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ABSTRACTS of the
XXIV INTERNATIONAL CONFERENCE
***INTERACTION OF INTENSE
ENERGY FLUXES WITH
MATTER***

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In this book abstracts of the XXIV International Conference “Interaction of Intense Energy Fluxes with Matter” (Elbrus, March 1–6, 2009.). The reports are devoted to the modern investigations in the field of extreme states of matter, including reviews of results obtained during the last 30 years since the 1st All-Union meeting on the problem of equation of state (Cheget, October 1978).

The following questions are covered:
models and theoretical calculations of equations of state at high concentrations of energy;
physics of shock and detonation waves;
experimental methods of diagnostics of rapid processes;
interaction of strong ion and electron beams, intense laser, x-ray and microwave radiation with matter;
methods of generation of intense impulse energy fluxes; electrical explosion of conductors under the action of powerful current pulses;
low-temperature plasma physics;
different physical and energetic aspects and technologies.

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CONTENTS

CHAPTER 1. POWER INTERACTION WITH MATTER

<u>Zhigilei L.V., Lin Z., Tahir E., Thomas D.A., Ivanov D.S.</u> Atomic-level simulations of laser interactions with metals . . .	20
<u>Ashitkov S.I., Agranat M.B., Anisimov S.I., Inogamov N.A., Komarov P.S., Ovchinnikov A.V., Petrov Yu.V., Sitnikov D.S.</u> Dynamics of expansion of front and rear surfaces of thin metallic film heated by femtosecond laser pulses	21
<u>Inogamov N.A., Ashitkov S.I., Zhakhovskii V.V., Petrov Yu.V., Khokhlov V.A., Agranat M.B., Anisimov S.I., Nishihara K., Komarov P.S.</u> Band structures of simple and noble metals and their material properties in a two-temperature state with hot electrons overheated above a cold crystal lattice by an ultrashort laser pulse	22
<u>Zhakhovskii V.V., Inogamov N.A., Ashitkov S.I., Agranat M.B., Petrov Yu.V., Nishihara K.</u> Ideal material strength, nanopallation, and molecular dynamics simulation by adequate EAM interatomic potential	23
<u>Inogamov N.A., Zhakhovskii V.V., Ashitkov S.I., Petrov Yu.V., Khokhlov V.A., Agranat M.B., Anisimov S.I., Nishihara K.</u> Ablation of simple (aluminum) and noble (gold) metals under action of femtosecond laser pulses	24
<u>Khishchenko K.V., Kostenko O.F., Levashov P.R., Povarnitsyn M.E., Veysman M.E., Andreev N.E., Fortov V.E.</u> Transport and optical properties of Au under femtosecond laser irradiation	25
<u>Povarnitsyn M.E., Andreev N.E., Khishchenko K.V., Kostenko O.F., Levashov P.R.</u> Simulation of ultrashort double pulse laser ablation of metals	26
<u>Andreev N.E., Fortov V.E., Kazakov E.D., Khishchenko K.V., Kostenko O.F., Kuehl Th., Levashov P.R., Povarnitsyn M.E., Rosmej O.N.</u> Interaction of PHELIX laser pulses with nanostructured targets: experiment and modeling	27
<u>Andreev N.E., Fortov V.E., Kuznetsov S.V., Tsirlina E.A., Veysman M.E., Cros B., Maynard G., Mora P.</u> Laser-plasma acceleration of relativistic electron bunches	27
<u>Khokonov M.Kh., Bekuliva I.Z., Keshev R.M.</u> Radiation spectrum of relativistic electrons in the high intensity limit of the external laser field	28

<u>Kostyukov I. Yu.</u> Electron dynamics in the relativistic plasma wake generated by short laser pulse: theory, simulation and experiment	29
<u>Kostyukov I. Yu.</u> , <u>Nerush E.N.</u> Oscillations of the plasma wake generated by tightly focused few-cycle laser pulse	30
<u>Komarov P.S.</u> , <u>Ovchinnikov A.V.</u> , <u>Fedorov V. Yu.</u> , <u>Kandidov V.P.</u> Filamentation of femtosecond laser pulse with 1.24 μm wavelength in air	30
<u>Petrovsky V.P.</u> , <u>Agranat M.B.</u> , <u>Ovchinnikov A.V.</u> Experimental researches of “SONY” CCD camera linear array response under action of femtosecond laser pulses	31
<u>Zmitrenko N.V.</u> , <u>Gus'kov S. Yu.</u> , <u>Demchenko N.N.</u> , <u>Doskoch I. Ya.</u> , <u>Rozanov V.B.</u> , <u>Stepanov R.V.</u> , <u>Tishkin V.F.</u> , <u>Vergunova G.A.</u> , <u>Yakhin R.A.</u> Mathematical modeling of the fast ignition laser targets and the HiPER project	32
<u>Grinenko A. Yu.</u> , <u>Gericke D.O.</u> Collisional absorption of laser light in strongly coupled plasmas	32
<u>Kurilenkov Yu.K.</u> , <u>Taranov V.P.</u> , <u>Gus'kov S. Yu.</u> Inertial electrostatic confinement and DD nuclear synthesis at interelectrode media of nanosecond vacuum discharge	33
<u>Gasilov S.V.</u> , <u>Pikuz T.A.</u> , <u>Faenov A. Ya.</u> , <u>Skobelev I. Yu.</u> , <u>Boldarev A.S.</u> , <u>Gasilov V.A.</u> , <u>Fukuda Y.</u> , <u>Kando M.</u> , <u>Kotaki H.</u> , <u>Daito I.</u> , <u>Homma T.</u> , <u>Kawase K.</u> , <u>Kameshima T.</u> , <u>Kawachi T.</u> , <u>Bolton P.</u> , <u>Daido H.</u> , <u>Kimura T.</u> , <u>Tajima T.</u> , <u>Kato Y.</u> , <u>Bulanov S.V.</u> Soft x-rays emission from fs laser plasma of the cluster jet targets based on the mixture of molecule and atomic gases	34
<u>Pikuz Jr. S.A.</u> , <u>Loupias B.</u> , <u>Gregory C.</u> , <u>Faenov A. Ya.</u> , <u>Pikuz T.A.</u> , <u>Nagorskiy N.M.</u> , <u>Benuzzi-Mounaix A.</u> , <u>Brambrink E.</u> , <u>Rabec le Gloahec M.</u> , <u>Koenig M.</u> x-ray backlighting and proton radiography imaging for diagnostics of shock waves and supersonic jets in intense laser plasma	35
<u>Bakhmutova A.A.</u> , <u>Lukyashin V.E.</u> , <u>Schardt D.</u> , <u>Martino G.</u> , <u>Pikuz Jr. S.A.</u> , <u>Golubev A.A.</u> Development of dosimetry methods for purpose of radiation therapy and ionography of biological objects	36
<u>Smirnov B.M.</u> , <u>Zhirnov K. V.</u> Kinetics of cluster growth in laser generation of metal clusters	37
<u>Kostenko O.F.</u> , <u>Andreev N.E.</u> Enhancement of k- α yield from the target with a clustered surface	38

<i>Azizi N., Malekynia B., Hora H., Miley G.H., Ghoranneviss M., He X.T.</i> Laser nonlinear force driven fusion energy from HB(11) by block ignition	39
<i>Kouhi M., Ghoranneviss M., Hora H., Malekynia B., Azizi N.</i> Alpha particle energy absorption in uncompressed DT for laser driven fusion	39
<i>Habibi M., Ghorbanalilu M.</i> Effects of ramp density profile on the relativistic self-focusing an intense laser beam	40
<i>Saleh Kotahi M.O., Moslehi Moslehabadi A.M., Mohammadi M.O.</i> Quasi mono-energetic soft x-ray beam produced by ultra-intense laser-produced electrons	40
<i>Loktionov E.Yu., Protasov Yu.Yu.</i> Experimental investigation of plume macrostructure and radiative gasdynamic processes of laser-matter interaction	41
<i>Bulgakova N.M., Bulgakov A.V., Zhukov V.P.</i> Ambient gas breakdown effects in ultrashort pulsed laser ablation of solid materials	42
<i>Kostin V.A., Silaev A.A., Vvedenskii N.V.</i> Ionization-induced generation of broadband terahertz radiation	43
<i>Silaev A.A., Vvedenskii N.V.</i> Phase effects in ionization-induced phenomena of the quasi-dc current excitation in the laser-produced plasma	44
<i>Krivko O.A., Klassen N.V., Kedrov V.V., Kudrenko E.A.</i> Particularities of laser destruction of microparticles of rare earth compounds	45
<i>Gatskevich E.I., Ivlev G.D., Malevich V.L.</i> Nanosecond laser ablation of silicon	46
<i>Privalov V.E., Raybul S.V., Shemanin V.G.</i> Polymer laser ablation destruction dynamics studies	47
<i>Kostanovskiy A.V., Presnyakov D.V., Kostanovskaya M.E.</i> Radiance temperature and normal spectral emissivity at 650 nm of hafnium at the melting point by a thin plate method . . .	49
<i>Kostanovskiy A.V., Kostanovskaya M.E.</i> Speed of the heating of high-temperature metals and parabolic model of heat conductivity	49

<u>Chernenko A.S., Anan'ev S.S., Bakshaev Yu.L., Bartov A.V., Blinov P.I., Dan'ko S.A., Kazakov E.D., Kalinin Yu.G., Kingsep A.S., Korolev V.D., Mizhiritsky V.I., Pikuz S.A., Shelkovenko T.A., Smirnov V.P., Tkachenko S.I., Ustroev G.I., Zelenin A.A.</u> Study of plasma parameters in hot points of megaampere X pinch	50
<u>Anan'ev S.S., Dan'ko S.A., Kalinin Yu.G.</u> Registration of temporal evaluation of characteristic x-ray radiation of multi-wire MA Z-pinch plasma	51
<u>Zelenin A.A., Akunets A.A., Anan'ev S.S., Bakshaev Yu.L., Blinov P.I., Chernenko A.S., Dan'ko S.A., Kazakov E.D., Korolev V.D., Pimenov V.G., Smirnova E.A., Ustroev G.I., Vikhrev V.V.</u> Neutron radiation from the constriction of fast deuterated Z-pinch	51
<u>Tkachenko S.I., Romanova V.M., Mingaleev A.R., Ter-Oganesyan A.E., Shelkovenko T.A., Pikuz S.A.</u> Study of material distribution in the dense core and rare plasma corona upon electrical explosion of wires	52
<u>Dyachenko S.V., Gasilov V.A., Krukovsky A.Yu., Tkachenko S.I., Olkhovskaya O.G., Bagdasarov G.A., Marchenko V.A.</u> Simulation of a tungsten wire heating by a current pulse	53
<u>Efremov V.P., Shurupov A.V., Polistchook V.P., Fortov V.E., Ivanov M.F., Kiverin A.D., Apfelbaum E.M., Iorish V.S., Khishchenko K.V., Dementiev Yu.A., Darian L.A.</u> Physical and numerical modeling of processes of the large power objects explosion	54
<u>Dudin S.V., Kozlov A.V., Leont'ev A.A., Mintsev V.B., Ushnurtsev A.E., Fortov V.E., Shurupov A.V., Shurupova N.P.</u> A magnetic-cumulative generator with magnetic flux trapping and a primary circuit being switched off	55
<u>Dudin S.V., Lavrov V.V., Leont'ev A.A., Mintsev V.B., Ushnurtsev A.E., Fortov V.E., Shurupov A.V.</u> Initiation of explosive-magnetic generator with a help of explosive wires	56
<u>Aksenov A.G., Fortova S.V., Troshkin O.V.</u> Heavy ion targets for the inertial fusion and for experiments with high energy density in matter	57
<u>Kim V.V., Matveichev A.V., Tahir N.A.</u> Computer simulation of solid graphite Super-FRS fast extraction targets	58

<u>Zhilyakov L.A., Kostanovskiy A.V., Kulikauskas V.S., Pokhil G.P., Fridman V.B.</u> Oscillations current of the proton beams at passing through dielectric channel	59
<u>Pokhil G.P., Vokhmyanina K.A., Mironchik A.I.</u> Ion guiding through an insulating capillary	60
<u>Bakulin V.N., Ostriuk A.V., Romadinova E.A.</u> Wide-range elementary cell for heterogeneous material with disperse filler	61
<u>Bugay I.V., Ostriuk A.V.</u> Deformation and destruction of multi-layer elastic-plastic shells under combined thermal and mechanical actions of radiations and particles fluxes	62
<u>Gribanov V.M., Ostriuk A.V.</u> Estimation method of pressure impulses formed in irradiated heterogeneous material having frame	63
<u>Romadinova E.A., Ostriuk A.V.</u> Hybrid method of energy absorbing calculation for x-ray irradiated spheroplastics	64
<u>Rusin S.P.</u> Computer modeling non-stationary heat transfer through dispersion materials at high temperatures	65
<u>Bisti V.E.</u> Charge-density excitations in bilayer graphene graphene in high magnetic field	66
<u>Steinman E.A.</u> Investigation of structural defects in Si subjected to high pressure treatment	67
<u>Savintsev Yu.P., Savintseva S.A., Shevchenko V.S., Uraakaev F.Kh.</u> On the microwave assisted synthesis of selenium nanostructures in polymeric composites	68
<u>Nikolaenko I.V., Kedim N.A., Shveikin G.P.</u> Microwave synthesis of ultra-nanopowders of tungsten oxide	69
<u>Gurentsov E.V., Eremin A.V.</u> Nonequilibrium radiation during iron clusters formation at room temperature	70
<u>Maikov I.L., Torchinsky V.M., Zaitchenko V.M.</u> Modelling of wave influence on the gascondensate system	71

CHAPTER 2. SHOCK WAVES. DETONATION. COMBUSTION

<u>Kanel G.I.</u> Mechanism and criterion of steady detonation without chemical spike	73
<u>Kovalev A.E., Kanunova L.I., Khishchenko K.V., Komissarov V.V., Lomonosov I.V., Mezhevov A.B., Novikov M.G., Zhernokletov M.V., Fortov V.E.</u> Measurement of sound velocities in shock-compressed tin at pressures up to 150 GPa	74

