAG laser with 532 nm wavelength was used as an excitation source. The scattered radiation passed through a holographic filter was directed to a diffraction grating (600 line/mm), and its spectrum was recorded by a cooled CCD camera. The number of scans was 30.

Additionally IR transmittance spectra of the samples were measured in  $5000\text{--}225 \text{ cm}^{-1}$  spectral range at the resolution  $4 \text{ cm}^{-1}$  using Thermo Nicolet Nexus FTIR spectrometer (Thermo Fisher Scientific, USA). The number of scans was 128.

As it follows from TRR the changes in reflectivity  $R$  are absent for both wavelengths of probing radiation at energy density  $W$  less than  $0.06 \text{ J/cm}^2$ . This value of  $W$  is likely corresponded to the threshold of laser-induced melting of the surface of the solid solution under consideration. The  $R$  increase at  $\lambda=1.06 \mu\text{m}$  is observed at  $W$  higher than the threshold. It can be explained by the formation of compositional melt. At the same time  $R$  does not change at  $\lambda=0.53 \mu\text{m}$ , that likely connected with the weak change of  $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$  optical parameters at  $\lambda=0.53 \mu\text{m}$  under transition in molten state, i.e. under phase transition crystal (semiconductor)–melt (semiconductor). The time dependence of the existence of  $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$  molten layer on  $W$  is obtained.

The Raman spectra showed that the laser-induced phase transitions lead to the modification of irradiated structures and to  $x$  changes. IR transmittance spectra do not change.

# EXPERIMENTAL STUDY OF IRON ATOMS FORMATION AFTER LASER PHOTOLYSIS OF IRON PENTACARBONYL

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Laser photo-dissociation of metal carbonyl compounds is an attractive technique of atom vapor production for chemical processes study [1]. This method can also be used for metal nanoparticles synthesis [2]. Photo-dissociation of metal carbonyls is very complex physical and chemical process which has a lot of uncertainties, such as complex structure of poly-atomic molecules and energy exchange between various excited states.

This study is devoted to the investigation of iron atoms formation after KrF excimer laser pulse photolysis of iron pentacarbonyl (IPC) with the mixture of noble gases and CO. We observed the radiation of iron atom lines from a quartz reactor immediately after laser photolysis of IPC by use spectrograph combined with CCD camera. Peaks of emission signals were attributed to the different excited states of iron atoms. Experiments have shown that emission has lower intensity in the mixture of IPC with CO. This fact confirms that quenching of excited iron atoms occurs faster in collisions with CO than with argon or helium molecules [1].

Atomic resonance absorption spectroscopy (ARAS) technique was used to measure the iron atoms concentration. It was supposed that the increase of iron atoms concentration in the ground state is resulted by a quenching of their excited states in collisions with noble gas, CO and parental IPC molecules. Decrease of iron atoms concentration occurs when they are taking part in reaction of recombination and others secondary reactions. Based on performed ARAS measurements the kinetic mechanism of small iron cluster growth induced by pulse photolysis of IPC was developed. Comparison of experimental data with kinetic modeling results has allowed determining the rate constants of basic reactions responsible for iron atoms formation and consumption.

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# CLUSTERING AND RECOMBINATION OF POINT DEFECTS IN Mo UNDER IRRADIATION. MOLECULAR DYNAMICS SIMULATION

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The evolution of self-interstitial atoms (SIA) and vacancies is the first stage of the defective structure relaxation after the cascade formation. This stage plays an important role in the nucleation process of the dislocations and voids. The modern kinetic theory of the radiation damage describes the kinetics of these processes in terms of the interaction radius [1]. But there are no accurate values of these parameters, because of the complex mechanism of SIA and SIA or SIA and vacancy interaction. The theoretical prediction of the interaction radius becomes complicated by the one dimensional (1D) diffusion of SIA in some metals, for example in Mo. The diffusion of SIA in Mo is strongly 1D up to 1000–1500 K. It is shown by means of kinetic Monte Carlo that 1D diffusion can change the kinetics of the interaction between SIA and sink strength dramatically. In the case of SIA and vacancies it is possible to observe the similar effect.

The present work is devoted to the molecular dynamics simulation of evolution of the system with SIA and vacancies. The new accurate potential is used [2], which parameterization includes the formation and migration energy of the defects. The clustering and annihilation is investigated in terms of the concentration changing of defects during the calculation time. The rate constants are evaluated. The comparison with theory of the diffusion controlled reactions is carried out. The results include the investigation of the influence of 1D diffusion on kinetics. The effects of temperature and defect concentrations on the reaction rates are also studied.

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## ATOMISTIC SIMULATION OF TRACK FORMATION BY HEAVY ION IN NUCLEAR MATERIALS

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There is a large interest in understanding of the mechanisms of track formation of swift heavy ions in various materials. In this work, the fission track formation in nuclear materials (U, Mo and UO<sub>2</sub>) is investigated by classical molecular dynamics simulation. The passage of the swift heavy ion (xenon) through nuclear material is simulated with use of two-temperature atomistic model. This two-temperature model describes lattice subsystem by means of classical molecular dynamics while the electron subsystem is considered in the continuum approach. The simulation results show the important role of an electronic pressure at description of track formation. The various mechanisms of destruction of the crystal during the track formation were examined. The comparison to the experimental data was performed.

## GRAIN BOUNDARY INFLUENCE ON VANADIUM CRYSTALLITE BEHAVIOR UNDER RADIATION LOADING

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The molecular dynamics simulation of the grain boundary influence on the atomic displacement cascade development in vanadium crystallite was carried out. Interatomic potentials were described in the scope of Finnis-Sinclair method. As a grain boundaries symmetrical tilted boundaries of special type ones were used. The analysis of damaged region was performed by means of Frenkel pairs calculation.

It was discovered that extended interfaces could significantly effect on the atomic displacement cascade development character caused by radiation exposure. Analysis showed that point defects generated in a bigger amount in crystallite with grain boundaries in compare with ideal crystallite with ideal structure with the same primary knocked atom (PKA) characteristics (PKA impulse magnitude and direction). At that the closer atomic displacement cascade was to the boundary the more number of

point defects generated at all stages of cascade development. The majority of generated structural defects formed in the grain boundary region which was an effective barrier for the atomic displacement cascade propagation.

The study of influence of grain boundary farness from the PKA on the cascade development was performed. The threshold distances from PKA to grain boundary at which formed cascade do not spread throw the interface were defined for various PKA energies. It was shown that the threshold distance rises with the PKA energy but the threshold distance raising rate decreases as during dissipation process the cascade region increasing occurs in all directions.

The work was carried out with the partial financial support of the RFBR grant #11-08-00423-a.

## KINETICS OF METAL EVAPORATION AND CONDENSATION UNDER THE HIGH-CURRENT ELECTRON IRRADIATION

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Metal evaporation by high-current electron beam and consequent condensation of the obtained metal vapor can be used for generation of ultrafine metal particles [1, 2]. Electron irradiation usually leads to incomplete evaporation of metal—a part of material remains in condensed phase state in form of liquid drops. These drops become the condensation centers and determine size of resulting ultrafine metal particles.

In this report we numerically investigate kinetics of evaporation and condensation of metal irradiated by high-current electron beam. Metal is treated as a two-phase medium consisting of vapor bubbles in liquid metal in the first stage of evolution and of liquid drops in vapor in the second stage. The size of bubbles and drops ( $\sim 0.1 \mu\text{m}$ ) is less than the typical length scale of the problem (the last one is of the order of electron range in substance  $\sim 10 \div 100 \mu\text{m}$ ). It allows using of continuous approximation in which both phases are described by continuous fields of parameters: concentration and radius of bubbles (drops), pressure, temperature, density, chemical potential and volume fraction of liquid and vapor phases in each point of space. Estimations show that the phases must have approximately the same velocities both in the first stage (bubbles in liquid)

and in the second stage (drops in vapor); therefore we use a one-velocity approximation. Substance dynamics is described by continuum mechanics equations. The beam action is taken into account through energy release of fast electrons. Generation and growth of vapor bubbles and consequent evolution of drops are described by kinetic equations for phase transition. A simple scheme of transition from the bubbles in liquid to the drops in vapor (a percolation problem) is constructed.

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## **ACTION OF HIGH-ENERGY ELECTRON BEAM ON ECOTOXIC POLYCHLORINATED COMPOUNDS ADSORBED ON SURFACES**

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High-energy electron beams are used for clearing air from volatile toxic components:  $\text{SO}_2$ ,  $\text{NO}_x$  and various volatile organic compounds (VOCs). In some cases, the compounds can be adsorbed on surfaces, including surfaces of dust particles. Action of high-energy electron beam on the substances adsorbed on inorganic materials has the specificity and demands separate research.

For modeling such processes we used the substances adsorbed on thin plates for thin layer chromatography (TLC), covered with layers of adsorbents such as:  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$  and  $\text{TiO}_2$ . As objects of research have been chosen known ecotoxines as: polychlorinated phenols, polychlorinated benzenes and polychloro-biphenils. The last were used as isolating oils and there is a problem of recycling their.

For the researches the portable electron accelerator RADAN with the following parameters was used: electron energy—180 keV, beam current—400 A, pulse duration—3 ns, pulse repetition rate—up to 10 Hz. For the analysis of products the method of gas chromatography with mass-selective detector (GC/MS) was used. Preliminary experiments have shown, that phenols and their chloro-derivatives under action of an electron beam in adsorbent layer are exposed to binding in to the structures with the dou-

ble amount of carbon atoms. Polychloro-biphenils lose atoms of halogen. Dechlorination is reversible, therefore it is important to select the reagents intercepting chlorine. Search of such reagents is the purpose of the further investigations.

The found regularities allow to carry out analogies between compound radiolysis under action of  $\gamma$ - radiation, photolysis in natural conditions and radiolysis under action of High-energy electron beam with application of the compact electron accelerator, and also modeling processes of ageing. The received data will be useful to development of new technologies of ecotoxines destruction, also will help to make assumptions about evolution of chlorine-containing ecotoxines on dust in Nature.

The work is supported by RFBR (project No. 10-08-01085a).

## **2D-CALCULATION OF HEATING CARRYING OVER COMPOSITE DESIGNS HEATED UP BY RADIATIONS AND PARTICLES FLUXES**

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Action of radiations and particles fluxes (RPF) on composite designs materials causes various physical and chemical transformations (PCT). The RPF set changes at transition from one enough narrow class of materials to another. For most composite materials heat-physical properties of binding and filler differ from each other. Therefore character of their thermal destruction will be essentially various and the mathematical model should consider material structure. In particular Such model is the model of a layered composite [1]. The model contains two sources of lamination. They are physical and constructional types.