<u>Milyavskiy V.V., Ten K.A., Borodina T.I., Valiano G.E., Zhulanov V.V., Kulipanov G.N., Lukyanchikov L.A., Prueuel E.R., Titov V.M., Tolochko B.P., Fortov V.E.</u> Hugoniot of C ₇₀ fullerite via synchrotron radiation technique	75
<u>Bezruchko G.S., Kanel G.I., Razorenov S.V., Savinykh A.S., Milyavskiy V.V., Khishchenko K.V.</u> Graphite transformation in the different structural state to the diamond-like phase in dependence to loading direction	76
<u>Savinykh A.S., Kanel G.I., Razorenov S.V., Bezruchko G.S., Khishchenko K.V.</u> Influence of initial temperature of graphite on parameters and kinetic transformations into diamond at shock-wave loading	77
<u>Belyatinskaya I.V., Fel'dman V.I., Milyavskiy V.V., Borodina T.I., Belyakov A.A.</u> Rock-forming minerals transformations in conditions of step-like shock compression of crystal schist	78
<u>Shakhray D.V., Molodets A.M., Khrapak A.G.</u> Mechanism of aluminium hydride AlH ₃ electroconductivity at high multy shock pressures	79
<u>Avdonin V.V., Shakhray D.V., Zhukov A.N., Palnichenko A.V., Sidorov N.S.</u> Study of superconductivity properties of magnesium diboride after its shock wave loading up to 65 GPa	80
<u>Golyshhev A.A., Molodets A.M.</u> Thermal conductivity of indium at high pressure and temperature of shock compression	81
<u>Novikov M.G., Kovalev A.E., Zhernokletov M.V., Khishchenko K.V.</u> Temperature in shock-compressed samples and equation of state of epoxy resin ED-5 at high dynamic pressures	81
<u>Kolesnikov S.A., Golubev A.A., Demidov V.S., Demidova E.V., Dudin S.V., Kantsyrev A.V., Mintsev V.B., Smirnov G.N., Turtikov V.I., Utkin A.V., Shutov A.V., Fortov V.E., Sharkov B.Y.</u> Application of charged particle beams to shock-wave and detonation studies: first results	82
<u>Glazkov V.S., Ignatova O.N., Malyshev A.N., Nadezhin S.S., Podurets A.M., Raevskiy V.A., Tyupanova O.A.</u> Peculiarities of high-rate deformation of copper upon convergence of cylindrical channels by action of shock waves	83
<u>Zeldovich V.I., Shorokhov E.V., Frolova N.Yu., Zhgiliev I.N., Kheifetz A.E., Khomskaya I.V., Nasonov P.A., Ushakov A.A.</u> Dynamic channel-angular pressing of titanium at high temperature	84

<u>Skripnyak V.A., Skripnyak V.V., Tyulina N.A.</u> Mechanical response of ultrafine grained metal alloys to influence of shock waves	85
<u>Skripnyak E.G., Skripnyak V.A., Pasko E.G.</u> Simulation of mechanical behavior of ceramic nanocomposites under shock wave loadings	86
<u>Naimark O.B.</u> Structural-scaling transitions in mesodefekt ensembles and nonlinear aspects of plasticity and failure in shocked solids	87
<u>Bayandin Yu.V., Uvarov S.V., Naimark O.B.</u> Mesodefekt induced mechanisms of plasticity and failure in shocked solids	88
<u>Uvarov S.V., Bayandin Yu.V., Naimark O.B., Oborin V.A.</u> Structure properties and structural-scaling transition in the armco iron under plate-impact loading	89
<u>Adushkin V.V., Dubovskoy A.N., Pernik L.M., Popel S.I.</u> Nano- and microscale knockings of rocks in experiments of fracture by successive explosions	90
<u>Zolnikov K.P., Parfenov N.A., Psakhie S.G.</u> Influence of internal structure on metal behavior under uniform pulse loading . .	91
<u>Kryzhevich D.S., Zolnikov K.P., Psakhie S.G.</u> Simulation of electrothermal pulse dispersion of a crystal-structured metal wire	92
<u>Kuksin A.Yu.</u> Molecular dynamics simulation of void growth in crystals under tensile loading	92
<u>Zhilyaev P.A., Kuksin A.Yu., Yanilkin A.V.</u> Atomistic simulations of dislocation nucleation in Al under high strain rate .	93
<u>Zhilyaev P.A.</u> Atomistic modeling of spall fracture near melting curve	94
<u>Norman G.E., Pisarev V.V., Stegailov V.V.</u> Spall kinetics in liquids at high strain rates	94
<u>Sosikov V.A., Utkin A.V.</u> Tension features of liquid and solid matter near melting point by shock waves	96
<u>Izvekov O.Y.</u> Fragmentation model of elastic media with damage accumulation	97
<u>Radchenko P.A., Radchenko A.V.</u> Modeling of destruction of materials with preferential properties orientation under dynamic loads	98
<u>Gorelski V.A., Khorev I.E.</u> Mechanisms of spall fracture of targets at high velocity impact	99
<u>Shipachev A.N., Zelepugin S.A.</u> Simulation of high-speed orthogonal cutting of metals using finite element method	100

<u>Konyukhov A.V., Likhachev A.P., Fortov V.E.</u> Numerical study of viscous shock wave behaviour in the regions of ambiguous representation of the shock wave discontinuity	101
<u>Konyukhov A.V., Likhachev A.P., Fortov V.E., Khishchenko K.V., Lomonosov I.V.</u> Numerical simulation of converging shock waves in thermodynamically non-ideal media	102
<u>Fortova S.V.</u> The cascade mechanism in free shear flows	103
<u>Simonov I.V.</u> Examination of collision of jets with ultrahigh velocities using various equations of state	103
<u>Shutov A.V.</u> Extension of acoustic Riemann solver for elastic body on case of Riemann invariants jump on contact discontinuity	104
<u>Ivanov A.V., Parshikov A.N.</u> Parallel implementation of smoothed particle hydrodynamics	105
<u>Lozitski I.M.</u> Numerical modeling of transient temperature fields in blanket of heavy ion fusion reactor chamber	106
<u>Piskunov V.N., Davydov I.A., Rudenko V.V., Veselov R.A., Voronin B.L., Demin D.A., Petrov A.M.</u> Method of cluster dynamics for simulation of dynamic processes of continuum mechanics	106
<u>Levashov P.R., Povarnitsyn M.E., Khishchenko K.V., Zakharenkov A.S.</u> 1D gas-dynamic simulation of shock-wave processes via Internet using different models of equation of state	107
<u>Barenbaum A.A.</u> The tectonic processes caused by fallings of large space bodies (according to geological data)	108
<u>Ten K.A., Titov V.M., Lukyanchikov L.A., Prueel E.R., Zhogin I.L., Tolochko B.P.</u> Synchrotron diagnostics the density distribution at the detonation front	109
<u>Prueel E.R., Kashkarov A.O., Merzhievsky L.A., Lukyanchikov L.A.</u> Density evolution during the initiation of detonation in porous PETN	109
<u>Kuper K.E., Ten K.A., Prueel E.R.</u> High explosives examination by high-resolution x-ray computed tomography on the VEPP-3 synchrotron radiation	110
<u>Yankovskiy B.D., Milyavskiy V.V.</u> Action of the water content on the scattering dynamics of detonation products of water-containing explosives	111
<u>Balagansky I.A., Hokamoto K., Manikandan P., Matrosov A.D., Stadnichenko I.A., Miyoshi H.</u> Phenomena of energy focusing in explosive systems, which include high modulus elastic elements	112

<i>Ivanov M.F., Kiverin A.D., Galburt V.A., Petukhov V.A.</i> Influence of the shock wave impact on the combustion regimes . .	113
<i>Ivanov M.F., Kiverin A.D.</i> Combustion of explosive mixtures of various composition	114
<i>Ivanov E.N., Ivanov M.F.</i> The statistical correlated parameters of axially turbulized medium inside combustion chamber under moveable piston	116
<i>Burov Yu.M., Smekhova A.G.</i> High pressure influence on velocity of monomolecular reaction	117
<i>Ziborov V.S., Efremov V.P., Fortov V.E., Shumova V.V.</i> Energy exchange in shock waves propagating in helium containing a small concentration of Mo(CO) ₆	118
<i>Golub V.V., Semin N.V.</i> On air compression with the help of detonation	119
<i>Ivanov K.V., Baklanov D.I., Volodin V.V., Golub V.V.</i> Experimental investigation of acoustic influence on the ignition of oxygen-hydrogen mixture	120
<i>Mikushkin A.Y., Golovastov S.V., Golub V.V.</i> Inhibition of spontaneous decomposition of acetylene by hydrocarbon and hydrogen by initial pressure 1–2.5 bar. An experimental investigation	121
<i>Semin N.V., Golub V.V., Laskin I.N., Bazhenova T.V.</i> Solution for a practical problem in hydrogen safety program	122
<i>Molkov V.V., Makarov D.V., Bragin M.V.</i> Physics and modelling of under-expanded jets and hydrogen dispersion in atmosphere	123
<i>Emelianov A.V., Eremin A.V., Fortov V.E., Makeich A.A.</i> Detonation wave of condensation	124
<i>Drakon A.V., Eremin A.V., Kulikov S.V.</i> Monte-Carlo and kinetics modeling of nonequilibrium processes in shock wave front	125
<i>Eremin A.V., Makeich A.A.</i> The application of ARAS and shock wave technique for investigation of small iron clusters formation in different gas-diluters	126
<i>Bronin S.Y., Emelianov A.V., Eremin A.V., Khrapak A.G.</i> Charging of carbon nanoparticles formed during shock wave pyrolysis of C ₃ O ₂	127
<i>Falyakhov T.M., Volodin V.V., Golub V.V., Golovastov S.V., Semin N.V., Tarasenko I.N., Baklanov D.I.</i> Compression of air behind the piston driven by detonation: experimental investigation	128

<u>Lenkevich D.A., Volodin V.V., Golovastov S.V., Golub V.V., Baklanov D.I., Ivanov K.V.</u> Experimental investigation of hydrogen self-ignition at the discharge into air	129
<u>Golovastov S.V., Laskin I.N.</u> Numerical investigation of mechanisms of acetylene spontaneous self-decomposition	129
<u>Kraiko A.N., Valiyev Kh.F.</u> The cylindrical and spherical fast intense compression of ideal gas with the adiabatic exponents from 1.2 to 3	130
<u>Maikov I.L., Director L.B.</u> Numerical simulation of dynamics of viscous liquid drops ensemble in a gravitational field	132
<u>Bessmertnyh A.V., Director L.B., Markov A.V., Shpilrain E.E., Zaitchenko V.M.</u> Bioconversion: power technological complexes	133
<u>Kosov V.F., Maikov I.L., Sinelshchikov V.A., Sokol G.F., Zaitchenko V.M.</u> Study of pyrocarbon formation in the binary mixtures of methane and its homologues	133
<u>Kosov V.V., Kosov V.F., Maikov I.L., Sinelshchikov V.A., Zaitchenko V.M.</u> High-calorific gas mixtures produced by pyrolysis of peat	135
<u>Sumskoi S.I., Efremov K.V., Lisanov M.V., Sofyin A.S.</u> Numerical modeling of severe accidental emission's consequences in industry	136
<u>Andrievskaya V.U., Dikinov H.J., Adzhiev A.H., Zashakuev Z.T.</u> Influence of spectral structure of aerosol particles in an atmosphere on a degree of absorption of electromagnetic radiation	137

CHAPTER 3. EQUATIONS OF STATE FOR MATTER

<u>Shpatakovskaya G.V.</u> Periodic orbits in atomic-ion systems	139
<u>Novikov V.G., Grushin A.S., Ovechkin A.A.</u> Quasizones and resonances in the selfconsistent field models of dense plasma	140
<u>Lomonosov I.V.</u> Equations of state for copper, silver and gold	141
<u>Degtyareva V.F., Degtyareva O.</u> Structure of beta-brass CuZn at high pressure to 90 GPa	142
<u>Levashov P.R., Sin'ko G.V., Smirnov N.A., Khishchenko K.V.</u> Thermal excitation of electrons and applicability boundary of pseudopotential approaches	142
<u>Veysman M.E., Levashov P.R., Khishchenko K.V., Andreev N.E.</u> Thermodynamics of electrons in metals under femtosecond irradiation	143

<u>Stegailov V.V.</u> Ab initio modeling of metals with hot electron sub-system	144
<u>Vorob'ev V.S., Apfelbaum E.M.</u> The critical points of several metals determined on the basis of their connection with unit compressibility line (Zeno-line) parameters	144
<u>Smirnov B.M., Berry R.S.</u> Phase transitions in metal clusters . .	145
<u>Baturin V.A.</u> EOS and chemical composition in the Sun through the helioseismology	146
<u>Gorshkov A.B., Baturin V.A.</u> Element diffusion during evolution of the Sun	147
<u>Ostrik A.V.</u> Numerical investigation of nucleation in the first-order phase transitions	147
<u>Borzov D.N.</u> Optical vibrations of hydrogen in disordered palladium-gold alloys	148
<u>Kuzovnikov M.A.</u> Vibrational properties of hydrogen impurity in high-pressure palladium deuteride	149
<u>Mutailamov V.A., Murtazaev A.K.</u> Dynamic critical behaviour of Heisenberg model with strong easy plane anisotropy	150
<u>Khizriev K.Sh., Murtazaev A.K.</u> Magnetic ordering in model of superlattice Fe/V with the negative interlayer exchange interaction	152
<u>Koptseva A.A.</u> Dimensional dependence of surface energy of ionic dielectric of the nanodimensional scale	153
<u>Gordon E.B., Kashtanov P.V., Smirnov B.M.</u> Equation of state for compressed inert gases	154
<u>Efimchenko V.S.</u> High-pressure hydrogen hydrates	155
<u>Shemyakin O.P., Levashov P.R., Khishchenko K.V.</u> Thermodynamic characteristics of metals with basis on Hartree–Fock–Slater model	156
<u>Kheifets O.L., Melnikova N.V., Shakirov E.F., Shabashova O.A., Babushkin A.N.</u> Electrical properties of copper chalcogenides CuInAsS ₃ , CuInAsSe ₃ and CuInSbS ₃ at low temperatures and high pressures	157
<u>Melnikova N.V., Kheifets O.L., Babushkin A.N., Sokhareva N.S., Pinigina K.S.</u> Cation conductance of the some glasses in system Cu–Ag–Ge–As–Se	158
<u>Karpenko S.V.</u> The size effects of the metallization pressure of alkali-halide crystals with small dimensions	159

<u>Mamchuev M.O.</u> Phase transition dielectric–metal in massive alkali-halide crystals in the conditions of hydrostatic compression	160
<u>Zubov V.I.</u> The third, molecular, form of carbon—fullerenes, fullerenes and fullerides. Pre-history, discovery and physical properties	161
<u>Basharin A.Y.</u> Investigation of the liquid carbon: new approach and fundamental results	162
<u>Basharin A.Y., Dozhdikov V.S., Turchanin M.A.</u> Structure of non-graphite carbon phases quenched from liquid carbon . .	163
<u>Basharin A.Y., Lysenko I.Y., Sobina O.A., Turchanin M.A.</u> Determination of the contact angle: liquid carbon and graphite	164
<u>Basharin A.Y., Lysenko I.Y., Sobina O.A., Turchanin M.A.</u> Vapor-crystal and vapor-liquid-crystal graphite growth mechanisms	165
<u>Polistchook V.P., Asinovsky E.I., Kiselev V.I., Mendeleev V.Y., Samoylov I.S., Skovorod'ko S.N.</u> Development of procedures and an experimental study of phase transformations on the surface of graphite at temperatures up to 3.3 kK	165
<u>Klimovskii I.I.</u> Physical synthesis of carbide. Thermodynamic background, challenges, and results	166
<u>Andreev V.G., Baev V.P., Dobrinskiy E.K., Klimovskii I.I., Malashin S.I.</u> Thermodynamically non-equilibrium material	167
<u>Verzhichinskaya S.V., Bukharkina T.V., Klimovskii I.I., Dobrinskiy E.K., Malashin S.I.</u> Synthesis of the new carbon modification by quenching carbon vapor and condensed particles in argon atmosphere	168
<u>Khokonov A.Kh., Kochesokov G.N., Dolov M.Kh.</u> State equation of krypton and xenon on the graphite surface	169
<u>Ustyuzhanin E.E., Shishakov V.V., Reutov B.F., Abdulgatov I.M., Frenkel M.M.</u> Scaling models of the saturation pressure in the critical region: possibilities and limits	170
<u>Starikov S.V., Stegailov V.V.</u> Peculiarity of surface melting of Al and Fe at high pressure	171
<u>Sergeev O.V., Stegailov V.V.</u> Density fluctuations and the kinetic spinodal in a simple liquid	172
<u>Nasretdinov Y.A., Stegailov V.V.</u> Modelling of methane hydrates using molecular dynamics	173

<u>Kislenko S.A., Samoylov I.S., Amirov R.H.</u> Molecular dynamics simulation of the electrochemical interface between graphite surface and ionic liquid [BMIM][PF ₆]	173
<u>Saakyan A.G., Peletsky V.E., Shur B.A.</u> Experimental study of thermodynamic properties of construction materials with the method of subsecond resistive heating	174
<u>Pikalov G.L., Kiseev S.V.</u> Use of physical models for experimental ratings of protective properties of engineering	175
<u>Dinariev O.Yu., Kudinov I.V., Evseev N.V.</u> Modeling interfacial phenomena in multicomponent mixtures using gradient terms introduced in free energy	176

CHAPTER 4. PHYSICS OF LOW TEMPERATURE PLASMA

<u>Levashov P.R., Filinov V.S., Bonitz M., Fortov V.E.</u> Wigner representation of quantum mechanics and conductivity of dense hydrogen plasma	178
<u>Iosilevskiy I.L.</u> Plasma polarization in massive astrophysical objects	178
<u>Reinholz H., Adams J., Lorenzen S., Raitza Th., Röpke G., Sengebusch A., Wierling A.</u> Diagnostics of dense Coulomb systems via transport and optical properties	179
<u>Zaporozhets Yu.B., Mintsev V.B., Gryaznov V.K., Reinholz H., Röpke G., Fortov V.E.</u> The angular dependence of s- and p-polarized reflectivities of explosively driven dense plasma . .	181
<u>Winkel M., Reinholz H., Wierling A., Röpke G.</u> Dynamical collision frequency in warm dense matter	182
<u>Vichev I.Yu., Novikov V.G., Solomyannaya A.D., Zaitsev V.I., Volkov G.S., Fedulov M.V.</u> Emission spectra research of the plasma mix	183
<u>Zakharov V.S., Novikov V.G.</u> Extra EUV emission from the xenon ions	183
<u>Norman G.E., Lankin A.V.</u> Crossover between excited atoms and free electrons	184
<u>Lankin A.V.</u> Description of recombination in strongly coupled plasmas	185
<u>Lankin A.V., Norman G.E., Saitov I.M.</u> Influence of pair fluctuations on the equation of state of nonideal plasmas	186
<u>Shumikhin A.S., Khomkin A.L.</u> High-temperature and low-temperature chemical models of dense metal vapor plasma .	187

<u>Apfelbaum E.M.</u> The calculation of the transport coefficients of noble gases under high pressure	188
<u>Goncharov A.V., Kashtanov P.V., Smirnov B.M.</u> Numerical simulation of cluster magnetron discharge plasma	189
<u>Hihluha D.R., Zelener B.V., Zelener B.B., Manykin E.A.</u> Velocities coefficients for excitation and deexcitation at collisions between Rydberg atoms and slow electrons	190
<u>Myasnikov M. I.</u> Kinetics of transitions between Rydberg states in low temperature plasma	191
<u>Shapoval S.Yu., Barabanenkov M.Yu., Ganiev A.S., Severov D.S.</u> Reflection efficiency of two-dimensional square symmetry unmagnetized plasma photonic crystals in microwave wavelength range	192
<u>Kosarim A.V., Shevelko V.P., Smirnov B.M.</u> Resonant charge exchange involving nitrogen and oxygen	193
<u>Vlasov A.N., Kolesnikov S.A., Manoshkin A.B., Panin V.V., Potashevsky S.S.</u> Exploding wire spirals rolled up in toroidal form	194
<u>Konovalov V.S., Kozlov A.N., Novikov V.G.</u> About the stationary and pulsing modes of the ionizing gas flow in the channel of the quasi-steady plasma accelerator (QSPA)	195
<u>Tereshonok D.V.</u> Thermal flow control	196
<u>Fortov V.E., Petrov O.F., Vaulina O.S.</u> Dust-plasma liquid in statistical theory of liquid state: experiments an simulations . .	197
<u>Antipov S.N., Maiorov S.A., Petrov O.F., Fortov V.E.</u> Dusty plasma structures in supersonic ion flow: experiments with dc glow discharge	198
<u>Maiorov S.A.</u> Dust particle charging in the upper atmosphere . .	198
<u>Prokopiev E.P., Grafutin V.I., Zakharov A.F., Razinkova T.L.</u> About opportunities of positron diagnostics for research of dust space plasma	199
<u>Vorona N.A., Gavrikov A.V., Petrov O.F., Vasiliev M.N.</u> Ultra-high charging of particles and coulomb explosion in dusty plasma induced by electron beam	200
<u>Bayandina D.V., Vasiliev M.N., Mamohin A.A., Postovarov P.I.</u> Experimental study of electron beam passing through the layer of aerosol which contains solid particles	201
<u>Vladimirov V.I., Deputatova L.V., Bogachev S.S., Rykov V.A.</u> Experiments with dusty plasma generated by a proton beam . .	202

<u>Vasilyak L.M., Vetchinin S.P., Polyakov D.N., Morfill G.E., Ivlev A.V., Pustynnik M.Y., Thomas H.M.</u> Dust cluster response to the high voltage nanosecond pulses	203
<u>Filippov A.V.</u> Electrostatic interaction of spherical conducting macroparticles in a plasma	204
<u>Vasiliev M.M., Antipov S.N., D'yachkov L.G., Petrov O.F.</u> Dynamics features of dust plasma structures in magnetic fields in a dc discharge	205
<u>Vasilieva E.V., Timirkhanov R.A., Gavrikov A.V., Petrov O.F.</u> The dynamical and structural features of dusty plasma structures in rf discharge	206
<u>Timirkhanov R.A., Vasilieva E.V., Gavrikov A.V., Petrov O.F.</u> Experimental study of dusty plasma with rod-like macroparticles	206
<u>Zobnin A.V.</u> The impact of dusty cloud on the dc discharge positive column structure	207
<u>Savin S.F., D'yachkov L.G., Vasiliev M.M., Petrov O.F., Fortov V.E.</u> Coulomb clusters of charged diamagnetic macroparticles in inhomogeneous magnetic fields	207
<u>Kostanovskiy I.A., D'yachkov L.G.</u> Charging and screening of small dust particles in plasmas over a wide range of collisionality	208
<u>Schweigert I.V., Aleksandrov A.L., Ariskin D.A.</u> Effect of transport of growing nanoparticles on crcf discharge dynamic	209
<u>Ariskin D.A., Schweigert I.V., Aleksandrov A.L.</u> Mode transition in capacitively coupled radio-frequency discharge in argon/acetylene mixture	210
<u>Abdrashitov A.V., Zolnikov K.P., Psakhie S.G.</u> Behavior of charged dusty particle systems of spherical and cylindrical symmetry under pulse loading	211
<u>Chikina J.V., Nazin S.S., Shikin V.B.</u> Dynamics of charged clusters in liquids in the pseudo-steady regime	212
<u>Norman G.E., Stegailov V.V., Timofeev A.V.</u> Kinetic temperature of charged dust particles in nonideal dust plasma	212
<u>Koss X.G., Vaulina O.S.</u> Criteria of formation of new layers in dusty plasma with isotropic pair interaction potentials	213
<u>Lisin E.A., Vaulina O.S.</u> New technique for restoration the pair potential of interacting particles in non-ideal systems	214

<u>Pinchuk M.E., Bogomaz A.A., Budin A.V., Rutberg Ph.G., Petrenko M.V., Losev S.Yu., Pozubenkov A.A., Kuznetsova I.V.</u> Radiation characteristics of high current pulsed discharge in high density hydrogen in visible and soft x-ray spectral ranges	215
<u>Petrov A.A., Amirov R.H., Samoylov I.S.</u> On the nature of cathode erosion in Trichel pulse negative corona	216
<u>Belevtsev A.A., Goryachev S.V., Chinnov V.F., Isakaev E.Kh.</u> The phase state of a tungsten cathode surface in high current atmospheric pressure electric arcs	217
<u>Kozlov A.V., Darian L.A., Luzganov S.N., Povareshkin M.N., Polistchok V.P., Uchvatov A.N., Tsyba N.E., Shurupov A.V.</u> Study of gas formation in the transformer oil in the pulse arc discharge	219
<u>Egorov O.G.</u> Engineering foundation of pulsed generator on inductive storage and combination of vacuum interrupter and plasma opening switch	220
<u>Shurupova N.P., Malyshev A.V., Shakaryan Yu.G., Novikov N.L., Kozlov A.V., Luzganov S.N., Povareshkin M.N., Uchvatov A.N., Shurupov A.V., Fortov V.E.</u> The inductive limiter of a short-circuit current	221
<u>Shurupov M.A., Rainish V.A., Shurupov A.V.</u> On fractional separation of submicron size powders with the help of plasma discharge	221
<u>Bardin A.A., Polushkin E.A., Kovalchuk A.V., Shapoval S.Yu.</u> Low temperature ECR plasma technology towards nanoscale devices creation	222
<u>Rud A.D., Kuskova N.I., Ivaschuk L.I., Fruchart D., Boguslavskii L.Z., Oreshkin V.I.</u> Utilization of high energy electric discharge techniques for production of carbon nanomaterials . .	223
<u>Amirov R.H., Isakaev E.Kh., Kiselev V.I., Merkulov V.V.</u> Development and experimental investigation of the carbon nanotubes synthesis process using a plasma torch	224
<u>Glazkov V.V., Merkulov V.V., Mordinsky V.B., Sinkevich O.A., Shustov Ye.N.</u> Experimental and theoretical investigation of the plasma torch with expanding channel for the coating purposes	225
<u>Kuznetsov D.L., Surkov Yu.S., Uvarin V.V., Filatov I.E.</u> Device for frequency pumping of Ar-Xe-laser by a non-self-sustained discharge	226

<i>Kuznetsova I.V., <u>Volkov S.A.</u></i> Plasma needle with fiber system for input-output an optical radiation	227
AUTHOR INDEX	229
ORGANIZATION LIST	237
PARTICIPANT LIST	244

**ATOMIC-LEVEL SIMULATIONS OF LASER
INTERACTIONS WITH METALS**

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Active expansion of femtosecond laser techniques into the area of micro- and nano-scale material processing calls for a better theoretical understanding of the connections between the basic mechanisms of laser interaction with materials and the final microstructure of materials treated by laser irradiation. Atomic-level computer modeling has the ability to provide detailed information on the complex processes induced by the fast laser energy deposition and can assist in the advancement of laser-driven applications. Recent progress in the development of computational methods for simulation of laser interaction with metals, as well as the results obtained for laser melting, spallation and ablation will be reported in this presentation. The simulations performed for one-component metal targets (Au, Ni, Cr) provide information on the kinetics of the laser-induced melting and resolidification [1],[2],[3], generation of crystal defects [3], as well as the mechanisms of material ejection from the targets. Recent simulations performed for targets composed of 30 nm Au or Ag films deposited on a bulk Cu substrate predict that the higher strength of the electron-phonon coupling in Cu, as compared to Au and Ag, results in a preferential sub-surface heating and melting of the Cu substrate [4]. The final concentration profiles in the resolidified targets are strongly affected by the kinetics of the melting process. The transient modification of the electron temperature dependences of thermophysical material properties due to the thermal excitation of the lower band electrons [5] are found to have important implications for quantitative computational description of the laser-induced processes.

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DYNAMICS OF EXPANSION OF FRONT AND REAR SURFACES OF THIN METALLIC FILM HEATED BY FEMTOSECOND LASER PULSES

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Absorption of femtosecond laser pulses of moderate intensity in a skin-layer of metal target leads to heating of electrons during action of laser pulse to temperatures of an order of several eV. Further heat energy is transmitted into the bulk of target owing to the electron heat conductivity, and also is transferred to lattice by means electron-phonon heat exchange. The feature of interaction is an isochoric heating and formation of a region with high pressure in a superficial layer of a target. According to molecular dynamic simulations [1], interaction of laser pulses of 100 fs duration and fluence 2 J/cm² with aluminum film leads to formation of the layer by thickness 100 nm heated to temperatures of several thousands degrees at a pressure approximately 20 GPa. This pressure leads to ablation of a material at the heated surface of the sample and generation of a shock wave propagated into the bulk of a target.