The two-dimensional equations of energy carrying over multilayered barrier are formulated for each layer of model in cylindrical system of coordinates. Energy redistributed by gaseous products of thermo-destruction and PCT are considered in these equations. The mass stream of gases caused by binding decomposition is calculated approximately. We assume that all weight of gas formed in the material depth until to some section passes with small speed through this section. Power allocation took place in volume RPF absorption is calculated by a method of Monte-Carlo [2]. Inflow (drain) of heat formed in a material as PCT result is defined by total thermal effect of corresponding transformations. Recurrence and multi-variant combinations

of actions of energy fluxes having various physical natures are considered.

The formulated problem is solved by final differences method and the implicit scheme realized splitting of spatial variables. Transformation of spatial variables is used at calculation of mobile PCT boundaries.

Results of 2D-calculations of multilayered composite designs treated to joint action of ionizing radiation and electrons fluxes are represented. Criteria of applicability one-dimensional assumption in problems of prognostication of parameters formed at thermal RPF action are offered. Values of parameters entering into these criteria are defined by a rated way.

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## **ACTION OF RADIATIONS AND PARTICLES FLUXES ON MULTILAYERED ORTHOTROPOUS COMPOSITE SHELLS**

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Numerical modeling of consequences of action of energy fluxes of the various physical nature on thin-walled bearing elements of flying machines designs includes thermophysical, thermomechanical, gasdynamical and mechanical aspects [1]. A features set complicating carrying out of researches possesses has thermal and mechanical action of fluxes of radiations and particles (RAP) on composite designs. First of all them concern anisotropy of thermo-physical and mechanical properties and rather low thermal stability of composites that to lead to binder thermal destruction and generation of coke when material layers are warmed up at thermal action of RAP energy fluxes.

At the same time calculations of thermal and mechanical actions, and also deformations and design destructions, can be spent independently because characteristic gasdynamic time of mechanical loading formation, as a rule, is much less than time of thin-walled design deformation, and it in turn can be a little in comparison with time of propagation of phase transitions boundaries and time of warming up of a composite material thickness. This circumstance allows to reduce a problem of forecasting of consequences of RAP action on thin-walled designs to the solutions of



three concerning independent problems. They are thermal problem (to calculation of a temperature profile and ablation), gasdynamic problem (to calculation of thickness of a splitting off and existential characteristics of loading) and mechanical problem (to calculation of dynamic durability of a heated-up design of a variable thickness). Calculation of parameters of thermal and mechanical actions is realized in quasi-one-dimensional approach (thickness of designs, warming up, having broken away much less sizes of a stain of influence). Deformation and destruction of shells are considered in the most general three-dimensional statement [2].

Results of calculations of joint thermal and mechanical actions of RAP energy fluxes on composite elements of vehicle designs are resulted in a final work part.

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## THE MONTE CARLO METHOD FOR MODELING OF IONIZING RADIATION ABSORPTION IN OBJECTS OF COMPLICATED GEOMETRY

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Prognostication of parameters of mechanical ionizing radiation (IR) action on heterogeneous coverings (HC) having structure represents considerable practical interest [1]. Correct calculation of power allocation in structure GP components partially defines accuracy of an estimation of these parameters. The Monte Carlo method is often used for calculation of IR power allocation in multilayered barriers having HC in one-dimensional approach. The hybrid approach to a problem of definition of power allocation in HC structures is offered in [2]. This approach allows to consider redistribution of energy between HC components by secondary electronic radiation in not one-dimensional geometry.

The numerical 3D-code for calculation of distribution and IR absorption in multicomponent materials of objects having complicated geometry is offered in the present work. The offered algorithm consists of several stages. This algorithm uses a Monte Carlo method that takes account of

the basic processes of interaction of radiation and substance (photo absorption, elastic and non-elastic dissipations, fluorescence and secondary electronic radiation).

The interaction problem for set spectrum radiation and average structure covering (homogeneous approach) is realized at the first stage. Spectral and angular power distributions of an IR impulse are calculated in various HC sections. This data is used further as the distributed IR sources located in zones 3D-structures.

Net splitting of three-dimensional elementary HC cell is a following stage. This splitting is carried out on corresponding algorithms using tasks of the closed covers dividing homogeneous cell parts.

The final stage consists of calculation of set of problems for the chosen covering sections. Its purpose is definition of distribution of power allocation in components of elementary HC structure.

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## NUMERICAL CODE FOR SEARCH OF RATIONAL PARAMETERS OF THIN-WALLED MULTILAYERED COMPOSITE DESIGNS WORKING IN EXTREME CONDITIONS

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Operating conditions of modern composite vehicles designs appear extreme in some cases [1]. In particular it takes place when action of fluxes of radiations, micro- and macro-particles (RMMP) [2] is supposed besides flight loadings. Ultimate goal of designing of such designs of the raised firmness to streams of energy of the various physical nature is the rational choice of a sheeting, its structure, and also configuration of heat-shielding and carrier layers. This choice should provide the set reliability level having the minimum weight expenses for protection. Achievement of this purpose demands attraction of versatile methodical technique.

The numerical code of search of rational parameters is offered in work. This code realizes in uniform algorithm calculation of parameters of RMMP action by techniques [1, 2] and definition of reaction of the

damaged and warm shell [3]. At calculation design parameters vary for maintenance of criterion function minimum.

To notice that the approach accepted in work is new. In this approach rational parameters of a multilayered thin-walled shell are defined on the basis of the data on parameters of reaction of a protected design on RMMP action. As a rule, only one covering is optimized separately from a protected design. Such optimization is possible at aprioristic preset values of passage factors and as much as possible admissible impulses of the pressure formed in a covering. The limiting temperature of a carrier layer is set also in this case.

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## **ABOUT PRINCIPAL POSSIBILITY OF ASTEROID 99942 APOPHIS REDIRECTION TO THE MOON SURFACE**

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According to astronomical observations and to calculations results asteroid Apophis will fly in 2029 at 40000 km distance from the Earth centre without its collision. However the know risk of collision can take place in 2036. The correction purpose is collision prevention in 2036 and only. But forecasting of consequences of such correction for the long time period after 2036 is not obviously possible. As a result the final solution of a problem of asteroid Apophis by means of its deviation from a collision orbit will not be reached.

In [1, 2] the problem of qualitative change of an asteroid orbit with the termination of its independent movement in solar system is put as the purpose. Instead of passive protection tactics variant of use of an asteroid is considered for statement of large-scale space experiment on shock action by an asteroid on the Moon. The organization of space scale collision will allow to solve a number of physical questions concerning the

Moon. The impact on the Moon surface was already used for physical experiments [3].

Principal possibility of the organization of such space experiment is shown in the present work. As a result of calculations on a method [4] it is received that correction of an Apophis orbit is necessary on January, 9th 2013. This correction is an increment of speed on 7.4 m/s that provides passage of asteroid Apophis on April, 14th 2029 on distance from the Moon surface hardly more than its radius. Repeated correction will allow to provide the guaranteed collision with the Moon surface. We notice that strong sensitivity of the solution to indignations doesn't allow to carry out correction with the guaranteed result in one stage.

Possibility of use of thermonuclear explosions and shock-kinetic actions for carrying out of offered changes of asteroid orbit is estimated. The variant of X-ray action on Apophis surface is considered [5].

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## **DEVELOPMENT OF DIRECT DOSIMETRY METHOD FOR PURPOSE OF RADIATION THERAPY**

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As complementary ion beam dosimetry for the radiobiology experiments at TWAC-ITEP the track detectors CR-39 are used. This type of plastic detectors provides data not only the mean range of energy and energy loss in the target but also the density distribution of the beam cross-section, numbers and the energy spread of the beam.

The charged particles passing through the detector loss their energy, producing the radiation damage of the target matter. Therefore along the particle trajectory there is the area with the modified structure of the matter that possessing of increased solubility. This is a latent track. The special selected chemical reagents lead to formation of hollow conical

or cylindrical channels outcoming from the surface to the depth of the detector. These are the revealed tracks. Data acquisition and processing of detectors is carried out using the system PAVICOM (LPI) [1].

Using plastic detectors the parameters of the ion beam can be developed. The plastics are axially oriented  $Z$ . There are two different approaches to measure intensity, the energy release and define the inhomogeneity of the beam. The first one is one or assembly of several plates that positioned in the middle of the beam. The second one is four plates that positioned on the field of the beam.

The measurements are performed at the entrance of the target, at the end of plateau of energy loss and at a maximum point of energy loss. This method is used as additional dosimetry for the radiobiology experiments.

The intensity of the beam and energy release were determined and compared with the data from fast current transformer and ionization chamber. The intensity variation and energy distribution of the beam are defined.

The description and experimental results are presented.

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## MICROWAVE SYNTHESIS OF BIOCOMPATIBLE NANOSELENIUM

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Elemental selenium, discovered by J.J Berzelius in 1817, in crystalline state was the widespread semiconductor and photoconductor of last century. Selenium is element with toxic properties. But nowadays its significance was established, especially in human and animals life. Low environment selenium content is the reason of specific diseases in some regions, such as children cardiomyopathy, osteoarthopathy etc. Homo sapiens body contains more than 25 selenoproteins and its isomers, working as biocatalysts, enzymes. They are responsible for prevention of cardiovascular diseases, heavy metals detoxication, cerebral, reproduction, and immune system functions, protection of tissues against oxidative stress thanks to its antioxidan properties, destruction of cancer cells owing to its oxidative properties. According last investigations nanoselenium, having reduced toxicity, can be successfully incorporated with these enzymes, de-

veloping antioxidant, anticancer and other useful properties. That is why nanoselenium and polymeric composites on its base are the interesting substances for study as chemopreventive and chemotherapeutic drugs for human cancer. We believe, polymeric composites are appropriate form of nanoselenium for applications mentioned above, but the process of synthesis and its products should be friendly environmental. Microwave stimulation of these procedures was applied as convenient to control energy supply and gaseous atmosphere. For polymeric media polyvinyl alcohol and polyvinyl pyrrolidone were used. Its water solutions were mixed with surfactants solutions (sodium dodecylsulfate and similar compounds), solutions of selenious acid and reducing agent (glucose, saccharose, ascorbic acid) and placed in reactor, situated in microwave furnace. Thus transparent composite solutions of different grades of red color have been produced. According chemical analysis data there were no any toxic compounds in composite solutions (soluble selenium forms). All selenium was in colloid nanoscale state. Systems obtained were investigated by UV-VIS spectroscopy, polymeric films produced after drying of solutions on glass slides were studied with electron microscopy and X rays. Therefore microwave assisted synthesis was successfully applied for production of acceptably environmental agents, having possibility be applied in human life.