In a present work the ultrafast time-resolved interferometric microscopy was used to measure the dynamics of front and rear surfaces expansion of thin aluminum film on a glass substrate under action of femtosecond laser pulses at moderate intensity of order $2 \cdot 10^{13}$ W/cm². This pump-probe technique allows to determine two-dimensional profile of high-speed surface deformations with temporal resolution of 10^{-13} s and out-of-plane spatial resolution of 0.5 nm using 40 fs, 400 nm probe pulses. The measurements show the ultrafast melting of superficial layer on the front heated surface at a time scale of several picoseconds and subsequent expansion of matter with maximal velocity of order 1 km/s. The deformation of rear side of target due to shock wave was also detected.

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**BAND STRUCTURES OF SIMPLE AND NOBLE METALS
AND THEIR MATERIAL PROPERTIES IN A
TWO-TEMPERATURE STATE WITH HOT ELECTRONS
OVERHEATED ABOVE A COLD CRYSTAL LATTICE BY
AN ULTRASHORT LASER PULSE**

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An ultrashort laser pulse (UsLP) transfers metals into a two-temperature (2T) state with $T_e \gg T_i$. In the paper results of experiments and theory are presented. Comparison of experimental optical responses of simple (aluminum, Al) and noble (gold, Au) metals to pump irradiation at the incident fluences ~ 1 J/cm² shows qualitative differences. Fast increase of electron temperature T_e during a short time slice of pump action τ_L causes small changes of ε in Al (though T_e is high) and large changes in Au at similar T_e . Our analysis links this to two factors. (i) There is a difference in the band structures of Al $3s^23p^1$ and Au $5d^{10}6s^1$. (ii) There is decrease of a degeneration degree and a sharp growth of a collision frequency ν caused by this. Consequence of the ν -growth for absorption of the probe photons are different for Al and Au as the collision mechanisms are different. In gold at room temperature (r.t.) there are $Z = 1$ conduction and 10 d-electrons. A gap $E_g \approx 2$ eV separates an upper edge of the d-band and a Fermi level at r.t. $Z(T_e)$ increases in Au with increase of T_e . $Z \sim 2 - 3$ at our fluences. It is important that the collision mechanism depends on the band structure. This differs electron collisions in Al and Au. There are three main contributions: (1) ν_{ei} , (2) $\nu_{ee}^{inraband}$, (3) $\nu_{ee}^{interband}$, where ν_{ei} is electron-phonon or electron-ion collisions, $\nu_{ee}^{inraband}$ is collisions between a pair of electrons both from the conductivity band, $\nu_{ee}^{interband}$ is collisions between s, p and d electrons in Au, they are absent in Al. In case of Au our calculations show that $\nu_{ei} = [\alpha(T_e)/nk_B](T_i/\theta)(T_F/\theta)$ is a strong function of T_e , where θ is Debye temperature, α is an electron-ion energy exchange coefficient. This

allows to explain large changes in ε_{Au} at time scale $\sim \tau_L$ observable in experiments.

It is remarkable that the smallness of the ε_{Al} changes allows to observe kinetic of melting in the thin skin layer of the irradiated Al target.

The work is supported by the RFBR grant No. 07-02-00764.

IDEAL MATERIAL STRENGTH, NANOSPALLATION, AND MOLECULAR DYNAMICS SIMULATION BY ADEQUATE EAM INTERATOMIC POTENTIAL

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Irradiation of condensed matter by a femtosecond laser pulse tends to the fast heating of a target and produces the strong stress in it. When this stress relieves after the end of a laser pulse in a thin film it gives rise to a rarefaction wave at the irradiated frontal side of a target and a compression wave moving to the rear side of the film. Frontal side rarefaction wave leads to the frontal ablation of a target material if the laser irradiation fluence exceeds threshold value F_a . The compression wave in a thin film forms the rarefaction wave at its rear side when the wave achieves the rear side. Interaction of the compression and rarefaction waves at the rear side gives rise to cracks in a film and rear-side spallation starting with threshold value F_s higher than F_a . To describe both frontal ablation and rear-side spallation we need to take into account the kinetics of associated phase and structural transitions. The most suitable method to calculate these phenomena is molecular dynamics simulation because it doesn't need additional information of kinetics of phase transformation.

The realistic MD simulation requires the adequate description of interaction between particles forming a target material. For metal target we must take into account many body interatomic interaction due to the conduction electrons. In this work the new embedded-atom method (EAM) potentials for aluminum and gold are proposed. They adequately describe uniaxial deformations of materials under the action of laser irradiation in contrast with other EAM potentials giving a good description of only near-equilibrium states. The ablation threshold value for the bulk gold target and the crater depth in it are obtained which are in a good agreement with the experimental values, whereas the use of alternative interaction

potentials gives less satisfactory results. At the latest stage of ablation it is shown that the bubbles in cavitation zone can be trapped inside freezing melt. It results in the deformation of a target surface and formation of its stable nanorelief. Besides of numerical simulation of the action of femtosecond laser irradiation onto thin aluminum and gold films the first experimental investigations of the time evolution of rear side of a nickel and Al films irradiated by laser are made. The work is supported by the RFBR grant No. 07-02-00764.

ABLATION OF SIMPLE (ALUMINUM) AND NOBLE (GOLD) METALS UNDER ACTION OF FEMTOSECOND LASER PULSES

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When femtosecond laser pulse (fsLP) acts onto the metal target it causes first of all the strong heating of the conductivity electrons of the metal inside the near-surface skin layer. Then the absorbed energy transfers by the electron heat conductivity into the bulk target with the simultaneous energy exchange between electrons and ions. This process develops together with the non-equilibrium melting due to the strong crystal overheating, then transferring to the equilibrium regime of melting and solidification. At the later stage the spatial moving of a target matter takes place. It is accompanied by the phase transition of a target substance: equilibrium melting, nucleation/cavitation in the expanding liquid and finally by its freezing (nanosecond stage). Because of the finite characteristic time of electron-ion thermal relaxation, the absorption of fsLP with moderate intensity $\sim 10^{13} \text{W/cm}^2$ results in non-equilibrium melting of overheated crystal lattice and cavitation decay of metastable state. The modelling of these nonequilibrium processes and their experimental investigation are presented. Two-temperature hydrodynamics (with separate temperatures T_e and T_i for electrons and ions) and molecular dynamics simulation are used. When writing the hydrodynamics equations the two-temperature equation of state, electron-ion energy exchange, electron thermoconductivity are included. Molecular dynamics simulation is carried out for the many-body potential in the case of aluminum and gold

targets. Experimental setup with pump-probe technique is used to follow evolution of irradiated target by the short time step 100 fs probe fsLP with $\sim 1\%$ accuracy of reflectivity measurement and ~ 1 nm accuracy of the probe phase measurement. Strongly nonequilibrium state of a target matter with highly excited electrons at the stage of isochoric heating results in the optical characteristic differing greatly from that one of cold metal. Comparison of the theoretical calculation of reflection and phase shift of probe laser pulse from aluminum based on Fresnel formulae with the results of experiments is made. Helmholtz equation has been solved for the description of probe reflection from a target. Optical model for the dielectric permittivity of includes optical transitions between bound and free electron states. It shows that in solid Al the electron-electron collisions give a minor contribution into the dielectric permittivity as compared with collisions between electrons and ions. At the same time the e-e collisions are significant for decrease of thermal diffusion. Calculation of the optical characteristics of aluminum shows that the measured phase shift of reflected probe pulse during the time interval $0 < t < 4$ ps results from kinetics of melting and difference of optical constants of solid and liquid phases and also due to hot electrons population in liquid Al. The optical response of gold to a pump pulse exhibits the essential difference with that of aluminum. This discrepancy can be explained when taking into account the thermal excitation of d-electrons in gold.

TRANSPORT AND OPTICAL PROPERTIES OF Au UNDER FEMTOSECOND LASER IRRADIATION

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A theoretical model is developed for the interaction of intense femtosecond laser pulses with solid targets on the basis of the two-temperature equation of state for an irradiated substance [1, 2]. It allows the self-consistent description of the laser absorption and dynamics of the plasma formation and expansion. Comparison of available experimental data on the amplitude and phase of the complex reflection coefficient of gold [3] with the simulation results provides new information on the transport coefficients and absorption capacity of the metal over a wide range of temperatures and pressures.

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SIMULATION OF ULTRASHORT DOUBLE PULSE LASER ABLATION OF METALS

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The purpose of this study is to develop a physical model for simulation of laser-metal interaction. Our model describes two-temperature effects, laser energy absorption, mechanical fragmentation, thermal conductivity, electron-phonon/ion collisions and ionization. Previously we simulated interaction of a single femtosecond laser pulse with metals and obtained good agreement with experiment [1, 2]. Recent experiments with double pulse technique [3] may give additional information about ultrafast processes in matter and help in adjustment of complex semi-empirical models. In experiment the delay between $2 \times 2 \text{ J/cm}^2$ pulses varies from 0 ps to 100 ps and results in different depth of crater. For short delays ($\Delta \leq 1 \text{ ps}$) situation similar to single pulse with fluence of 4 J/cm^2 . For longer delays ($\Delta \geq 10 \text{ ps}$) substance ablated by the first pulse shields the second pulse. We performed simulation of double pulse laser ablation of Cu and Au and obtained good agreement with experiment in self-reflectivity data and crater depth.

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INTERACTION OF PHELIX LASER PULSES WITH NANOSTRUCTURED TARGETS: EXPERIMENT AND MODELING

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The role of the laser pulse contrast, prepulse generated by a powerful laser system PHELIX is analyzed by numerical modeling in view of the current and planned experiments in GSI, Darmstadt. It is shown that for the current contrast ratio of the picosecond PHELIX pulses (from 10^{-6} to 10^{-4} in a nanosecond range), nanostructured targets and thin foils will be destroyed by the nanosecond prepulse at the intensities of the main pulse in excess of 10^{17} W/cm². The progress in usage of the nanostructured targets, which can provide creation of effective sources of x-ray radiation, requires substantial increase of the contrast that can be achieved, e.g. by the use of the plasma mirror technique.

LASER-PLASMA ACCELERATION OF RELATIVISTIC ELECTRON BUNCHES

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The important features of the promising high-gradient laser-plasma accelerators are discussed. Consistent analysis of the bunch charge (beam loading effect) influence on the energy characteristics of accelerated electrons is presented [1]. In one dimensional approximation the simple analytical expression for the optimum electron bunch density is derived, which minimizes the electron energy spread when maximum bunch energy gain is achieved. For wide electron bunches all analytical predictions are confirmed by the results of numerical modelling. First self-consistent simulation results obtained by the code LAPLAC for the new scheme of the low energy bunch injection in front of the laser pulse are obtained and analyzed.

Simulations of the coupling of an incident laser pulse to a capillary tube are presented. Examples of the perfect Gaussian laser pulses and

an experimentally measured radial intensity distributions are studied in a vacuum capillary, as well as the excitation of the wakefield inside a gas filled tube. The presented technique with cone entrance, increasing aperture and acceptance of the capillary, can also help to overcome the problem of pointing stability of the laser [2].

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RADIATION SPECTRUM OF RELATIVISTIC ELECTRONS IN THE HIGH INTENSITY LIMIT OF THE EXTERNAL LASER FIELD

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The physics of interaction of ultra relativistic electrons with strong laser fields has become of practical interest in connection with recent progress in constructing powerful terawatt (TW) and petawatt (PW) lasers [1], [2]. Electromagnetic processes in the strong laser field are characterized by the invariant parameter $\nu = e\mathcal{E}/m\omega_0$, where \mathcal{E} is the laser field strength, ω_0 is its frequency, e and m represent charge and rest mass of an electron. In the experiments with 46.6 GeV electrons moving opposite the TW laser beam the value $\nu = 0.6$ was achieved [3]. In the case of PW laser $\nu > 10$.

Nonlinear effects of high harmonic generation take place in interaction of relativistic electron beams with lasers if $\nu > 1$ [4], [5], [6]. This leads to sharp peaks in the electron radiation spectrum.

We develop theoretically formalism which permits one to take into account the nonlinear effects of high harmonic generation using relatively simple expressions. By this approach we calculate in analytical form the radiation spectrum for the case of linear polarized plane wave interacting with relativistic electrons. Our approach is based on the semiclassical Baier-Katkov formalism with taking into account the quantum recoil effect due to radiation and influence of spin. Finally we show that in the limit of high intensity of the laser beam, when $\nu \gg 1$, the radiation formulas simplify essentially and the spectrum becomes of synchrotron nature. Such the synchrotron approximation turns out to describe the radiation spectrum perfectly for $\nu > 2$.

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ELECTRON DYNAMICS IN THE RELATIVISTIC PLASMA WAKE GENERATED BY SHORT LASER PULSE: THEORY, SIMULATION AND EXPERIMENT

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The laser-plasma wakefield electron acceleration is now fast developing area of science. It has attracted now a much attention due to the generation of quasimonoenergetic, dense and short bunches of relativistic electrons with energy up to 1 GeV. The high-gradient acceleration is possible due to very strong electromagnetic fields in plasma wake excited by short laser pulse. The ponderomotive force from the laser pulse pushes out the plasma electrons radially leaving behind the laser pulse the soliton-like plasma cavity—bubble with unshielded immobile ions. This is bubble or blow out regime of laser-plasma interaction. It is important that the part of the plasma electrons can be trapped in the plasma cavity. The phase velocity of the cavity is close to the speed of light and the trapped relativistic electrons can continuously accelerated in the plasma fields up to very high energy. It is now generally believed that self-injection occurs in the bubble regime. The self-injection essentially affects the quality of the electron beam generated in laser plasma. Despite great interest to laser driven electron acceleration, there is little theory of self-injection in the bubble regime.

We present the multidimensional model of the electron self-injection. The models predict the condition for the electron trapping. The model predictions are compared with results obtained by 3D PIC simulations. The recent experimental studies of ultrahigh intensity laser-plasma accel-

eration conducted at Petawatt laser system of Institute of Applied Physics are discussed.

This work has been supported by the Russian Foundation for Basic Research (No. 07-02-01239-a, 07-02-01265-a, 08-02-01209-a).

OSCILLATIONS OF THE PLASMA WAKE GENERATED BY TIGHTLY FOCUSED FEW-CYCLE LASER PULSE

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The dramatic increase of the laser intensity during last years led to new effects in relativistic optics. The further development of relativistic laser sources of few-cycle pulses allow to study the fundamental principles in detail. We investigate the wakefield generation during the interaction of tightly focused ultrashort (few-cycle) laser pulses with underdense plasma by means of 3D particle-in-cell simulations. It is shown that a plasma cavity generated by the laser pulse in the blowout regime undergoes transverse oscillations. The oscillation behavior is determined by the laser pulse polarization. The cavity oscillations strongly affect the dynamics of self-injected electron beam, that leads to the beam modulation. We present a simple model for the cavity oscillations.

FILAMENTATION OF FEMTOSECOND LASER PULSE WITH 1.24 μm WAVELENGTH IN AIR

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In present paper, filamentation in air of Cr:forsterite laser pulse with 1.24 μm wavelength is investigated experimentally and theoretically.

Experiment was performed with femtosecond terawatt Cr:forsterite laser system of Joint Institute for High Temperatures [1]. Generated pulse has wavelength 1.24 μm , duration 80 fs (FWHM), energy 80 mJ, and power 1 TW. At fixed distances from laser system measuring setup was built, which consisted of microscope objective (Plan-P, LOMO PLC, St.-Petersburg, Russia) and CCD-camera (SensiCam SVGA, PCO AG,

Kelheim, Germany). For energy flux in pulse transverse section registration, radiation refracted from thick glass plate was used. Dependencies of filament radius and peak energy flux on initial pulse energy were obtained. It was shown that filament radius for pulse with 1.24 μm is higher than filament radius for pulse with 0.8 μm obtained in known experiments.

Numerical simulation, performed on the basis of the general model for pulses with different wavelength [2], showed good agreement of theoretical estimations with experiment.

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EXPERIMENTAL RESEARCHES OF “SONY” CCD CAMERA LINEAR ARRAY RESPONSE UNDER ACTION OF FEMTOSECOND LASER PULSES

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Experimental results on studying of working capacity of “SONY” CCD camera linear array under action of femtosecond laser pulses with energy below and equal to ablation threshold are presented.

Experiments are carried on femtosecond laser complex of IHED. A radiation of titan-sapphire laser system has been used for investigation of experimental parameters of laser pulses leading to various mechanisms of CCD linear array malfunction. Laser radiation wavelength is 800 nm, pulse time duration of order 40–50 fs, energy is up to 2.5 mJ. The laser system operates at frequency of 1 kHz, and for realization of work in a single pulse mode a precision scheme of synchronization of a laser complex with CCD array is used.

A determination femtosecond laser pulse power parameters leading to CCD-array element ablation was carried out by means of pump-probe technique. In this scheme a pump pulse influences directly on CCD-array element, and by means of a probing pulse changes of intensity of the reflected signal after influence of a pump pulse are measured. A pump pulse wavelength was 800 nm and probe one was 400 nm. Pulse duration was 40 fs.

Laser radiation parameters, mechanism and response leading to temporary, long and full malfunction of “SONY” CCD camera linear array were determined.

MATHEMATICAL MODELING OF THE FAST IGNITION LASER TARGETS AND THE HiPER PROJECT

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In this presentation we talk about the main parameters of the contemporary project of a fast ignition laser fusion realization. There are many numerical simulations of such the approach. In this report the set of the key moments is analyzed. These issues are: achievement of the high compression degrees, fast electron generation and their transport and energy deposition, thermonuclear burning. To simulate these problems one dimensional as well as many dimensional hydrodynamical codes are used. Two dimensional simulation is necessary to describe an ignition process, which is realized within this scheme by one laser beam of a high intensity. We demonstrate the results of a set of the calculations, devoted these problems. We confirm the high gain achievement. We more accurately determine the regions of parameters, which can reached also.

COLLISIONAL ABSORPTION OF LASER LIGHT IN STRONGLY COUPLED PLASMAS

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A new theoretical approach for collisional absorption of laser energy in dense plasmas which accommodates arbitrary frequencies and high intensities of the laser field is presented. We establish a connection between laser absorption by inverse Bremsstrahlung and the stopping power. This relation is then applied to include strong correlations beyond the mean field approach. The results show an excellent agreement with molecular dynamics simulations up to very high coupling strength.

**INERTIAL ELECTROSTATIC CONFINEMENT AND DD
NUCLEAR SYNTHESIS AT INTERELECTRODE MEDIA
OF NANOSECOND VACUUM DISCHARGE**

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The generation of energetic ions and DD neutrons from microfusion at the interelectrode space of a low energy nanosecond vacuum discharge has been demonstrated recently. However, the physics of fusion processes and some results regarding the neutron yield from the database accumulated were poorly understood. This work presents a detailed PIC simulation of the discharge experimental conditions using a fully electrodynamic code. The dynamics of all charge particles was reconstructed in time and anode cathode space. The principal role of a virtual cathode (VC) and the corresponding single and double potential well formed in the interelectrode space are recognised. The calculated depth of the quasistationary potential well of the VC is about 50 keV, and the deuterium ions being trapped by this well accelerate up to energy values needed to provide collisional DD nuclear synthesis. Correlation between the calculated potential well structures (and dynamics) and the neutron yield observed is discussed. In particular, ions in the potential well undergo high frequency (about 80 MHz) harmonic oscillations accompanied by a corresponding regime of oscillatory neutron yield. Both experiment and PIC simulations illustrate very favourable scaling of the fusion power density for the chosen inertial electrostatic confinement scheme based on nanosecond vacuum discharge.

**SOFT X-RAYS EMISSION FROM FS LASER PLASMA
OF THE CLUSTER JET TARGETS BASED
ON THE MIXTURE OF MOLECULE AND ATOMIC GASES**

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Development of ultrafast x-ray sources is an important problem nowadays. Such sources are useful investigation tool both in fundamental and applied research fields. For instance, soft x-ray radiation in 300–550 eV spectral region (the water window) is particularly attractive for biology applications. Here absorption from carbon compounds can be distinguished from water contributions. Femtosecond laser plasma appears to be one of the most bright point soft x-ray (SXR) source with a table-top size. Parameters of the generated plasma and soft x-ray emission are strongly depend on the target type and material.

In the current work we propose to use cluster media (mixture of 90% atomic He and 10% molecular CO₂ gases) irradiated by fs Ti:Sa laser pulses to create bright debris-free x-ray source which emits mainly in the 10–50 Å spectral region. Atomic gas is necessary for enhancement of clusterization of the CO₂ gas. We used He because it is transparent for the SXR radiation so no additional absorption takes place in the area surrounding plasma. Especially designed supersonic gas jet nozzle was used in our experiments to produce clusters. Numerical simulations were made to optimize the size of produced clusters [1], which allowed to increase SXR output from the cluster targets. Two focusing spectrometers with spatial resolution were set up to measure plasma parameters. Experiments show that x-ray flux in the individual lines exceeds $3 \cdot 10^{10}$ photon/sr/pulse while total x-ray flux is at least 10^{12} photons/sr/pulse, peak brightness $1.6 \cdot 10^{23}$ ph/s/mm²/mrad²/0.1%BW, source size is about 100x100 λm. The possible application of this source is the metrology and qualitative analysis of thin foils and biological objects with nanoscale thickness.

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X-RAY BACKLIGHTING AND PROTON RADIOGRAPHY IMAGING FOR DIAGNOSTICS OF SHOCK WAVES AND SUPERSONIC JETS IN INTENSE LASER PLASMA

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Tunable high-luminosity scheme to obtain x-ray monochromatic shadowgraphy images was developed based on spherically bent quartz dispersion element. The key features of the scheme are in that angle of radiation incidence to the crystal is far from normal and the radiation source is located inside Rowland circle of the crystal. Therefore, the scheme can work in wider spectral range of backlight and provide image magnification factor up to 10. Due to spectral selection of illuminating radiation providing by spherical crystal, the density of the object can be measured in precise. Absorption properties of soft x-ray radiation allows to investigate low-contrast structures such as turbulences, jets and shock waves in laser plasma. As it was demonstrated by ray tracing simulation, developed x-ray backlighting scheme provides spatial resolution up to 10 μm for 2D images and up to 5 μm in single direction of main interest (for ex., transverse to shock wave front)

The scheme was applied for diagnostics of super sonic jets and shock waves in plasma initiated by ultra-intense (PW/cm^2) 1 ns nanosecond laser pulses in LULI Ecole Polytechnique. Shadowgraphy images with spatial resolution up to 8 μm were obtained in V He α spectral line with photon energy about 5 keV. The important data on compression rate of 2.8 and wave front velocity of 20 km/s are presented for shock waves propagating inside plastic media.

In the case x-ray source cannot be generated with enough intensity the channel of proton radiography was realized. Illuminating proton flow with energy of about 5 MeV was generated by intense picosecond laser pulse in aluminum foil. It allows to providing the images of low-contrast plasma jets in plasma during its propagation in ambient media. The evolution of jets in time and birth of secondary structures in plasma are investigated. Proton radiography data analysis proves the demand on further progress in monochromatic x-ray radiography methods for the purposes of laboratory astrophysics and warm dense matter investigations. Work was supported

in parts by Program of fundamental research of RAS Presidium # 12 and CRDF BRHE # Y5-P-11-02 project.

DEVELOPMENT OF DOSIMETRY METHODS FOR PURPOSE OF RADIATION THERAPY AND IONOGRAPHY OF BIOLOGICAL OBJECTS

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In view of wide use of ion fluxes in technique, medicine and imaging diagnostics the development of concepts that relate the absorption of ionizing radiation in matter to the geometry and nature of the affected structures is the actual aim.

Based on requirement to provide precise measurement of absorbed dose in every microscopic biological volume the microdosimetry approach was used. The description and experimental results of tissue equivalent proportional counter calibration to perform microdosimetry measurements on ion beam at GSI SIS-18 facility are presented. Calibration with α -particles and 300 MeV/u pencil-like ion beam demonstrates linear response of the detector in wide flux range. Thus, the conversion factor of the linear energy to the absorbed dose in microscopic volume of the matter was determined. The possibility of adaptation the similar diagnostic methods in wider energy range and for the purposes of ion radiography is discussed.

We have focused to create a precise and effective control system of beam parameters with 3D spatial resolution. New segment ionization chamber was developed and applied to define physical dose absorbed in biological matter irradiated by carbon beam with short pulse lead-out and fluence from 10^6 to 10^{10} particles per pulse (time length 1 μ s) at the ITEP-TWAC facility.

The segmentation of electrodes allowed to define the beam inhomogeneity in different points across beam focal spot during the irradiation. Also, the developed chamber provides the measurements for beam fluxes up to $2 \cdot 10^8$ particles, which in order exceeds the dynamic range of commercially available detectors. The chamber was used in the experiments of radioresistant melanoma cells irradiation and the value of the absorbed dose was obtained.

KINETICS OF CLUSTER GROWTH IN LASER GENERATION OF METAL CLUSTERS

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Laser generation of cluster generation results from irradiation of a metal surface by a laser pulse [1, 2]. We analyze the kinetics of subsequent stages of this process. The first stage is absorption of laser radiation, and when the pulse duration is small compared to a time of heat propagation inside the metal volume. Then the energy of laser pulse is consumed on evaporation of atoms from the metal surface and heating of evaporating atoms. Correspondingly, an absorbed laser pulse heated the metal surface, and the temperature of an irradiated spot determines the flux of evaporated atoms, so that the pressure of free metal atoms near the surface coincides with the saturated vapor pressure of this vapor at the surface temperature.

On the second stage of the evaporated process free atoms are characterized by a semi-Maxwell distribution function with the surface temperature. On the next stage near the surface this atomic flux is transformed in an atomic beam [3, 4]. As a result, the temperature of the atomic system drops, and the atomic beam moves with the sound speed for the beam temperature. Because at this temperature The vapor pressure exceeds significantly the saturated vapor pressure at this temperature, metal atoms are transformed into clusters and clusters grow.

We analyze kinetics of cluster growth for two regimes, when an atomic beam propagates in a vacuum or in a buffer gas. The size distribution function of clusters formed as a result of expansion of an evaporated vapor in a vacuum or in a buffer gas depends both on the initial temperature of a heated metal surface that determines the initial number density of metal atoms and on the angle of beam expansion.

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ENHANCEMENT OF K- α YIELD FROM THE TARGET WITH A CLUSTERED SURFACE

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A narrow-band picosecond pulse of K- α x-rays is the promising tool for probing dense plasmas [1], but the conversion efficiency of laser energy comes short of the values achieved for the He- α and Ly- α radiation [2]. That is the reason why an optimization of processes of hot electron formation, which determine the efficiency of K- α generation, is of current importance. Several mechanisms of hot electron generation, essential in a different ranges of laser pulse and target parameters, are known [3].

It is shown that K- α yield when a massive metal target was irradiated by femtosecond laser pulses of JIHT facility [4] in a definite range of parameters is described by the model of vacuum (Brunel) heating of electrons [5]. Within the framework of this model, the number of K- α photons increases considerably when the target with a clustered surface is used due to driving electric field enhancement at a cluster surface and more favorable conditions for K- α photons output from the wafer.

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LASER NONLINEAR FORCE DRIVEN FUSION ENERGY FROM HB(11) BY BLOCK IGNITION

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Controlled fusion energy from burning hydrogen with boron-11 is of interest because no neutrons are produced. Following the scheme of ignition by spherical irradiation by laser or particle beams is extremely difficult. A new approach following the scheme of block ignition with laser pulses of picosecond duration and more than petawatt power led to the possibility of plane geometry irradiation of the fuel using the anomalous effect of block ignition for deuterium tritium (DT) based on updated conditions for the initial computations by Chu (1972). We present the extension for HB(11) resulting in a very less dramatic difference to DT than in the case of spherical pellet geometry. Ignition thresholds may be only about one order of magnitude higher and the needed temperatures of about 50 keV are no problem for the skin layer acceleration by nonlinear forces for the block generation.