## **LOW-TEMPERATURE PYROLYSIS FOR SOLID HYDROCARBONIC FUEL UPGRADING**

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Low-temperature pyrolysis (torrefaction) is an effective way to upgrade thermotechnical characteristics of biomass solid fuel. As a result of thermal treatment (heating up to the temperature near 300°C) not only moisture removing happens but also partial destruction of hemicellulose (one of the biomass components) has place. This gives rise to formation of hydrophobic product, increment of density and combustion heat of produced fuel in comparison with initial raw materials. The paper is devoted to experimental research of heat treatment operating conditions effect (temperature and holding time) on thermotechnical characteristics of granulated fuel made of different biomass sorts. Experiments were carried out on thermoanalyzer SDT Q600 which enables performing of differential scanning calorimetric (DSC) and thermogravimetric analysis. Initial raw material heating was performed in inert-gas blanket with 10°C/min heating rate up to temper-

atures of 230, 250 and 270°C with following holding in isothermal conditions. Data on hygroscopic properties, content of volatile compounds and combustion heat of torrefied fuel received in the different heat treatment conditions are presented. Based on DSC data the influence of the heat treatment operating conditions on combustion dynamics of torrefied fuel is discussed. Structure changing of initial raw material during the heat treatment progress is also presented.

## CONDITIONS OF FORMATION CARBYNE THIN FILMS BY MAGNETRON SPUTTERING OF GRAPHITE TARGET

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There are a number of works on obtaining allotropic forms of carbon such as graphite, diamond-like films, etc. Usually, carbon thin films are obtained by chemical vapor deposition and ion sputtering of graphite.

In this paper we studied the conditions for the formation of a thin film carbyne, one of the allotropic forms of carbon with the influence of the activating radiation from a black body model at high temperatures. Deposition of the film occurred at a graphite target magnetron sputtering of graphite DE-24. The films were deposited on a silicon substrate heated to a temperature of 800 K. The power of the DC magnetron sputtering system was 1.5 kW.

The phase composition of the transparent films with a thickness of 50–200 nm, was investigated by Raman scattering. Raman bands showed the presence of 1950  $\text{cm}^{-1}$  double bonds and 2149  $\text{cm}^{-1}$  conjugated triple bonds, which indicates the presence of carbyne phases in the films [1].

Snapshot of the film surface, obtained by electron-optical microscope FEI PHENOM revealed two regions with the highest exposure to radiation and decreasing the intensity of the Gaussian. It is clearly seen that in a region where the film surface is illuminated by radiant flux greater intensity of radiation, there are certain crystal structures.

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**LOW TEMPERATURE NON-THERMAL PLASMAS  
AT ATMOSPHERIC PRESSURE: DIAGNOSTICS  
AND MEDICAL APPLICATIONS**

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This study was devoted to diagnostic of low temperature plasma non-thermal plasmas produced at atmospheric pressure and investigation of its bactericidal effect against bacteria in biofilms and within eukaryotic cells. The profile of gas temperature near the torch outlet was measured. The spectrum in a wide range of wavelengths was derived by the method of optical emission spectroscopy. Probe measurements of the floating potential of plasma were carried out. The estimation and adaptation of parameters of plasma flow (temperature, velocity, ion number density) according to medico-technical requirements were produced. The model of immersed surface-associated biofilms formed by Gram-negative bacteria, *Pseudomonas aeruginosa* and *Burkholderia cenocepacia*, and Gram-positive bacteria, *Staphylococcus aureus*, was used to assess bactericidal effects of plasma treatment. Reduction in the concentration of live bacteria in biofilms treated with plasma for 5 min was demonstrated by measuring Live/Dead fluorescent labeling and using direct plating. The intracellular infection model with the pathogenic bacterium, *Chlamydia trachomatis*, was used to study the efficacy of microwave argon plasma against intracellular parasites. A 2 min plasma treatment of mouse cells infected with *C. trachomatis* reduced infectious bacteria by a factor of  $2 \times 10^6$ . Plasma treatment diminished the number of viable host cells by about 20%. When the samples were covered with  $MgF_2$  glass to obstruct active particles and UV alone was applied, the bactericidal effect was reduced by  $5 \times 10^4$  fold compared to whole plasma.



**Z-PINCH IN HELIUM AT INITIAL PRESSURE  
OF 10–25 MPa**

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Research results for discharge in high density helium with current amplitude of 0.5–1.5 MA, current rise rate  $10^{10}$ – $10^{12}$  A/s, at initial pressure of 10–25 MPa are presented. Experiments were carried out on two installations. On the first experimental set-up with current rise rate  $\sim 6 \cdot 10^{11}$  A/s discharge channel characteristics are measured by shock wave velocity, generated by discharge channel, and conductivity and pressure in channel. The conductivity is lower than Spitzer conductivity due to own magnetic field influence. On the second one with current rise rate  $\sim 3 \cdot 10^{10}$  A/s a discharge channel contraction is observed. In our opinion, the observed contraction is determined by excess of radiative critical current (generalized Pease–Braginskii current) and agrees with prediction of radiative collapse model.

**PLASMA CHANNEL STRUCTURE DURING THE  
HIGH-VOLTAGE GENERATOR WITH THE PICOSECOND  
PULSE FRONT DISCHARGE TO THE MICROWIRES**

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The main objective of the suggested work is the experimental investigation of the efficiency of the peculiarities of the non-ideal plasma generation under the impact of the electromagnetic pulse (EMP) with the subnanosecond rise on microconductors. The high-voltage impulse generator “RADAN-220” (with characteristic impedance of 50  $\Omega$ ) was discharged to the inhomogeneous 15 cm long and 10 cm internal diameter coaxial line (vacuum chamber). To the central conductor there were placed 5–15 mm long microwires of Cu ( $d = 20 - 300 \mu\text{m}$ ), Ni ( $d = 25 \mu\text{m}$ ) and W ( $d = 24.5 - 100 \mu\text{m}$ ). Voltage pulse amplitude  $U_0 = 220$  kV, pulse rise duration  $\tau_f = 200 - 500$  ps; energy stored in the generator  $w = 1$  J.

Pressure in the camera varied as  $P = 10^{-4} - 760$  Torr. Input voltage was measured via the capacitance voltage divider installed into the vacuum oil, electric current – via shunt with the impedance  $R_{sh} = 0.4 \Omega$  and up to 5 GHz bandwidth, both signals registered via the digital oscilloscope with 1GHz bandwidth.

It is shown that microconductors destruction via the EMP with  $\tau_f < 1$  ns is caused by the electrodynamic processes, arising within their surface layer and its vicinity. The discharge channel has a complex structure: plasma crown, dense core – non-ideal plasma and a transitional layer in between, where vortex and helical structures, clear luminous spots and plasma jets are observed. It is shown that the emission spectrum at the moment of plasma crown formation is continuous. The most intense Cu spectral lines (510.554, 515.324, 521.82) nm, arise just about  $\sim 3$  ns after the plasma crown was formed. Using the spectral lines intensities ratio was acquired the electron temperature evaluation:  $T_e \sim 0.7$  eV.

The work is carried out under the partial financial support of the RFBR (projects No. 10-08-00691-a and No. 11-08-00434-a) and the Presidium of the Ural Branch of Russian Academy of Science within the integration projects, carried out by joint efforts of UB, SB and FEB of RAS (project No. 09-C-2-1002), and also within the Programs for basic research of the Presidium of Russian Academy of Science (projects No. 09-II-2-1016 and No. 12-II-2-1005).

## DIFFERENT SCENARIOS OF THE CORE-CORONA FORMATION DURING WIRE EXPLOSION

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In the numerical calculations it was obtained that, during the explosion of a single aluminum wire, the core material remains for a long time in the state of a dense nonideal plasma with a temperature of 1–3 eV. Only after shunting the main part of current to the corona, the core goes into a two-phase liquid-vapor state in the expansion process. However, if shunting of the current occurs at an early stage of the explosion, for example, when the wire material is still in liquid state, it is possible another scenario of core structure formation. In this case, due to a sharp drop of the compressive magnetic pressure, the core material can come into a state of the stretched melt during unloading. In accordance with the molecu-

lar dynamic calculations this metastable state decays, that resulting in to formation of a complex core structure: the outer cylindrical liquid shell filled with low-density foam. The foam decays into liquid droplets before the outer shell breaks apart. Simulated density profiles demonstrate good qualitative agreement with experimental high-resolution X-ray images showing the complex hollow structures within the long-living dense core.

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## DENSE PLASMA IN HIGH CURRENT SYSTEMS WITH LARGE DENSITY OF ENERGY

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Dense plasma is applied in high current systems with high density of energy as the tool for formation of voltage pulses and for transformation of energy. Explosive breakers and plasma dynamic sharpeners, installations with accelerating, braking and pinching plasmas have relation to such systems. Occurrence of pulse voltage is typically for all these systems when pulse deformation of plasma volume happens. Three questions arise in such cases. The first, what determines amplitude of pulse voltage. The second, what time moment is connected to a maximum of pulse voltage. The third, what mechanism is in the reason of its origin. For the analysis of a situation we considered the equation of energy for elementary volume of plasma:

$$\frac{\partial}{\partial t}(\mu_0 H^2/2 + \epsilon_0 E^2/2) + \operatorname{div}(\bar{E} \times \bar{H}) \pm P \operatorname{div} \bar{u} = \frac{(n-1)}{(\gamma-1)} P \operatorname{div} \bar{u} + \operatorname{div} \bar{q}.$$

The traditional designation of included quantities is accepted in this equation. This energy equation is possible to integrate at observance of some conditions and receive the equation of balance of density of flows of energy:

$$\bar{E}_{max} \times \bar{H} \pm P \bar{u} = \frac{(n-1)}{(\gamma-1)} P \bar{u} + \bar{q},$$

where  $\bar{E}_{max} \times \bar{H}$ —density of a flow of electromagnetic energy,  $P \bar{u}$ —density of a flow of mechanical (kinetic) energy,  $\frac{(n-1)}{(\gamma-1)} P \bar{u}$ —density of a flow on change of internal energy of plasma,  $\bar{q}$ —density of a heat flow lost in the

volume of plasma. Work of high current systems is connected to management of energy flows. In this view point, the interest is represent members in the left part of the energy equation, which describe influence on current plasma of external conditions. For example, by pressing of the button it is possible to connect an additional source of electromagnetic energy or to deform a plasma volume by external mechanical act. If pressing of the button we assign a flow of mechanical influence on plasma with a current the member  $P\bar{u}$  carries character of the reason of quantitative change of other flows then the following parities take place:  $q < Pu$ ,  $\frac{(n-1)}{(\gamma-1)} < Pu$ ,  $(E_{max}H) < Pu$ . From here follows, that the amplitude of a generated impulse voltage is limited to magnitude of density of an energy flow of mechanical influence, when deformation of plasma volume with the current takes place. Results of all known experiments with explosive breakers and plasma dynamic sharpeners are in the full consent with this restriction.