ALPHA PARTICLE ENERGY ABSORPTION IN UNCOMPRESSED DT FOR LASER DRIVEN FUSION

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The alpha particle created in the DT fusion reaction has initial energy of several MeV (3.5 MeV) whereas the plasma has the temperature in the range of keV (about 8 keV). The fraction of the alpha particle energy was absorbed by the plasma electrons and ions. This process caused reheating DT plasma, so it is very impotent for ICF investigation. The deposition of energy by alpha particles has been re-evaluated by early analysis including later discovered collective stopping power. Besides, binary collisions model has been applied to compare results with collective model for block ignition laser driven fusion by the hydrodynamic theory of Chu

[Phys. Fluids 15, 413 (1972)] and the advantage of this model has also been studied.

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EFFECTS OF RAMP DENSITY PROFILE ON THE RELATIVISTIC SELF-FOCUSING AN INTENSE LASER BEAM

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The propagation of a Gaussian beam in an underdense plasma with upward increasing density ramp is analyzed. We have showed that the spot size of the laser beam decreases as the beam propagates in the plasma. In these conditions we showed that the spot size oscillations of laser beam increases and the beam-width of the laser decreases with proper plasma density ramp. The analytical calculations are presented and showed more reliable results in comparison to the previous works.

QUASI MONO-ENERGETIC SOFT X-RAY BEAM PRODUCED BY ULTRA-INTENSE LASER-PRODUCED ELECTRONS

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Quasi mono-energetic x-ray beams are generated from thin targets by interaction of mono-energetic electron beams from 600 mJ, 80 fs laser pulse. A micron-scale laser-produced plasma creates and accelerates relativistic mono-energetic electron bunches. As such electrons propagate in the ion channel produced in the wake of the laser pulse; the accelerated electrons can interact with different targets with various atomic numbers and densities and generate soft x-ray radiation of keV energy and MeV/cm² flux.

In the present work the data produced from Monte Carlo simulations of x-rays spectra and contributions of bremsstrahlung and characteristic x-ray in these spectra are presented.

**EXPERIMENTAL INVESTIGATION OF PLUME
MACROSTRUCTURE AND RADIATIVE GASDYNAMIC
PROCESSES OF LASER–MATTER INTERACTION**

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Generation of plasma plumes, hypersonic flows and powerful shock-waves has numerous scientific and technological applications. To define macro scale technological performance of different initial regimes experiments should be conducted, as theoretical investigation is too complicated as compared to basic experimental techniques. Materials chosen are usually used for flows generation, construction and heat insulation. The results of experimental investigation of solid targets laser induced plasma macrostructure (POM, PTFE; Cu, Nb, Al, Mo; Al₂O₃-ceramic; $\lambda=532, 1064$ nm; $\tau_{FWHM}=18$ ns; $E/S=0.1-20$ J/cm² @ $d\sim 1.5$ mm) based on shlieren registration ($\Delta t=0.2-5000$ μs) and emission spectrometry are presented. Velocities defined from shlieren-graphs for shockwave front and from electric probe measurements for plasma front (41.7 km/s to 4.5 km/s at the initial stage). Plume macrostructure is considered according to shlieren-graphs photometric analysis. Emission spectra show presence of continuum at early stages and numerous secondary ions near above plasma threshold. Exposure superposition at near-surface zone with pulse repetition rate increase (1–10 Hz) is demonstrated. The results of experimental and theoretical investigation are presented and discussed.

AMBIENT GAS BREAKDOWN EFFECTS IN ULTRASHORT PULSED LASER ABLATION OF SOLID MATERIALS

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Ultrashort laser ablation of solid targets is strongly affected by the presence of an ambient atmosphere due to several effects including pressure confinement, ambient plasma formation, gas-phase chemistry, and plasma-surface interaction. To gain insight into gas breakdown effects, we have developed a combined 2D model describing laser-induced generation of the ambient plasma in a focal region in front of the irradiated target, plasma decay, and dynamics of the ambient gas perturbed by a heat release resulted from plasma recombination. The model treats the involved processes in two stages. In the first stage, laser beam propagates through the ambient gas toward a solid target with further reflection, creating in a focal region a strongly non-equilibrium ambient plasma via a multi-photon ionization process. The ionization/recombination dynamics of the generated plasma and its energy evolution are described within the frames of kinetic rate equations. For simplicity we assume that the second stage, laser-induced motion of the ambient gas, starts after plasma decay which occurs in several nanoseconds after the laser-target interaction. The temperature distribution obtained in the first-stage modeling presents initial conditions for the gasdynamic problem. The simulations have been performed for a platinum target in argon and air irradiated by laser pulses of duration below 100 fs in the range of laser fluences 1–5 J/cm². The following features of the breakdown effects are analyzed: laser energy balance (losses for ambient gas ionization, ambient gas heating, target absorption, recombination radiation), shock wave formation in the ambient gas and its dynamics, heat exchange between the target and the ambient gas. The simulation results demonstrate an intriguing picture of laser-induced ambient gas motion with superposition of a strong semispherical shock wave propagating from the laser focus region and a cylindrical compression wave moving radially from the laser beam trajectory. Additionally, we discuss the surface plasma chemistry issues such as plasma surface etching and modification as well as possible impact on the ablation process.

IONIZATION-INDUCED GENERATION OF BROADBAND TERAHERTZ RADIATION

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We present the results of recent studies of the phenomenon, during which broadband terahertz radiation is generated in various schemes of gas ionization (including atmospheric air) by intense femtosecond laser pulses. In such schemes, the radiating medium is a sufficiently dense laser plasma, which can be a small-scale (dipole) oscillator formed when a short-focus spherical lens focuses laser pulses into a low-pressure gas, or a sufficiently long laser spark (from 1 to 10 cm, and longer) formed either when a conical (axicon) lens performs the focusing, or when a filamentation (self-focusing) instability arises. Therein, the pumping field supplying energy to terahertz waves is either the field of the ionizing laser pulse itself [1]–[4], or some external field, in whose presence the optical breakdown occurs [5]–[8]. In the first case (*self-induced* generation), acceleration of free electrons and generation of low-frequency (terahertz) currents in the generated plasma are performed by either the averaged ponderomotive force of the laser pulse [1, 2], or by its electric field which imparts some quasi-constant component of the velocity to electrons at the moment of ionization [3, 4]. In the second case (*forced* generation), static (or microwave) electric fields [5, 6] or the second-harmonic field of the laser pulse itself (which is obtained by using a frequency-doubling crystal) [7, 8] are regarded as the external field.

The developed theoretical models agree well with the experimental results and include quantum-mechanical and semiclassical approaches to calculations of the low-frequency currents excited in plasma in the process of the optical breakdown, as well as self-consistent models for calculation of the parameters of terahertz waves generated by these currents, which are based on solving exact Maxwell equations. Optimal conditions for the most efficient generation of terahertz waves and possible schemes for generation of superpower radiation (of a gigawatt power level) by using ultrashort ionizing laser pulses are determined.

This work was supported by the Russian Foundation for Basic Research (project nos. 07-02-01265 and 07-02-01239) and the Ministry of Education and Science of the Russian Federation (project no. MK-3923.2008.2).

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**PHASE EFFECTS IN IONIZATION-INDUCED
PHENOMENA OF THE QUASI-DC CURRENT
EXCITATION IN THE LASER-PRODUCED PLASMA**

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We discuss ionization-induced phenomena of the quasi-dc current excitation in the plasma produced by femtosecond laser pulses. These phenomena are caused by the alternating electric field of the laser pulse accelerating the newly born electrons and imparting them a large constant velocity component along with the oscillatory one. The value and the direction of the former depend on the phase of accelerating field at the moment of ionization. As a result, in the general case, the non-zero electron current density remains in the produced plasma after the passage of the pulse. Under some optimal conditions, the value of the density of the residual quasi-dc current can reach $\sim 10\%$ of maximum available oscillatory-current density [1, 2]. This residual quasi-dc current is the initial push leading to the polarization of the created plasma and excitation of radiating oscillations in this plasma. These oscillations can have terahertz frequencies at the wide range of ionized gas pressure and maximum plasma density. At present, this phenomenon is of interest due to the possibility of using it to achieve high-efficiency conversion of laser pulses into high-power terahertz waves and to determine carrier-envelope phase of few-cycle laser pulses.

In this work we consider two possible realizations of ionization-induced phenomena of the quasi-dc current excitation, used in recent experiments [3, 4]: 1) when a gas is ionized by multicycle laser pulses (with the duration of 30–100 fs), the excitation is achieved by superimposing the light pulses with their own second-harmonic radiation which can be produced by using a beta barium borate (BBO) crystal; 2) when few-cycle laser pulses (with the duration of 3–10 fs) are used, the quasi-dc current is ex-

cited by the electric field of the ionizing laser pulse itself. In both cases, in purpose to achieve maximum values of the quasi-dc current density, some optimal phase conditions for ionizing laser pulses should be satisfied. In the first case this is the condition for the phase difference between the fields at the doubled and fundamental frequencies, in the second case the carrier-envelope phase of the ionizing laser pulse should be matched in a proper way. We develop quantum-mechanical models to find the residual quasi-dc current, which are based on the solution of the time-dependent Schrödinger equation, and compare obtained results with the results of the much simpler semiclassical models used earlier in Refs [1, 4, 5]. We find optimal conditions for obtaining maximum values of the efficiency of the quasi-dc current excitation and determine the range of applicability of semiclassical models.

This work was supported by the Russian Foundation for Basic Research (project nos. 07-02-01265 and 07-02-01239) and the Ministry of Education and Science of the Russian Federation (project no. MK-3923.2008.2).

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PARTICULARITIES OF LASER DESTRUCTION OF MICROPARTICLES OF RARE EARTH COMPOUNDS

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We have found a new process of laser destruction of transparent microparticles of rare earth compounds which differs essentially from laser destruction of bulk materials. Microparticles Gd_2O_2S (Tb), Gd_2O_2S (Eu), Y_2O_2S (Tb) with diameter about 20 micrometers have been irradiated with pulses of eximer laser (Xe-Cl, $0.308 \mu m$, 10 ns, $\sim 10^8$ Wt/cm²). These microparticles were separated from each other by liquid ethanol with triton surfactant. The average density of laser flow was regulated

by variation of frequency of laser pulses. At a certain density boiling of ethanol appeared, revealing sufficient heating of the particles, because the ethanol itself doesn't absorb this laser radiation. Then the particles were dried and analyzed by means of scanning electron microscope. Electron microscopy revealed several types of microparticles: a) non-damaged; b) cleaved; c) new particles of nanoscopic dimensions with the same chemical composition: separate particles having ideal spherical form with diameter 100–200 nm and agglomerations of nanoparticles with mean sizes about 50 nm. The cleaved surfaces are non-homogeneous: the center region with a width about a half of a total diameter has a boiling-like structure, whereas the edge regions look like non-damaged steps with crystallographic orientations. It is worth noting that typical dimensions of pores in the boiling-like structure in the center correspond to typical dimensions of separate nano-spheres.

It shows that the internal distribution of temperature in the microparticles induced by laser irradiation is essentially non-homogeneous. The material in the center is heated higher than the melting point, whereas the temperature of the subsurface regions is lower. This non-homogeneity can result from two reasons: strong flow of the energy to the external space via the surface and by non-linear enhancement of laser flow absorption in the central regions. The energy flow to the external space can proceed at least by two mechanisms: heat transfer to the surrounding liquid and thermal infrared emission. Non-linear enhancement of laser absorption can be induced by thermal broadening of the absorption edge of the material. The cleavage results from high pressure produced by over-heating of the central region of the particles. After it and corresponding decrease of the pressure the over-heated material is boiled in explosion-like way resulting in ejection of quickly solidified drops. This work opens a new way of creation of nano-particles by laser irradiation of micro-solids.

NANOSECOND LASER ABLATION OF SILICON

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High power laser ablation under short pulsed irradiation is a promising method for the formation of nanoparticles and nanostructures. The use of this method needs the detail study of the conditions at which laser ablation takes place. Our work is devoted to the investigation of the processes initiated in single-crystalline Si by 80-nanosecond ruby laser irradiation

with energy densities higher and lower than ablation threshold. Optical pyrometry diagnostics of laser-induced processes has been carried out by detecting thermal radiation at the effective wavelength of $0.53 \mu\text{m}$ and laser radiation reflected by the heated zone.

According to experimental data obtained, the peak brightness temperature of the melt surface increases linearly from 1600 up to 2800 K with change in irradiation energy density W from 1.8 up to 6.5 J/cm^2 . The values of peak temperature obtained indicate the considerable pre-ablation overheating (more than 500K) of liquid phase relative to the equilibrium boiling point 2900 K of Si. The brightness temperature measured, runs up 7000 K due to plasma generation under conditions of laser ablation ($W > 7 \text{ J/cm}^2$) at the energy density in laser spot about 9 J/cm^2 .

Numerical simulation of laser-induced heating, melting and ablation processes in silicon under conditions of the pulsed laser irradiation have been carried out. The calculated data have been compared with experimental results obtained.

POLYMER LASER ABLATION DESTRUCTION DYNAMICS STUDIES

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The laser ablation under power laser pulse on the substances surface studies is the important scientific problem and it plays the great role in the many technological applications [1, 2]. It demands the detail studies of the polymer target threshold parameters dynamics at the laser ablation destruction in the laser pulse energy density from 1 up to 100 J/cm^2 .

Therefore this report goal is the time dynamics of the polymer laser ablation destruction versus the incident laser radiation focusing conditions—dimension effect and time irradiating decay dependencies for the high pressure polyethylene and polytetrafluoroethylene experimental studies. The important problem in this study is the laser plasma plume formation on the target surface [2] recording procedure. The experimental laser ablation station detail description was given earlier in [1, 4]. The YAG: Nd laser radiation with pulse duration of 10 ns and energy up to 0.3 J at 1064 nm wavelength beam was focused by the special objective on the polymer target surface. The laser plasma emission intensity was measured by the FEU-79 type photomultiplier (PMT) through the glass filter with transmittance maximum at 532 nm wavelength [2]. The threshold energy den-

sity QT have been derived from the dependences of breakdown probability P versus laser pulse energy density Q at the condition of the probability P is equal to 0.5 as in our earlier work [1, 2] These threshold values for two targets were for PE—10.1 and PTFE—24.3 J/cm². The polymer sample with the maximal mass capacity c and minimal heat transfer coefficient λ —PTFE has the highest threshold energy Q value in accordance with the thermal model [1, 3]. But laser ablation process is too complex for the poor description in terms of the thermal process without of plasma formation and its interaction with irradiating laser pulse [3]. And the laser pulse absorption increases in plasma plume due to this absorption has strong dependence from plume dimensions and its flight away velocity. It can be explained by laser plume plasma ionization ratio magnification, its temperature raising and the laser energy portion absorbed in plasma plume increasing coincidentally as it demands by thermal model. The laser plasma integral emission pulse spectral distribution dynamics experimental studies can serve as the additional confirmation of this fact because these spectra were not equivalent to the black body ones. And this plasma integral emission time decay was about 100 ns as in [5].