## CRYSTALLIZATION OF PROTONS IN A DENSE HYDROGEN PLASMA

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We perform a first-principle analysis of Coulomb crystallization in neutral two-component mass asymmetric plasmas by large-scale path integral Monte Carlo simulations for a dense hydrogen plasma in a broad density range. We observe two jumps in the relative distance fluctuations of protons that are connected with qualitative changes in the behavior of the proton pair distribution function and are attributed to the crystal-liquid and liquid-plasma phase transitions.

## VAPOR-LIQUID AND DIELECTRIC-METAL TRANSITIONS IN ALKALI METALS VAPOR

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In the present study, the physical model of alkali metals vapor taking into account effects of metallization of an atomic component is under

construction. The bases of the theory of an atomic gas metallization are made in works of Wigner-Seitz and J. Bardeen. In this work the concept of cohesive energy is extended to gaseous state. Within the framework of the unified approach the model described gaseous and liquid-metal phases, including vapor-liquid transition. The model explicates the model of gaseous metals of Likalter. Difficulties of application of Wigner-Seitz-Bardeen theory to liquid alkali metals are connected with necessity of the account of the ionic core. Numerical simulation and various extrapolation approaches, for example a quantum defect method, are used. In the present study, we offered the Kratzer potential to use as interatomic potential of alkaline atoms. Kratzer potential successfully used earlier for the description of the ionic molecules. By analogy to Lenard-Jones potential it is possible to term it as (2-1) potential. On long distances it has a Coulomb asymptotic, and on short distances contains the repulsion that modeling the ionic core. The Schrödinger equation with the Kratzer potential has the exact solution that allow to define a factor of repulsive term, having equated the energy of a ground state of an isolated atom analytically founded to the experimentally measured one. Cohesive energy is calculated for alkali metals in whole range of Wigner-Seitz cell sizes using the theory of Wigner-Seitz-Bardeen for the ordered system of atoms with interatomic Kratzer potential. This energy has two extremum: a minimum at liquid-metal densities and a small maximum at lower one. It's occurs when the radius of a classical orbit of the bound electron is equal to radius of Wigner-Seitz cell, passed through a zero between them. The density at which binding energy vanished is close to the critical one. The thermodynamics of vapors calculated using the thermodynamic perturbation theory for a one-component system taking into account excluded volume and the metalized binding energy of atoms. The model contains vapor-liquid phase transition (Van der Waals loop) which parameters qualitatively agree with known values. Conductivity is calculated with use of Joffe formula. Conductivity at near critical temperatures shows metal-dielectric transition. Correlation of this transition and with vapor-liquid transition is considered.

# THE ELECTRONIC TRANSPORT COEFFICIENTS IN Ag AND Au PLASMA

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The electronic transport coefficients of metals (conductivity, thermal conductivity and thermal power) play important role in fundamental tasks and applications. So there are many theoretical and experimental investigations of the considered coefficients under various densities  $\rho$  and temperatures  $T$  [1]. Even the area of dense plasma ( $T > 5-10$  kK and  $\rho < \rho_n$ ,  $\rho_n$  is the normal density) has become accessible for measurements during past two decades [2, 3]. But among the noble metals only Cu has been studied in appropriate way. Up to now for Au conductivity in plasma area several models have been published (see [4]) and only one experimental isochore [5]. For Ag conductivity no any data has been published for  $T > 5-10$  kK up to present time. The published data about other two coefficients have been also absent both for Ag and for Au in plasma region.

Recently these coefficients have been calculated within the relaxation time approximation [4]. The ionic composition, necessary for this calculation, has been obtained within the generalized chemical model [1, 4]. The results of calculations are in good agreement with available experimental and theoretical data. But the model itself is limited by density from above because of used approximations. Here we used the generalized Ziman formalism [6] to go beyond this limit. The results of calculations has been compared with available data of others researchers.

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# PERMITTIVITY OF ALUMINUM PLASMA: QUANTUM STATISTICAL AND KINETIC APPROACHES

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Permittivity of aluminum plasma is calculated both by wide-range model based on kinetic approach and by linear response approach in quantum statistical (QS) theory. It is demonstrated, that both approaches give the same results for weakly-coupled plasmas and for optical laser frequencies.

In the region of strongly coupled non-degenerate plasmas (for solid-density aluminum the corresponding electronic temperatures are  $T_e \sim 20\text{--}200$  eV), the kinetic approach with Rutherford electron-ion collision cross-section gives lower values of effective collisional frequency  $\nu_{ef}$  and imaginary part of permittivity  $\varepsilon$  than the QS approach. This is connected to the fact that Rutherford-like cross-sections don't take into account strong collisions with electron scattering on the large angles, which are essential in the region of strong coupling. The ways to improve results of the kinetic theory in the region of strongly coupled plasmas are discussed.

In the region of low frequencies of laser radiation,  $\omega < \Re\nu_{ef}$ , QS theory based on the calculations of J-J correlation functions within one-moment approach underestimates the values of  $|\Re\varepsilon|$  and  $|\Im\varepsilon|$ . In order to obtain correct description of permittivity in this region, higher-order moments of distribution function should be used in calculations of correlation functions.

# LASER RADIATION INTERACTION WITH STRONGLY CORRELATED PLASMA

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The analysis of the response of dense plasma to electromagnetic waves of moderate intensity can be used as a tool to investigate the validity of the physical models describing the behavior of matter under extreme conditions [1, 2]. However, to interpret correctly the results of reflectivity measurements it is necessary to know parameters of a transitive plasma layer. 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 explosively driven dense xenon plasma are presented. The study of polarized reflectivity properties of plasma was accomplished using laser light of wavelength  $\lambda = 694$  nm and  $\lambda = 532$  nm at incident angles up to  $\theta = 70^\circ$ . With density  $\rho = 3$  g/cm<sup>3</sup>, pressures  $P = 12$  GPa and temperatures up to  $T = 3 \cdot 10^4$  K of the investigated plasma, conditions with strong Coulomb interaction (the nonideality parameter up to  $\Gamma = 2.4$ ) were present.

For determination of the equilibrium properties of explosively driven plasma, appropriate gas dynamics calculations were carried out. The plasma composition was calculated within a chemical picture [3]. The integration of Maxwell equations are based on an interpolation formula for dc conductivity [4], obtained from a systematic quantum statistical treatment of different limiting cases. Results of the calculations with layer temperature profile and ea-collisions as factor are presented too.

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# IMPROVEMENT OF WAVE PACKET MOLECULAR DYNAMICS USING PACKET SPLITTING

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The method of classical molecular dynamics (MD) is widely used to simulate equilibrium and nonequilibrium nonideal plasmas. At the same time the applicability of MD is restricted to non-degenerate and fully ionized plasmas. Such a model is often too rough if applied to real experimental conditions. One of the possibilities to improve the method of MD without losing its performance benefits is to consider electrons as wave packets [1]. In this case the problem of choosing effective electron-ion interaction potential does not arise, the accuracy of simulation of an individual particle collisions is increased and ionization-recombination processes are represented in a better way. Furthermore the exchange interaction between electrons in the Hartree-Fock limit can be taken into accounts using antisymmetrized wave packets [2]. This method was named Wave Packet Molecular Dynamics (WPMD).

Problems of the existing implementations of this approach are the poor accuracy for a bound state of electron an ion and spreading of wave packet for a weakly bound electron [3]. We propose to address both issues using a new technique based on expansion of the wave function for each electron in the bases of multiple Gaussians. Calculations of the ground state energies of H and He show that this method provides accuracy of less then 1% for even three Gaussians per electron. Another advantage of the new technique is the possibility to study quantum effects related to the wave function splitting such as penetration through a potential barrier. As a test case we consider tunnel ionization of a hydrogen atom in a short laser pulse. It is shown that the results of the new method are in a good agreement with quantum-mechanical calculations.

In future it is planned to apply the new method to model bound states of electrons and ions in nonideal plasmas and combine it with the classical Coulomb interaction model for free electrons.

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# GPU-ACCELERATED MOLECULAR DYNAMICS SIMULATIONS OF NONIDEAL PLASMAS

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The molecular dynamics (MD) simulation allows discovering various properties of nonideal (strongly coupled) plasmas. However, the performance of an MD code is highly dependent on the number of particles due to the long-range Coulomb interactions. This type of interaction requires calculation of the full interaction matrix and disables the neighbor list optimization that is routinely used for the short-range potentials. It makes the task numerically heavy, even for a relatively small number of particles in the system. In addition the need to know the coordinates of all particles in the system for force calculations makes ineffective the standard method of code parallelization (space decomposition) that is used on distributed memory architectures. It causes problems with effective loading of high performance computing clusters with the distributed memory.

Alternative way to speedup calculations is the use of modern Graphical Processing Units (GPUs) [1, 2]. Contemporary GPUs provide tremendous peak computational power but at the same time require specific highly parallelized codes. In contrast to the conventional clusters the GPU has shared memory architecture which implies it is more effective in the case of MD simulations with long-range interactions.

In the present work we discuss developing of the GPU-enabled MD code for the electron-ion nonideal plasma. The code is applied to simulations of the sodium clusters ionized by a short laser pulse [3]. As the numbers of atoms in a nanocluster is less than one million the dynamics of ions and ionized electrons can be modeled directly for the whole system. The benchmarks for the CPU and GPU simulations are considered depending of the number of particles in the range  $N = 50 - 2 \cdot 10^5$ . For this particular problem the Nvidia Tesla 2050M GPU is found to be 100 times faster than Intel Xeon E5520 CPU at the maximum system size. It allows us to increase the cluster size and consider smooth transition of the plasma properties from finite nanoplasma to bulk plasmas.

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## RATE OF RECOMBINATION IN STRONGLY COUPLED ION PLASMA

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The goal of this works is to study of the recombination process in the plasma of positive and negative ions produced in the afterglow of gas discharge. Experimental study of the recombination process in this system showed a strong suppression of the recombination rate compared to the classical model [1] for the ion plasma consisting of F<sub>2</sub> or SF<sub>6</sub>. Explanation for these results is possible within the framework of approaches based on the use of molecular dynamics simulation. An earlier study of the recombination process [2] showed that the increase of the plasma nonideality parameter should strongly suppress the recombination process. In this case, the recombination rate should be described by the following formula:

$$K\tau = \begin{cases} 0.3 \cdot \Gamma^{9/2} & \text{for } \Gamma < 0.488 \\ 2.7 \cdot \Gamma^{9/2} \exp(4.5 \cdot \Gamma) & \text{for } \Gamma > 0.488 \end{cases} \quad (1)$$

where factor  $A = 4.5$ . The resulting ratio is consistent for the rates of recombination in an ultracold plasma. In the case of ion plasma this ratio also must maintain its applicability. This model is sufficient to describe the recombination processes in ion-plasma SF<sub>6</sub> [1]. However, the magnitude of the factor  $A$  in this case exceeds the value of the electron-ion plasma and is equal to  $A = 6.75$ .

If in the case of SF<sub>6</sub> proposed model can well describe the dependence of the recombination rate from the nonideality parameter, in the case of F<sub>2</sub> decrease the recombination rate with increasing non-ideality is significantly stronger than predicted by the model [1]. The explanation for these results can be done under the assumption that the recombination process is strongly coupled ion plasma occurs in two stages. In the first stage is reversible formation of a loose ion pair, in which the recombining ions are separated by solvate shell. A second stage is a transition of loose ion pair in a tight ion pair with its subsequent recombination. In cases where the loose ion pair is unstable then the two-stage nature of the recombination has little effect on its kinetics and it is described by the model [1]. If the

activation energy of the decay of a pair is sufficiently high the rate-limiting phase is the second stage. Which leads to an additional reduction in the rate of recombination in strongly coupled plasmas.

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## **STOCHASTIC PROPERTIES OF IONIC LIQUID**

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The emergence of irreversibility and stochastic properties have been studied only for simple liquids and plasmas. Ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate ([bmim]<sup>+</sup>[BF<sub>4</sub>]<sup>-</sup>) is explored in this work. The interatomic interaction potential is more comprehensive in this case. Classical molecular dynamics method is used. The dynamic memory times and K-entropy are estimated which correspond to different degrees of freedom: center of mass translation, rotation, bond stretching, angle oscillations.

The approach used is based on the divergence of the MD trajectories of the centers of mass of ions and allows to calculate the diffusion coefficient. It is an important property of the liquid. The diffusivity determines the properties of ionic liquid [bmim]<sup>+</sup>BF<sub>4</sub><sup>-</sup> as the solvent and the rate of charging and discharging supercapacitors made on its basis.

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

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Ionic liquids are usually organic salts. Irregular shape of ions results in lower binding energy in the crystalline state and melting temperature 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. In addition, the supercapacitor practically does not degrade during charging/discharging cycle.

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 to be studied using quantum approaches. In this work we apply methods of classical molecular dynamics to study diffusivity of the bulk system composed entirely of the ionic liquid.

Two types of ionic liquids are studied: 1-butyl-3-methylimidazolium tetrafluoroborate ( $[\text{bmim}]^+[\text{BF}_4]^-$ ) and N-methyl-N,N,N-triethylammonium tetrafluoroborate ( $[\text{tema}]^+[\text{BF}_4]^-$ ). Data are obtained showing anomalous time dependence of the mean square displacement of the centers of mass of ions. Quite long transition between ballistic regime and diffusion obeying Einstein—Smoluchowski relation is observed. Two (or even three) different diffusion coefficients are calculated relevant to ps and ns timescales. Space or time non-locality is discussed. Special attention is paid to the statistical error of the molecular dynamics simulation results quantification. Experimental data are considered.

## DIAGNOSTICS OF LOW TEMPERATURE PLASMA AT ATMOSPHERIC PRESSURE FOR TREATMENT OF HEAT-SENSITIVE OBJECTS

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In plasma medicine various plasma sources, such as Narrow jet, Direct barrier discharges (DBD), Microwave plasma are used. The sources of cold plasma with a temperature preferably not higher than 40°C are used for sterilization and acceleration processes of tissue healing. In our work with a use of device MicroplaSter we generated a microwave discharge with a frequency 2.45 GHz with magnetron power from 80 to 150 W. Buffer gas was pure Argon. To obtain a profile of temperature in the torch we used a thermocouple. It was screened for minimization of ambient plasma effect on precision of measurements. For a detection of presence of plasma in

various distances from the edge of plasma torch we carried out a probe diagnostics. We used a grid probe with 6 sm in diameter with a mesh size 2.5 mm. Under standard parameters of the discharge we measured a floating potential of the probe. A probe potential in dependence of distance from plasma torch was obtained. It was revealed that even in the distance of 45 mm there are charged particles, because the floating potential of the mesh grid was not equal to zero. For the spectral diagnostics of plasma torch we used a spectrometer Avesta. The measuring of the spectrum was carried out in continuous operation in a range of waves from 220 to 900 nm through a quartz fiber optics, positioning of which was carried out with the help of optical table with micrometric screws. Calibration of the spectrometer was carried out on deuterium and halogen lamps. Analysis of spectral lines showed a presence of well-defined line of hydroxyl OH and nitrogen N<sub>2</sub> as well as a line of plasma-supported gas Ar in plasma jet. For diagnostics of intensities of spectral lines we made a plasma torch with quartz windows, which allowed measuring them in the region of plasma generation. Through these windows we made spectral measurements in various distances from the electrodes. Also we measured SHF radiation of plasma torch. At some regimes of Microplaster power of SHF radiation exceeded 10 mW. This value corresponded SHF radiation density of about 1 mW/cm<sup>2</sup>.

## **COULOMB ENSEMBLE OF CHARGED DIAMAGNETIC MACROPARTICLES IN A MAGNETIC TRAP UNDER MICROGRAVITY CONDITIONS**

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Physical properties of strongly coupled Coulomb systems (SCCS) are of considerable interest in various fields of science and technology. After first experimental observations of ordered structures of dust particles in gas discharges, similar dusty plasma structures are frequently considered as a macroscopic physical model of SCCS which can visually be observed. Using such structures of charged dust particles, one can investigate the processes of phase transitions, waves, and instabilities on kinetic level. For confinement and investigation of strongly coupled systems of charged dust particles, we propose to use a trap based on the known possibility of

the levitation of diamagnetic bodies in a nonuniform steady-state magnetic field. For the investigation of Coulomb clusters of diamagnetic particles in nonuniform steady-state magnetic field the experimental setup with the region of stable levitation about  $400 \text{ cm}^3$  and magnetic field gradient of  $0.04 \text{ T/cm}$  was produced. Preliminary experiments were carried out on the board of International Space Station with carbon particles with sizes of 100, 200, 300 and  $400 \text{ }\mu\text{m}$  in the argon atmosphere under atmospheric pressure. The preliminary analysis of the experiments allowed us to determine the formation of large cluster of carbon particles in the magnet trap. A number of particles in the cluster was about 2000. The oscillations of the cluster were observed, the maximum amplitude of the oscillations was  $0.49 \text{ cm}$ , the oscillation period— $10 \text{ s}$  and damping factor— $0.07 \text{ s}^{-1}$ . From the balance of electrostatic and magnetic forces the dust charges were evaluated. The charge value for the particles with size of  $400 \text{ }\mu\text{m}$  was  $4 \cdot 10^4 e$ . This work was supported by the Research Program of the Presidium of the Russian Academy of Sciences “Thermophysics and Mechanics of Extreme Power Actions and Physics of Highly Compressed Matter” and by the Russian Foundation for Basic Research, Project No. 10-02-90056, No. 10-02-01428 and Project No. 11-02-01051.

## DYNAMIC DUST PARTICLE CONFINEMENT IN GAS FLOW

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The purpose of this work is to study the possibility and conditions of the dust structure confinement in quadrupole traps at an atmospheric pressure in a corona discharge plasma or in a nuclear-excited plasma in a gas flows and gravitation field.

For simulation of dust structures we consider potential forces acting on dust particles. The influence of the buffer gas is taken into account by viscosity and random forces. The motion of dust particles is described by Brownian dynamics that takes into account the stochastic forces acting on dust particles from the neutral and plasma particles. In addition, the interparticle interaction and influence of trap electric field on these particles are taken into account. The equations of motion of dust particles are described by the Langevin equations:

$$m_d \frac{d^2 r_i}{dt^2} = F_{tr}(r_i) + F_{int}(r_i) - 6\pi\eta R_d \left( \frac{dr_i}{dt} - v_{flow} \right) + F_{Br}(r_i) + F_{mg} \quad (1)$$

where  $N$  is the number of dusty particles,  $i = 1, \dots, N$ ,  $R_d$  is the radius of a dust particle,  $\eta \approx 0.02$  mPa·s is the normal air dynamical viscosity,  $v_{flow}$  is the speed of the gas laminar flow,  $F_{tr}(r_i) = -\nabla_i \bar{U}$  is the force of interaction of the grains with the electrodes of the trap,  $F_{Br}(r_i)$  is the acting on dust particles the stochastic Gaussian delta correlated force resulting from a collision of plasma particles with a dust particles,  $F_{mg}$  is the gravity force,  $F_{int}(r_i) = -\nabla_i U$  is the force of the interaction between the grains and  $U$  is effective potential energy of dusty particle interaction. Description of numerical method of solving stochastic differential equations like (1) and its derivation are given in [1].

In this article we have suggested the improved quadrupole trap. At normal atmosphere conditions (pressure and temperatures) for reasonable choice of dust particle and trap parameters the results of our simulations allow finding the regions of the dust particle confinement and dependence of these regions versus the particle charge and applied to the trap electrodes voltage.