These results can be as the basic of the designing the new methods for laser ablation destruction dynamics for any polymer samples and estimation its parameters characterizing the ablation destruction mechanism.

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RADIANCE TEMPERATURE AND NORMAL SPECTRAL EMISSIVITY AT 650 nm OF HAFNIUM AT THE MELTING POINT BY A THIN PLATE METHOD

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Radiance temperature at 650 nm of hafnium at the melting point was measured by a thin plate method. To measure the melting point of hafnium the thin plate specimen laser heated from room temperature to its melting point in less than 0.7 s and measuring the specimen radiance temperature every 1 ms with a high-speed micropyrometer precalibrated by the black-body model. Melting of the specimen was manifested by a plateau the radiance temperature-versus-time function. The melting point radiance temperature for a specimen was determined by averaging the measured values along the plateau. The determination of normal spectral emissivity is based on the using Planck's law along with the knowledge of the true melting temperature. The results for radiance temperature and normal spectral emissivity at 650 nm of hafnium are as follows: 2270 K and 0.40. Based on the estimates of the uncertainties arising from use of pyrometry and specimen conditions the reported values is ± 12 K.

This study was supported by the Russian Foundation for Basic Research (project No. 07-08-00670-a).

SPEED OF THE HEATING OF HIGH-TEMPERATURE METALS AND PARABOLIC MODEL OF HEAT CONDUCTIVITY

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The first results of the analysis experimental termograms of molybdenum and of tungsten with the purpose of a substantiation of legitimacy application of parabolic model of heat conductivity are presented. Experiments with sources of heating which power changes in time are considered: pulse lasers and heating by a direct current in a circuit with the unloaded battery. The mode of free cooling of samples also was analyzed. Rate of change of temperature for tungsten has made $2 \cdot 10^1 \div 8 \cdot 10^7$ K/s, for molybdenum $3 \cdot 10^2 \div 5 \cdot 10^4$ K/s. Use of Criterion Maxwell-Cattaneo-Vernotte allows to show, that for the specified metals at rates of change

of temperature $\leq 5 \cdot 10^4$ K/s the parabolic model of heat conductivity is realized.

This study was supported by the JIHT RAS program.

STYDY OF PLASMA PARAMETERS IN HOT POINTS OF MEGAAMPEARS X PINCH

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The experiments were performed in the S-300 facility (2.3 MA—the amplitude of current, 0.15 Ohm—the impedance of generator, 150 ns—the rise time of current). The results of experimental investigations into the dynamics of plasma produced in the multiwire X pinch at currents up to 2.3 MA are presented. The materials, diameters, and the number of wires are varied. At such currents, the power of the soft x-ray radiation with the photon energy from 1 to 2 keV increases to 120 GW, and, since the size of a hot spot is less than 20 μm , it corresponds to a source brightness of $\sim 10^{15}$ W/(cm² sr). The energy recorded in lines of neon-like molybdenum (in the range of 2.5–3 keV) is higher than 10 J. Hard x-ray radiation detected in experiments with tungsten and molybdenum X pinches has the photon energy more than 800 keV. It was stated that the hot points of X pinch plasma have extremely high parameters: $T \sim 1200\text{--}1400$ eV, $n_i \sim 10^{22}$ cm⁻³ that corresponds to $n_e \sim 2.5 \times 10^{23}$ cm⁻³.

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**REGISTRATION OF TEMPORAL EVALUATION
OF CHARACTERISTIC X-RAY RADIATION
OF MULTI-WIRE MA Z-PINCH PLASMA**

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The experimental technique of x-ray lines hydrogen- and helium- ([H]- and [He]-) like aluminium ions registration with time resolution is described in the presented work. The experiments were carried out at S-300 machine [1] using aluminium wire arrays as a load in conditions of great electromagnetic blast. Spectral lines of [H]- and [He]-like ions of aluminium were obtained by spherical focusing mica crystal. x-ray spectrum is transformed into the visible radiation by scintillator, applied on side of the optical fibre. The guiding fibre transfers the spectrum image to the photocathode light-guiding fibre of the streak-camera [2]. The spectral lines traces image was passed to the remote computer by means of the CCD camera and fibre-optic connection.

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**NEUTRON RADIATION FROM THE CONSTRICTION
OF FAST DEUTERATED Z-PINCH**

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On the S 300 installation at currents up to 2 MA with rise time 100 ns, the investigation of the formation process of high-temperature plasma in fast Z-pinch was carried out. The central part of the loads was made from agar-agar and represented a deuterated polyethylene cylinder with small density 50–100 mg/cm³ and 1–2 mm diameter. On the ICT images, obtained in optical and soft x-ray range of a spectrum with 3–5 ns exposition, it is visible that on the axis of the polyethylene cylinder at the current's rise time a cord is formed and it is separated into bright formations. They

were observed on a background of a luminous area which occupied the initial neck volume. On time-integrated pinhole pictures obtained in SXR range (1–4 keV), hot points with minimal size of 50 microns were registered. From the chronograms results, obtained by means of the optical high-speed-streak camera mount along the neck axis with time resolution 1 ns, it follows that luminous formations arise sequentially during the different time moments (in 10–30 ns). Occurrence of luminous formations was accompanied by x-ray radiation occurrence with energy more than 1 keV with short duration of 2–4 ns. Simultaneously with x-ray radiation neutrons with the maximal yield of $6.5 \cdot 10^9$ were registered. The average energy measured in 4 directions under angles with an axis of: 0° (above the anode), 90° , 180° (under the cathode) and 270° , were accordingly: 2.4 ± 0.2 , 2.5 ± 0.1 , 2.5 ± 0.1 , 2.5 ± 0.1 MeV.

STUDY OF MATERIAL DISTRIBUTION IN THE DENSE CORE AND RARE PLASMA CORONA UPON ELECTRICAL EXPLOSION OF WIRES

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The study of exploding wire material distribution is very interesting for many basic and applied scientific problems, which provides our motivation for studying the dense core and conducting plasma distribution that results from a current-driven wire explosion. Experimental results on electrical explosion of wires in vacuum and air with current density $j \sim 10^{12}$ A/m², current rise rate (dI/dt) ~ 50 A/ns and current pulse with amplitude ~ 10 kA are presented. The structure of the discharge channels in vacuum has been studied using laser shadow and schlieren imaging with 7 ns frames, UV pinhole images. It was studied and analyzed the different regimes of the wire explosions: the current in the circuit was interrupted at some moment of the pulse; the exploding wire was preheated before start of the main current pulse.

To plot the UV image, there was used a four-frame micro channel camera with 5-ns exposure duration, 10-ns interval between frames and maximum sensitivity in the ultraviolet range (> 10 eV quantum energy). The image was plotted with 1:2 magnification using a 4-pinhole of rather large diameter—400 or 200 μm . The spatial resolution in this case was not very good, but using a pinhole of large diameter provided the needed optical

efficiency. The information on the dense core material and the conducting plasma distributions was obtained in our experiments by analyzing and comparing the results obtained from all diagnostics.

The experiments have shown that the current-conducting plasma, which is observed in UV radiation, occupies the most of the discharge channel and has a higher expansion rate than the more dense part of the exploding wire material that is observed by laser probing. Development of $m = 0$ instabilities in the conducting plasma was also observed. A difference in the shock wave propagation in air and the expansion of the exploded wire dense core in interrupted- and uninterrupted-current regimes has been observed.

SIMULATION OF A TUNGSTEN WIRE HEATING BY A CURRENT PULSE

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There exist some insufficiently studied problems which complicate the calculation of wire ablation and formation of a plasma flow in the course of wire array heating by an intense current pulse. Among others we underline the problem of wire ablation accounting in coupled simulation of multiple-scale ablation-plasma motion processes. Note that in modern experiments carried out in multi-megaampere generators the typically used wires have a micron-size diameter while the diameter of the whole array is about of a centimeter. Another important problem consists in building the model able to describe the “cold start”, i.e. the wire heating by an electric current starting from the room temperature. It is possible to alleviate the mentioned problems by constructing a model of plasma source to incorporate it into the radiative-magnetohydrodynamic model. To simulate electric explosion processes of wire arrays correctly, it is primarily necessary to study the dynamics of the single wire explosion. Therefore at first we study the problem of heating 25 μm tungsten wire by a current pulse with rise-time about 400 ns and current maximum of 10 kA. For comparisons we used the experimental data which refer to a wire explosion in a vacuum (S.A.Pikuz et. al., 2008). The calculations through the whole computational domain including the wire material and its surroundings were done by virtue of homogeneous RMHD-model. The extremely

rarefied substance or vacuum were substituted by a model medium with density and conductivity sustained at some minimal level allowing correct MHD-calculations. The equation of state used in calculations was of the wide-range type: it was able to describe various phases of a wire material as well as metastable states (V.E. Fortov et. al., 1998). The electric conductivity was calculated according to semi-empirical model (H. Knoepfel, 1970). Two different codes were used for the wire evaporation modeling. The initial stage of wire explosion (~ 40 ns), was simulated using the 1-D conservative numerical technique with accounting for the phase transition. The following simulation was implemented in the frames of a two-temperature plasma model. The calculation at this stage was done by a Lagrangian-Eulerian RMHD-code RAZRYAD-2.5, (V.A.Gasilov et. al., 1990). We simulated the coupled expansion of a wire core and corona. The numerical results are in agreement with experimental data.

PHYSICAL AND NUMERICAL MODELING OF PROCESSES OF THE LARGE POWER OBJECTS EXPLOSION

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Improving of the stability, fire and explosion safety of the power objects is largely determined by the level of modeling of the probable accident scenarios. The aim of this work is the physical and numerical modeling of the oil filled transformer explosion.

Contemporary oil filled transformer is a complex power installation. The oil mass in such transformers can be about one hundred tons. The accident in so power-filled system has a wide influence range. It can result to destruction of not only transformer, but other objects. Reconstruction and resumption of the work are extremely expensive. Usually the transformer explosion is caused by a shortcut circuit. In this case the electrical breakdown of the dielectric oil occurs, the electrical arc is generated. Due to the electrical arc evolution the oil is vaporizing. As vapor-gaseous bubble is forming, the layers of cold oil are compressed and pressure in the oil filled tank is increasing. Time duration of gas generation and pressure increase is greater then period of acoustic relaxation of the transformer vol-

ume (d/c , where d —characteristic length scale of transformer, c —sound velocity in the oil). Exceeding of pressure limit of transformer leads to transformer destruction. Due to this, the safety is one of the most important and least examined problems in the transformer design and building practice. This work proposes modeling method of the transformer explosion. The testing of oil filled transformer using high voltage generators is replaced by the explosion of water filled transformer shell. This method can be put into practice of the equipment testing during the design phase. It is based on the similarity of the physical properties of water and mineral oil and on the assumption of the possibility to model an electrical breakdown in the oil by the explosion in the water. The energy deposition in both of phenomenon is expected to be equal. Explosion in the water is produced by the cylindrical load of condensed high explosive (HE).

The numerical simulation is used for more detailed interpretation and accompaniment of the real experiments. It allows to understand the evolution of the hydrodynamic processes in both of problems (electrical breakdown in the oil and explosion in the oil and the water). For the calculations the computational fluid dynamics computer codes are used. These codes are based on the model that includes the hydrodynamic transport of viscous compressible fluid and heat conduction. The transport coefficients and equations of state of real fluids were used. To describe the explosion in the water the Kuznetsov equation of state is used [1]. The equation of state for the transformer oil is based on the experimental data. The equivalence of the energy release in the HE explosion and electrical breakdown is used to calculate the mass and size of HE. It is shown that the generation of the maximum pressure is sufficiently reasonable in both tasks.

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A MAGNETIC-CUMULATIVE GENERATOR WITH MAGNETIC FLUX TRAPPING AND A PRIMARY CIRCUIT BEING SWITCHED OFF

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To feed an inductive load $\sim 0.1 \mu\text{Hs}$ with an electrical pulse with steep fast-head front (a leading edge no more $3 \mu\text{s}$) and output energy

~ 100 kJ, the circuit design with current switching is traditionally used, amplitude of a current being ~ 1.5 MA. The alternate solution can be use: a magnetic-cumulative generator with magnetic flux trapping (MCG FT) with a primary circuit being switched off. Modeling of such generator with a sliding contact point has been conducted with different dependences of inductances decreasing used. It has been shown the effective application of the MCG as small-sized power supply device, with an abatement of a HE weight twice. Theoretical and experimental results are presented for actual magnetic flux losses, coefficient of perfection, losses in the contact point of, and also for open switch resistance. The maximum parameters of the device picked on the basis of the executed calculations. With restrictions of a load voltage no more than 40 kV, MCG FT has been designed and investigated with cutout of a primary circuit. Generators were tested for a model loading by inductance $1.16 \mu\text{H}$. An explosive open switch cuts out a current by amplitude 3 MA no more than $3 \mu\text{s}$, that ensured front of a build-up of a voltage pulse on a loading $\sim 2 \mu\text{s}$. The intercepted magnetic flux in primary circuit 0.086 Wb, the electrical pulse in a loading has been registered with parameters: energy 86.3 kJ, a magnetic flux of 0.45 Wb. Coefficient of flux conservation —0.6. The leading edge of the current and the shape of the voltage on the load have matched to desired values. The tests under consideration have demonstrated a high performance and an opportunity of MCG FT application in the power supply of the impulse plasma accelerator.