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## EXPERIMENTAL INVESTIGATION OF EQUILIBRIUM STRUCTURAL PROPERTIES OF DUST MONOLAYERS IN RF-DISCHARGE

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In case of isotropic pair interaction thermodynamic and transport properties of non-ideal systems (such as pressure, energy density, thermal capacity, viscosity and heat-conduction coefficients etc.) are defined by pair correlation function  $g(r)$  (where  $r$  is a distance between two particles) which, in turn, depends on a type of potential of interaction,  $U(r)$ , between particles and ambient temperature,  $T$ . Information about pair function  $g(r)$  is necessary for the solving of the integral equations of statistical physics and also can be useful for the analysis of phase state and a prediction of phase transitions in non-ideal systems.

In present work the results of experimental verification of a simple one-parametrical model [1] offered for the description of spatial correlation of particles in strongly non-ideal systems with a wide range of pair potentials are presented. The mentioned model is based on dependence of the form



of pair correlation function  $g(r)$  from a value of a root mean squared displacement of separate particles at specific sites in the lattice of a crystal.

Experiments were performed in near-electrode layer of rf-discharge in argon at pressure  $P = 0.1\text{--}0.3$  Torr with discharge power  $W = 2\text{--}30$  W. The dust component was provided by particles of monodispersed (melamine formaldehyde) spheres of radius  $\sim 6.37\mu\text{m}$ . It is shown that theoretical model is in a good agreement with experimental data and represents all features of behavior of measured pair correlation functions. In addition the results of measurements with close values of parameter are in a good accordance with data of numerical simulation of the problem.

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## MEASURING THE CHARGE OF DUST PARTICLES IN WEAKLY IONIZED GAS DISCHARGE PLASMA

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The particle charge is an important parameter determining physical properties of complex plasmas, and has a significant influence on the thermal energy acquired by a dust particle due to various mechanisms. The magnitude of charge is crucial for particle trapping and levitation as well as for the formation of ordered dusty structures in a laboratory plasma.

The results of measurements of the charge on dust suspended in laboratory rf-discharge plasma are presented. Experiments were performed for both small-size clusters of particles (consisting of 11–29 particles) and large quasi-two-dimensional systems (monolayers of about 1500–2000 particles) forming in the sheath region of rf-discharge in a wide range of dusty plasma conditions (with different sizes, kinetic temperature and concentration of dust, coupling parameter, pressure of neutral gas, and etc). The magnitudes of dust charges were derived from the interaction potential profiles of dust particles, their characteristic oscillation frequencies and the confining field parameters obtained by two methods: one based on a solution of the inverse Langevin problem [1] and another one on studying mass-transfer processes in dusty subsystem [2].

The values of the particle charge  $Z$ , obtained by the ways above, are their lowest estimate, because the results of measurements at distances

close to the mean interparticle distance does not fully take into account the possible screening of the particles. A highest estimate of the particle charge was derived from equations of the near-electrode layer theory [3].

To compare the particle charges, obtained in the considered experiments, with the collisionless theory we estimated their values in the OML approach for isotropic and anisotropic plasma. Finally, we compared the experimentally obtained particle charges with the results of calculations of the dust charge in argon using the molecular dynamics technique in the case of isotropic plasma with an electron temperature 2.5 eV.

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## THE POSSIBILITIES OF CRYOGENIC TEMPERATURES FOR DUSTY PLASMA STRUCTURE FORMATION

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Levitation of dust particles and formation of ordered dust structures were observed in plasmas of the most various kinds: in thermal plasma, in gas discharges of various kinds and configurations, in nuclear-induced plasma. Dusty plasma structures were also observed in the cryogenic dc gas discharge. Such systems received the name of cryogenic complex (dusty) plasma, i.e. dusty plasma where heavy neutral component is cooled down to cryogenic temperatures. Considerable interest in cryogenic temperatures as conditions of dusty plasma structures formation is caused by the assumption that cryogenic dusty plasma allows to combine two approaches in study of strongly coupled Coulomb systems: first, the cooling the particle system and second, the increasing the energy of particles interaction in plasma.

The present work is devoted to investigation of specific features of super dense dust structures formation in a dc glow discharge at cryogenic temperatures. Results on the experimental investigations of new phenomenon of spheroidizing (process of the dust structure transition to compact glob-

ular shape at cryogenic temperatures) were presented. Possible nature of such phenomenon is discussed.

## SECOND ORDER PHASE TRANSITIONS IN CRYOGENIC DUST PLASMA OF GLOW DISCHARGE

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Cooling of dust plasma to cryogenic temperature leads to diminishing of distance between dust particles [1, 2] and to formation of non regular chain clusters in glow discharge. In this work the phase diagram “pressure–current” for dust structures from 4.14  $\mu\text{m}$  MF dust particles in cryogenic neon plasma at temperature of liquid nitrogen and pressure 0.14–1.4 torr is represented for the first time. The regions of transition from chain-ordered clusters to homogeneous structures and regions of clusters melting are registered. The distance between dust particles and shapes of dust clouds are observed to have complicate dependence versus ion temperature, gas pressure and discharge parameters. At plasma cooling to 200 K the formation of dense core similar to the “center of crystallization” was observed in the center of dust structure. The vertical oscillations of dust particles were observed with amplitude depending on gas pressure. Further plasma cooling led to the formation of dense uniform structures with distance of 25–40  $\mu\text{m}$  between dust particles, or chain clusters with the distance of 125–150  $\mu\text{m}$  between clusters. In contrast to observations in air, clusters in neon were observed to form regular structures resembling points of hexagonal lattice. With increase of discharge current, clusters were observed to melt, the distance between particles and the amplitude of particle longitudinal oscillations increased. The border of cluster melting versus current and pressure approximately coincides with the border of transition from sub-normal to normal glow discharge. The increase of gas pressure leads to the coagulation of clusters into dense uniform structures, while the increase of discharge current results in diminishing of longitudinal size of dust structure and increase of its diameter. Unlike experiments at room temperature, the dust structures with central zone free of particles [3] were not registered in cryogenic plasma in this range of discharge current.

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**INFLUENCE OF DUST PARTICLES ON THE  
CURRENT-VOLTAGE CHARACTERISTICS OF POSITIVE  
COLUMN OF GLOW DISCHARGE IN NEON**

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Presence of charged dust particles and dust structures in gas discharge plasmas change plasma properties owing to the electron losses on the dust particle surface. Increased electron losses are followed by increase of ionization frequency and electron temperature and result in increase of electric field strength. Such processes take place in plasma in order to conserve the total discharge current, necessary for the self-maintained discharge and result in increase of electron drift and positive column voltage. These facts were recently confirmed in a number of experimental and theoretical studies. In this work the experimental data on the influence of dust particles and their dynamical stability in dust structure on the voltage of glow discharge positive column in neon are represented for the first time. Experiments were carried out at neon pressure of 0.35 and 0.6 torr. The discharge glowed in a cylindrical discharge tube of 16.5 mm i.d. with the hollow cathode and cylindrical anode. Two ring electrodes were glued into the tube walls with distance of 4 cm between them for measuring the voltage drop in the positive column. Electrodes were situated in front of the region of formation of dust structure. Dust structures were formed from mono dispersed melamine-formaldehyde dust particles of 2.55  $\mu\text{m}$  diameter. Registered were images of dust structures, corresponding current-voltage characteristics of discharge and the same characteristics of free discharge without dust particles. The optical registration of dust structure was carried out by means of a microscope equipped with video camera and diagnostic laser. The highest difference of current-voltage characteristics from free discharge was registered for discharges with large-scale dust structures containing large number of dust particles or spatially stable structures. Such structures were observed in the region of non-monotonous behavior of current-voltage characteristics at current of 0.5–1 mA. These values of current correspond to the sub-normal glow

discharge region. When instabilities in the form of dust acoustic waves were developed in dusty plasma, the difference between current-voltage characteristics of discharge with and without dust particles was not registered even at a very large total number of dust particles in structures that increased one in spatially stable structures.

## **GLOW DISCHARGE POSITIVE COLUMN IN AIR WITH THE CLOUD OF DISPERSE PARTICLES**

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The study of low pressure–low current glow discharge positive column with the cloud of disperse micron size particles was motivated by need to simulate changes of plasma parameters induced by introduction of dust cloud. These aspects are important at high density of particles, e.g. at cryogenic temperatures or in systems with a large number of particles, observed in microgravity conditions [1]. The simultaneous measurement of discharge and dust cloud parameters is carried out in this work and the diffusion model, explicitly described in [2, 3] is developed on the base of new results.

Dust structures in positive column of glow discharge in air were obtained at pressure of 0.1–0.6 torr and discharge current of 0.1–3 mA. The experimental setup is described in more details in [4]. The most stable dust structures were observed at a current of 0.6–2 mA and pressure of 0.4–0.5 torr with particle concentrations of  $(0.2\text{--}3.0)\cdot 10^5\text{cm}^{-3}$ . For these conditions the current-voltage characteristics of discharge with and without dust component were measured. The numerical model for the dust cloud with the specified geometry and particle concentration was developed, basing on diffusion approximation for description of plasma component and orbit-motion-limited approximation for particle charging. The influence of dust cloud size on radial electron and ion profiles were simulated. The cloud of particles, working as an additional factor of free electron losses in the bulk of plasma, was shown to be a discharge stabilizing factor with variable parameters. The smoothing of electron concentration over the discharge cross section under the action of dust cloud was demonstrated. The excess of ion concentration over electron increases with the size of dust cloud. Dust structures may be used as a tool to create a trap for positively charged ions without increase of discharge current.

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**RESONANCE EFFECTS OF NANOSECOND PULSE  
ACTION ON DUSTY STRUCTURES IN GLOW  
DISCHARGE PLASMA**

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Within researching processes of an appearance of ordered structures and phase transitions in non-ideal dusty plasma the behavior of dust structures under the action of nanosecond electric pulses in the DC glow discharge has been studied. The search of resonance effects, stabilization, precipitation and destruction of dust structures is carried out. We performed experiments to study the action of nanosecond electric pulses with pulse repetition frequencies from 4 to 300 Hz. The analysis of a particle fluctuation amplitude has revealed the resonant frequency of 7.1 Hz. The investigation of a mechanism of particle fluctuations was of great interest. It was revealed that nanosecond pulses change the background plasma near the particle and do not get an impact on the displacement of particles. In the previous experiments with the RF discharge a stabilization of particles was observed at the pulse repetition frequency of 16 Hz. The similar experiment has been made in the DC glow discharge. The stabilization effect of self-excited fluctuations and waves was observed at a pulse repetition frequency of 200 Hz. Such behavior of particles is due to that an application of the capacitor nanosecond discharge forms an additional local ionization of plasma and artificial striation in which the dust cloud is stabilized. The further increase of nanosecond pulses frequency caused the effect of the dusty crystal melting and subsequently a precipitation of particles. We found experimentally that when a dusty cloud contains particles of two sizes it is possible to separate a heavier fraction by the partial trap destruction.

# EXPERIMENTAL INVESTIGATION OF DUST PARTICLE DYNAMICS IN CORONA DISCHARGE

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The behavior of dust particles in corona discharge has been studied. The search of the possibility of dust particles with diameters of 50–150 microns to keep charge and to move in corona discharge in open and closed volumes was investigated. The quartz discharge tubes with various internal diameters 12, 16, 29 mm were used as closed volume. The bottom brass electrode has been made in the form of the cylinder. The top electrode has been made from molybdenum wire with diameter of 0.8 mm with radius of the round edge about 50 microns. The distance between electrodes was 28 mm. The design of the discharge cell allowed carry out researches of dust particles dynamics in corona discharge in various gases. The discharge cell with open volume consisted of two parallel copper plates. The gap between plates was 28 mm. Particles were located in discharge cells so that they covered with a thin layer a surface of a flat bottom electrode. Electrodes were connected to the high voltage source of a direct current. The voltage value can be changed up to occurrence of the spark discharge. Observation was carried out by high-speed camera Fast Hispec. The laser knife with thickness of a beam 150 microns on length of a wave of 550 nm was used for particle illumination. During performance of works it is established:

- The movement of dust particles in volume of discharge cell occurs only at the occurrence of corona discharge. If corona discharge is not present the movement of metal particles which are on a potential bottom electrode is not observed.
- Volume restriction of corona discharge by dielectric walls (discharge tube) improves conditions of lifting and moving of particles and prevents the escaping of particles from discharge zone.
- The favorable condition for lifting and movement of particles are realized in the flat geometry. In this case the dense cloud of levitation particles is observed. Moving particles with time leaved the discharge zone in area of weak electric field abroad electrodes and fell on the bottom surface.
- The estimated value of the particle charge is equal about million electron charges.

# THE POSSIBLE MECHANISM OF MACROPARTICLE MOVE FROM THE CATHODE IN STREAMER DISCHARGE

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The mechanism of metal macroparticles motion from the negatively charged electrode in a flat discharge gap with electric fields lower than the breakdown field is considered. In discharge gap with the distances between flat electrodes longer than 3 centimeters in air of atmospheric pressure the Taundsend breakdown is replaced by the streamer one. If the average intensity of electric field is insufficient to complete the breakdown then the streamers can start from the cathode and move in anode direction with high attenuation. These streamers will stop after some distance and they won't lead to breakdown in a spark stage. Macroparticles on the cathode surface increase the local intensity of electric field. As a result streamers start from the particle surface in anode direction. When the streamer stopped the local spatial charge of positive ions is formed near the particle. Electric field of this spatial charge in immediate proximity from the particle surface sum up with electric field in the discharge gap, and enhance it twice and even more times. This local non-uniform electric field and also polarization of metal particles in this field create conditions for a raising and moving of the small charged macroparticles from a cathode surface. Preliminary experiments show that in air in electric fields of 4.7–4.9 kilovolt per centimeter at occurrence of streamers the metal particles with diameter of an order 0.1 mm can leave the cathode. An estimated charge of particle is approximately equal about million electron charges.



# EXPERIMENTAL INVESTIGATION OF DUSTY STRUCTURES IN PLASMA CREATED BY PROTON BEAM

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In the dusty plasma studies one can distinguish works where the ionized medium is generated by fast charged particles incoming with the initial energy  $E$  from an external source into gas. In the slowing-down process in gas the non-equilibrium plasma is formed in the area of charged particle track with an expressed non-homogeneity in space and fast recombining in time. The medium molecule ionization results in the appearance of the first generation electrons, some part of them having energy sufficient for ionization of other atoms. Thus the spectrum of electrons is formed, including electrons of all subsequent generations. This spectrum has a non-equilibrium character with a non-Maxwellian electron velocity distribution. When getting into dust particles, electrons are absorbed, as a result grains acquire the negative electric charge and attract positive ions. However, because of a high mobility of electrons, dynamic equilibrium between the electron and ion flows is established at the negative charge of a dust grain. This charge, at a high energy of electrons, can be large enough for plasma to become highly non-ideal for the dust component, that forms the conditions for its crystallization. The work was devoted to experimental investigation of a behavior of dust particles in the track plasma generated by a beam of accelerated protons and obtaining ordered crystal-like structures of dust particles. The electrostatic proton accelerator has been used for the experiments. The experimental cell had the form of a rectangular parallelepiped with the basement of  $16 \times 16 \text{ cm}^2$  and height of 12 cm. The horizontal proton beam with energy 2 MeV and current of  $1 \mu\text{A}$  was passed via titanium foil and diaphragm of 8 mm diameter. Monodisperse melamine-phenol particles with radius of  $4.82 \mu\text{m}$  and polydisperse  $\text{CeO}_2$  particles were used in the experiments. The argon gas pressure was less than 10 Torr. At these conditions a number of dusty particles structures were formed. The structures were placed in the region between a dense dusty formation and the electrode to which a potential from 50 to 100 V was applied. The interparticle distances were increasing when approaching the electrode. The vortex movement and waves were noticed in the structures as well as a separation of particles on dimensions.

# SIMULATION OF DUST PARTICLES MOTION IN GAS DISCHARGE PLASMA

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In laboratory experiments it has been found that dust particles can acquire a kinetic energy of 10 eV and higher, significantly higher than the ion temperature and electron temperature in a gas-discharge plasma under certain conditions. The average kinetic energy of horizontal motion may significantly differ from the average kinetic energy of vertical motion of dust particles. Admissibility of the concepts of “temperature” and “kinetic energy” to describe the motion of dust particles and the equality of the average kinetic energy and “temperature” also raises many questions in the community. We attempt to simulate dust particles system in gas discharge plasma and clear considered questions.

A system of equations of motion of dust particles in a gas discharge is formulated in view many different effects, such as the charge fluctuations, features of near-electrode layer of the gas discharge, charging delay, charge dependence on distance from electrode, ion wake and others. A molecular dynamics simulation of dust particles motion is performed. Using molecular dynamics method allows us to take into account the aggregate effect of all the known phenomena, including nonlinear and stochastic, on the motion of dust particles. Varying the parameters of the equations of dust particles motion allows us to avoid the problem of the lack of exact values of some parameters of plasma-dust system. Varying the system parameters also allows getting approximation formulas for different characteristics, such as coupling parameter, kinetic energy, and interparticle distance.

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## BEHAVIOR OF BICOMPONENT DUST PLASMA CLUSTERS UNDER ELECTRIC PULSED LOADING

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Behaviour of bicomponent dust plasma clusters under electric pulsed loading using molecular dynamics method was investigated. The next phenomenological scheme was suggested for the description of dust particle charge changing after electric nanopulsed loading. The dust particle charges increased linearly 1.3 times from the initial value during 0.05 ms after electric nanopulsed loading, then particle charges decreased exponentially to initial ones during 0.15 ms. Yukawa potential was used to describe the interparticle interaction while a combination of the electrostatic field and gravity was used to describe confinement field.

Gain-frequency characteristics of dust particle clusters under electric pulsed loading were obtained. It was shown that resonance frequency is greatly affected by size of the dust cluster particles. Centre of mass oscillation of the bicomponent system is characterized by two resonance peaks. The position and the magnitude of each of them correspond to the position and the magnitude of resonance peak on the gain-frequency characteristics of the one-component system.

The work was supported by RAS Scientific Program “Thermal physics and mechanics of extreme energetic interactions and physics of strongly compressed matter”.

## TWO-STAGE EXPLOSIVE MAGNETIC GENERATOR WITH DISCONNECTING OF THE PRIMARY CIRCUIT CURRENT

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The design with open switch and with switching the load current is used most often to get in the inductive load of about 1  $\mu$ H the electric pulse with a steep leading front (front of the voltage pulse is not more than 3  $\mu$ s, the output energy of about 100 kJ). One of the alternatives is to use a

two-stage explosive magnetic generator with magnetic flux trapping (EMG MFT) and breaking of the primary circuit.

Results of experimental studies of EMG MFT with breaking and without breaking of the primary circuit are presented in the report. Generators tested at work on a model load inductance of  $1.16 \mu\text{H}$ . Experimental studies have shown that EMG MFT with breaking of the primary circuit has a higher efficiency in comparison with the EMG MFT without breaking of the primary circuit.

## EXPERIMENTAL STUDY OF GAS OUTFLOW FROM DISCHARGE CHAMBERS

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Gas outflow from discharge chamber is investigated experimentally. The discharge has been developed between two electrodes placed in the bottom of the chamber. Over the chamber the channel is placed and it is connected to atmosphere. The channel expands and heats surrounding gas. Channel expansion also causes formation of a shock wave [1]. Gas is able to expand only lengthwise the chamber channel which may cause interaction between gas and shock wave followed by gas. Gas characteristics depend also on the geometry of chamber channel. In current investigation were used: cylindrical channel, expanding channel, three holes channel. The aim was to investigate the influence of the channel geometry on the gas outflow.

The discharge conditions were created by the chain of 4 successive capacitors charged by high voltage impulse generator. Energy was altered in the range from 40 J to 369 J. For flow investigation Schlieren and Particle Image Velocimetry were applied. Due to Schlieren investigations length-time and shock wave velocity-time charts were obtained. Comparison of the charts has shown that shock wave propagation does not depend on channel geometry. Shock wave velocity-time charts have allowed to estimate energy input into the kinetic energy of the gas [2]. PIV data has allowed to divide outflow process into three phases. In the first phase gas velocity is high, jet has cylindrical shape. In the second phase vortex ring involves surrounding gas inside the streamer. The third phase begins when vortex ring stops its growth. Data analysis has shown that outflow from cylindrical channel has the highest velocity than outflows from other channels. Outflow from expanding channel has the highest velocity at the early

stages, but gas jet rapidly decelerates. The vortex in case of expanding channel has the biggest size. Interaction between three jets arose due to outflow from three holes channel leads to generation of single asymmetrical jet.

The author thanks to supervisor of studies Prof. E. Son and to the Streamer Ltd. company for partial financial support.

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## **ELECTRICAL DISCHARGE INFLUENCE ON PARAMETERS AND STRUCTURE OF GAS FLOWS IN EXTERNAL MAGNETIC FIELD**

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Experimental study of constricted electrical discharge influence on gas flows in external magnetic field is an important part of plasma aerodynamics. Motivation for investigations is to use the impact of the electrical discharge interaction with magnetic field [1] for vortex structures modification in tasks of flight control and for mixing intensification in tasks of plasma assisted mixing in practical applications. The objection of current work is to investigate influence of electrical discharge in external magnetic field on flow parameters, structure and mixing experimentally. Results of dynamical impact of the constricted electrical discharge in external magnetic field on gas flows are presented here.

One of experimental sections for the investigations is based on a construction described in [2]. The initial air flow comes into the test section. The electrical discharge is initiated between the central wire and annular electrodes. In external magnetic field under electromotive body force it moves and impacts the flow. Discharge parameters are measured by electric current and voltage probes. Discharge visualization is performed with high speed digital photo camera IDT Vision 3N. Velocity field measurements and flow structure visualization are performed with Particle Image Velocimetry technique. Data were obtained in plane of laser beam that was set at a distance of  $8.5 \times 10^{-2}$  m downstream from the central electrode and at a distance of  $0.5 \times 10^{-2}$  m from aerodynamical duct exit.

Under the discharge in magnetic field flow starts to rotate. Maximum value of tangential velocity for the case is  $\sim 1$  m/s that corresponds to estimation made with balance equation. It was observed that displacement of vortex center in opposite directions takes place for clockwise and anti clockwise discharge rotation. It can be explained by the angular momentum conservation law for the flow rotating in field of Archimedean force. There are no differences between time-averaged pictures of flow structure for the annular electrode-anode and cathode cases since discharge evolution is similar for the two cases under considered conditions [3].

The work is supported through Russia President Grant MK-3155.2011.8.

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## **DEVICE FOR REMOVAL OF CARBON DISULPHIDE FROM AIR BY STREAMER CORONA**

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Studies of conversion of carbon disulfide in gaseous ejections of chemical production began about 20 years ago. In Institute of Electrophysics UB RAS studies of conversion of CS<sub>2</sub> in plasma formed by pulsed electron beams and non-self-sustained discharges initiated by beams were carried out. It was explained that the mechanism of conversion and its products depend on parameters of beams and discharges. Conversion is achieved with low specific energy expenditures for removal of one CS<sub>2</sub> molecule [1].

However, the wide application of electron beams in real cleaning systems is held in control by three facts: by complexity and by high costs of electron-beam systems; by their insufficient reliability; and also by the need of creating the biological protection from ionizing radiation. In connection with this larger propagation obtain electric discharge methods, for example using a streamer corona, since similar installations are relatively cheap, reliable, simple in the operation and do not require the creation of the biological protection. Such advantages in the majority of the cases compensate the main disadvantage in the electric discharge systems—somewhat greater specific energy expenditures for conversion in comparison with electron-beam systems.

A device created by us is a special removable block attached to a multifunctional laboratory complex. The complex is described in [2].

The removable block is a cylindric gas chamber with a high-voltage thin wire metal electrode, located on the axis of the cylinder. A streamer corona discharge is ignited between the thin wire electrode and the cylinder. Discharge pulses in air have the following parameters: voltage at the discharge gap up to 135 kV, discharge current up to 500 A, discharge pulse duration up to 50 ns, energy of the discharge in one pulse about 0.5 J, pulse repetition rate up to 10 Hz.

The device presented here will make it possible to overcome the main disadvantages in the electron-beam methods. Furthermore, the optimization of the parameters of installation will make it possible to decrease specific energy expenditures for CS<sub>2</sub> removal.

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## THE GAS CLEANING ELECTRO FILTER EFFICIENCY IN THE SPARK AND ARC BREAKDOWN REGIMES

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It is necessary to support the voltage at the filter electrodes at the maximal possible level for the electro filter effective operation in the exhaust dust gaseous flow cleaning [1]. For this purpose it demands the unbroken voltage increasing at the filter electrodes which can be stopped in the voltage at the filter electrodes exceeds the discharge gap breakdown property and the breakdown was occurred in the electro filter cell-streamer, spark or arc breakdown.

At the spark breakdown that was characterized by the voltage decreasing to the zero value and the short-term current increasing the controlling system has to fulfill the next operation: The voltage at the filter electrodes was continuously watched up to the breakdown. The voltage level restoration after the breakdown was produced by the control angle value stating

as in formula in RF Patent 2399426

$$\alpha_f = K_1 - K_2 * K_2^2 + (1 - K_n), K_n = \frac{U_{max} - U_{min}}{U_{max}},$$

where  $K_1 = 5.5$ ;  $K_2 = 18$ ,  $U_{max}$ ,  $U_{min}$ —the maximal and minimal voltage values at the filter electrodes up to breakdown. After the voltage level restoration the controlling system has to form this angle with the taking into account the preceding operation calculated by the formula

$$\alpha_{ot} = \alpha_p - K_3(1 + \sin(\alpha_p) + \cos(2 * \alpha_p)),$$

where  $K_3 = 0.5$  at the spark and  $K_3 = 0.1$  at the arc breakdown. In the next the controlling system has to continue the opening angle increasing by the earlier stated program.

If the arc breakdown has been occurred in the electro filter cell characterized by the current through the discharge channel that was supported by the power supply id est this discharge current time duration and its value exceed the spark discharge values. In this case the controlling system has to take away the power thyristors control pulses for 1–2 half periods and then to fulfill the voltage restoration program as at the spark breakdown.

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## **ARC DISCHARGE BETWEEN GRAPHITE ELECTRODES AT LOW PRESSURE OF ARGON**

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Studied arc discharge arose after destruction of the sample which was heated by constant current within 5–30 minutes in argon atmosphere. The samples were made of rod of spectral graphite with diameter of 6 mm; the diameter of the central part of the sample on the length of 20 mm was reduced to 3 mm. During the exposure of the sample at filament current a gradual increase of the voltage on the sample and its temperature took place. When the sample temperature reached about 3.3 kK, the voltage on the sample sharply rose from 12 to 30 V; the integrity of the sample was violated, and arc discharge along the surface sample appeared.

Our study of this discharge at argon pressure of 10–90 kPa and the arc current about 100 A has shown that under these conditions the pressure of



argon weakly affects on the electrode processes. At pressure below 10 kPa the picture of these processes qualitatively varies. At the pressure above 10 kPa visible gap of 0.1 mm between cathode and anode part of the sample arose through 1–10 s after voltage jump, and the anode had look as a mace with a smooth surface. The maximum anode diameter increased by 10–20%. Anode temperature slightly changed along the surface and was about 3.5 kK. At low pressure the visible gap between two parts of sample arose through 30 s after voltage jump, and the anode part of the sample was covered by outgrowths with complex form. In these regimes the separation from the anode flat fragments with a size of about 3 mm was observed. Sharp drops of the temperature on the anode surface were about 0.5 kK. Thermogram of anode cooling after shutdown of arc had a peculiarity in the form of a plateau with duration of 30 ms at the temperature of 3.25 kK. Before shutting down the arc temperature of anode was about 3.4 kK; the argon pressure was 4 kPa. The origin of this plateau may be likely explained by the crystallization of the liquid carbon.

At the pressure above 5 kPa the cathode spot moved on the face surface with the speed about of 1 cm/s. Decrease of pressure was accompanied by expansion of the discharge on the lateral surface of the cathode. The cathode temperature was about 3.4 kK. In this mode the movement of the cathode spot stopped, and the cathode surface was quite smooth. When the pressure of argon was decreased below 0.3 kPa, the diffuse cathode spot destroyed, and moving cathode spot with size of 1 mm appeared. The speed of this spot was about 1 cm/s.

## **PULSE ARC DISCHARGE IN MINERAL AND ORGANIC OILS**

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In principle the explosion-safety of high-voltage oil-filled electrotechnical equipment (OFEE) can be enhanced through the use of some other insulating fluids instead of usual transformer oil. The arc discharge (AD) in organic (soy and canola) and transformer oils was investigated at duration of burning of 3–10 ms and the maximal current up to 50 kA. These conditions are typical for an initial stage of the AD which arises in OFEE after internal short circuit.

Experiments were spent in the discharge chamber with total volume of

61 l. The volume of oil was 35 l and the remaining volume was filled with nitrogen at atmospheric pressure. The AD was arisen at electric explosion of a copper wire with diameter of 0.1 mm, connecting parallel electrodes with diameter of 20 mm. The distance between electrodes was 48 mm. The energy released in AD reached about 100 kJ.

The diagnostic system included measurement of a current and a voltage of AD, pressure in oil and in nitrogen. The video shooting with a speed up to 2000 frames per second of development of the discharge and liquid-gas surface was spent. Propagation of the AD to oil was registered by means of potential probes. The contact probes were used to determine the oil velocity near the electrodes.

The maximal pressure in the liquids measured on distance of 0.2 m from AD column was about 2 MPa. At the same energy of AD the pressure in organic oils was noticeably greater than in mineral oil. Characteristic value of electric field strength in AD column was about 0.2 kV/cm. The electrical resistance of arc in organic oils with the same current was approximately twice as less than in the mineral one. In mineral oil gas producing factor in arc was about 0.11 l/kJ. In organic oils this factor was on 5–10% greater. The composition of the gases which have formed from the oils in the AD was defined.

## **PLASMA-DRIVEN MASS-SEPARATOR CONCEPT FOR NUCLEAR FUEL RECYCLING IN A CLOSED FUEL CYCLE**

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The recycling of a nuclear waste and spent fuel is a key technology for a closed nuclear fuel cycle. The plasma-driven mass-filtration is a promising technique [1, 2] for the segregation of heavy elements from a solid material. The benefits of this method are: the absence of a liquid active waste, compactness and the principal inability to segregate Pu, which is essential for the nuclear weapon materials security. The device under development functions basing on a principle of the nuclear fuel ionized particles (atoms and molecules) separation in the crossed electrical and magnetic static fields. The field optimization results are presented along with the collector, chamber and electrode systems design.

The productivity of the machine is estimated to be 100 g/h with the

starting ion energy of 3 eV, 1.5 kGs magnetic field tension, 1 kV maximum internal voltage and the characteristic chamber size of 1 m.

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*ING* — Institut Neel, Grenoble, France

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