INITIATION OF EXPLOSIVE-MAGNETIC GENERATOR WITH A HELP OF EXPLOSIVE WIRES

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Powerful pulsed sources on the basis of the explosive-magnetic generator (EMG) have found a wide application as in scientific investigations, so in solving the practical problems [1]. Nowadays there exists a necessity to apply such feeding sources in the field conditions, for example for testing the electro energetic objects, including high voltage lines, from the point of view of supplying the necessary lightning protection, for estimating the electrical conductivity of different kinds of soils [2, 3]. In the previous works [4] it was shown, that the explosive-magnetic generator successfully worked on the emulsion explosives (EHEs). The initiation of EHE is

a complicated experimental problem. It is connected with its low sensitivity and as a consequence—a high critical detonation diameter. In the work different methods of initiation, including the methods without using electro-detonators and intermediate charges of the state high explosive are tested. The methods are based on transition combustion regimes to low-speed detonation, with the use of dry compositions on the base of ammonium nitrate and sodium nitrate and the combination of these methods. The initial pulse was created by explosive wires.

The setup for initiation of emulsion high explosive with a help of explosive wires was developed and tested. The opportunity of use of the suggested scheme for initiation of the explosive-magnetic generator liner filled with EHE was experimentally represented. The energy characteristics of explosive wires and also time and detonation parameters, necessary for using of this device in mobile installation are determined [1].

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HEAVY ION TARGETS FOR THE INERTIAL FUSION AND FOR EXPERIMENTS WITH HIGH ENERGY DENSITY IN MATTER

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By means of the multi-dimensional multi-temperature code [1] we carry out calculations of the burning wave propagation for different types of fuels (DT, pure deuterium, and the hybrid deuterium target with the U238 shell) in the direct cylindrical targets. Such targets are as a natural scheme for the heavy ions driver due to a long ion’s braking path in compare with the laser irradiation. It is possible to conserve the necessary symmetry at the

compression. Also is possible to obtain the large enough gain. For fuel parameters ρ_{fuel} , $(\rho r)_{\text{fuel}}$ acceptable for the existence of the steady burning wave we can estimate requirements for the compression beams (10 MJ/cm, 10000 MJ/cm, and 500 MJ/cm for different types of targets) [2, 3, 4, 5, 6].

Obtained driver's parameters can be compared with these parameters for indirect spherical targets, irradiated by the x-ray obtained from the conversion of the driver with the energy ~ 10 MJ [7]. For the developing setting ups in GSI (Darmshtadt) and in ITEP (Moscow) with the beam's energy ~ 100 MJ we discuss the possibility for the obtaining of the high energy density in the matter with the pressure ~ 50 Mbar and the temperature ~ 40 eV. Such parameters are possible for the comparatively low total energy in compare with chemical explosions due to the high specific power [8, 9].

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COMPUTER SIMULATION OF SOLID GRAPHITE SUPER-FRS FAST EXTRACTION TARGETS

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Survival of the production target irradiated with high intensity uranium beam in successive experiments (with a repetition rate of 1 Hz) over an extended period of time is one of the key problems encountered in designing the Super-FRS (Superconducting Fragment Separator) at the future Facility for Antiprotons and Ion Research (FAIR) at Darmstadt. Because of the difficulties involved in construction of a liquid jet metal target, it is highly desirable to employ a solid production target at the Super-FRS. However, with the high beam intensities that will be available

at the FAIR, the production target may be destroyed in a single experiment due to high specific energy deposition by the beam in the target material. The level of specific energy deposition can be reduced to an acceptable value by increasing the beam focal spot area. However, the spot size is limited by requirements of achieving good isotope resolution and sufficient transmission of the secondary beam through the system. The resolving power of the fragment separator is inversely proportional to the X-dimension of the focal spot whereas the transmission depends on Y-dimension only. It has been previously shown [Tahir et al., 2005c] that an elliptic focal spot with appropriate dimensions, will fulfill the above two conditions simultaneously and will also have a large enough area to reduce the specific energy deposition to an acceptable level for certain beam intensities of interest. In this paper we present numerical simulations of thermodynamic and hydrodynamic behavior of a solid graphite target that is irradiated by 1 GeV/u uranium beam in the intensity range of 10^{10} – 10^{11} ions per bunch with a bunch length 50 ns.

These simulations have been carried out using a three-dimensional computer code, PIC3D, that includes elastic-plastic effects, in two and three-dimensions. This theoretical work has shown that up to a beam intensity of 10^{11} ions/bunch, one can employ a solid target while for higher intensities the target will be destroyed due to thermal stresses induced by the beam. It has also been found that a circular focal spot leads to minimum thermal stresses as it generates minimum pressure gradients compared to an elliptic focal spot, for the same specific energy deposition. Moreover, the stress level increases with an increase in the ellipticity of the focal spot. It is therefore recommended that one should use a circular focal spot for lower intensities provided that the criteria for isotope resolution and transmission are fulfilled.

OSCILLATIONS CURRENT OF THE PROTON BEAMS AT PASSING THROUGH DIELECTRIC CHANNEL

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The Phenomena of the passing beams accelerated charged particles through dielectric channels and connected with this physical processes at present are actively studied. Recently, was discovered that at passing ion beams through flat [1] and cylindrical channels [2], exist the oscillations

of the current of the beam. In presented work were also fixed oscillations of the current of the beams accelerated proton, passed through glass and fluoroplastic cylindrical channels. In experiment was noted that oscillations appear only under determined position of the cylinder for directions of the spreading the proton beam. Also, there were noted flashes of the phosphorescence in channel, correlated with oscillations of the current of the beam. At present explanations of the mechanism oscillations in literature is absent. The Nature oscillations points that they appear as a result of periodic formation on surfaces dielectric conducting channel moreover dependency of the appearance these channel from ion dose encountered on wall of the channel must have hysteresis, i.e. channels must appear under greater dose, than dose, under which they disappear. The Authors consider two mechanisms, which can be in charge of this phenomena: electric breakdown of the gas, adsorbed on surfaces, and sharp increase to surface conductivity of the material of the wall of the channel as a result of accumulations on surfaces of the critical concentration certain bistable defect. Under this concentrations must occur phase transition dielectric-metal. The japanese scientist Tarasava observed the Similar phenomena of the periodic arising the breakdowns solid dielectric at study of the anomalous behavior of the indicative x-ray radiation [3].

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ION GUIDING THROUGH AN INSULATING CAPILLARY

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We discuss the mechanism of ion guiding through insulating channel in this work. We suggest the model for explanation of the experimental angular dependence of the ion current transmitted through a flat capillary. The model is founded at the assumption that surface conductivity has very sharp dependence on surface charge under the ion irradiation. The conductivity rise up very sharply, if the surface density of charge become higher than any critical value σ_0 . In this case the beam creates and keeps

the density σ_0 at the interval l of the top plate if ions enter the capillary at any angle ϕ . The length l defines the value of that part of a beam, which is necessary for creation and keeping the density σ_0 at this interval. The rest part of beam comes through. And the length l is defined by necessity to bent the rest part of beam at the angle ϕ in the uniform field $2\pi\sigma_0$, which is created by surface charge. The angular dependence of the transmitted current can be parabolic or trapetsium just as in the experiment.

The flat capillary guides ions if we tilt the ion beam towards the capillary plane at a few degrees and it guides ions if we rotate the flat capillary around axis which is perpendicular to plates without changing the plane of the plates in the small angular interval too. We call this phenomena double guiding. In this paper the model for explanation the double guiding is suggested. The modeling shows that double guiding is due to creation the surface charge distribution with rather high shoulders along the ion trace. This charge creates the coulomb trap for transversal motion which keeps the ions in if the angle is rather small.

WIDE-RANGE ELEMENTARY CELL FOR HETEROGENEOUS MATERIAL WITH DISPERSE FILLER

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Quite a few non-equilibrium models of heterogeneous material cell absorbed intense ionizing radiation (IR) fluxes of different physical nature are constructed at the present time [1, 2]. These models have variant application regions and it can not used at all practically important interspaces of intense IR fluxes parameterizes [3].

The wide-range non-equilibrium model for elementary cell of heterogeneous material with polydisperse filler is constructed. It is assumed that cylindrical cell is existed in uniaxial deformational state. Stresses relax calculation for each cell is based on solution of elastic-plastic medium equilibrium equations and wide-range equations of states. Suggested model allows determining initial stress profile in all variation range of absorbed specific energy densities (small energy contributions than elastic-plastic deformation is important are as well as large energy contributions than phase transitions take place). This model takes into account effects of electrical micro-breakdown and thermal exchange between heterogeneous material components.

In our model we paid attention to structural specialties of multilayer micro-spherical fillers used for protection from IR in heterogeneous coverings. These specialties were taken to account by consideration of next processes: the loss in stability of thin micro-spheres than thickness-to-radius ratio is small; thick micro-spheres destruction; irreversible collapse of micro-spheres [4].

Calculations results of initial stresses profiles in heterogeneous coverings filled glass or carbon micro-spheres (they are covered heavy metals: tungsten or nickel) are presented.

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DEFORMATION AND DESTRUCTION OF MULTILAYER ELASTIC-PLASTIC SHELLS UNDER COMBINED THERMAL AND MECHANICAL ACTIONS OF RADIATIONS AND PARTICLES FLUXES

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Development of numerical methods for modeling of dynamic deformation and destruction of thin thickness constructions remains important throughout in despite of heady progress of calculation methods used in non-stationary deforming solid substance mechanics. It may explain, firstly, how capabilities of problem dimension decrease (in particular it allows to improve results demonstrativeness), secondly, how it is notorious that numerical modeling of non-stationary processes in thin thickness constructions requires powerful computer time expenditure beyond the framework of shell hypothesizes.

Universal numerical code for modeling of dynamic deformation and destruction of thin thickness constructions was suggested in [1]. This code

provides calculations of non-uniform heated shells having variable thickness. We regard that university includes: possibility provision for calculations of complex multilayer thin thickness constructions having various packets conformations, geometrical shell forms and sustentative elements; possibility provision for inclusion of different shell models (Kirhgoff-Love's hypothesis, Timoshenko's hypothesis and others of that ilk), material deformation and destruction models.

For numerical realization of shell model we use space variables splitting method and implicit finite-difference scheme. It will be observed that implicit type of the scheme provides possibility to achieve stationary regime. At every time step the solution for system of algebra equations that were obtained after Newton linearization method of initial equations in finite-difference form is made by matrix running method with main component choice by column. It's correct for any definite system of equations.

Calculations results allow to make conclusion that suggested numerical code may be employed to wide problem group referring to investigations of thin thickness constructions strength to combined thermal and mechanical actions of radiations and particles fluxes.

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ESTIMATION METHOD OF PRESSURE IMPULSES FORMED IN IRRADIATED HETEROGENEOUS MATERIAL HAVING FRAME

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Pressure impulse is of basic radiation mechanical action parameters that define destruction of irradiated construction. Because development of reasonably simple method allowed estimating this integral characteristics with admissible error (it's less 10 percentages [1]) is required. Efforts of different authors lead to integral formulas allowed calculating vapor and failure impulses. These formulas contain constants complex defined from experimental date or gas-dynamic calculations results. Selection of constants is happily realized if we have case of homogeneous material. However this selection is not correct for heterogeneous material.

In the present work above integral formulas are used in upgraded forms. In particular effective Grünaisen coefficient is applied in integrand in place

of agreeable parameter of homogeneous material. It will be noted that Grünaisen effective coefficient of heterogeneous material vastly differentiates from coefficient of average homogeneous material in many cases. It takes place if heterogeneous material has strongly marked frame. In addition effective Grünaisen coefficient changes in target space. In particular it's associated with energy redistribution by secondary electrons because in the making of radiation transfer spectrum becomes hard and electrons gab grows. Non-equilibrium elementary cells models [1, 2] are used for effective Grunaisen coefficient calculation.

Calculations results of pressure impulses in irradiated heterogeneous material having multilayer filler are presented. We consider micro-spherical filler covered heavy metals (nickel and tungsten). It's demonstrated that suggested method of pressure impulse estimation provides required accuracy.

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HYBRID METHOD OF ENERGY ABSORBING CALCULATION FOR X-RAY IRRADIATED SPHEROPLASTICS

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At the present time spheroplastics are considered as perspective heterogeneous coverings used for protection of vehicles from x-ray intense fluxes [1]. These materials diminish radiation by means of heavy metals inserted on filler surface. In addition irreversible collapse of micro-spheres provides mechanical impulse damping in irradiated covering. However numerical modeling realized of collective transfer of photons and secondary electrons in spheroplastics is difficult because in considered case insertions dimension are smaller than (or are comparable to) run length of secondary electrons. In particular direct application of Monte-Carlo method leads to colossal computer time expenditure.

Hybrid calculation method is suggested in the present work. Photons transfer is realized by Monte-Carlo method but energy redistribution by secondary electrons is determined analytically. According to this point of

view 'incuts' method [2] is used. It's suppose that x-ray flux insignificantly changes within heterogeneous material elementary cell that is photon run length is more then micro-sphere dimensions. Angular distributions of secondary electrons born in interaction processes (photo-absorbing and Compton scattering) are supposed isotropic [3].

Calculations results for specific energy absorbed in components of heterogeneous material having glass or carbon micro-spheres (they are covered heavy metals: tungsten or nickel) are presented. Accounting necessity of energy redistribution by secondary electrons that born in thin layers of heavy metals coverings is presented.

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COMPUTER MODELING NON-STATIONARY HEAT TRANSFER THROUGH DISPERSION MATERIALS AT HIGH TEMPERATURES

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The heat transfer under influence of high intensive thermal fluxes on dispersion materials is carried out by thermal radiation, thermal conduction on the particle, thermal contacts between particles, and thermal conduction through gas which fills in space between particles.

As a rule, an assumption about local thermodynamic equilibrium is carried out at a stationary state for materials strongly absorbing thermal radiation. Thus, it is possible to attribute radiation and conduction conductivity to the same temperature and to use the diffusion equation. In this state the effective conductivity coefficient characterizes thermophysical properties of the dispersion material. However, the assumption about local thermodynamic equilibrium has no place in many cases at a non-stationary state for translucent thermal conduction materials. Besides, it is necessary to take into account the fact that the speed of thermal radiation distribution is much greater than conduction speed of distribution of heat. In the present report the heat transfer in a dispersion material is simulated by system of opaque punched thermal conduction screens (shields).

As shown, the heating of screens with sudden high intensive thermal fluxes is carried out basically by thermal radiation firstly and afterwards by conduction heat transfer. In this case the heat transfer through a dispersion layer limited with two opaque shields is determined in such parameters as emissivity, specific heat capacity, volumetric density of dispersion particles material and volumetric density of the dispersion particles layer. Due to small sizes of particles and large thermal resistance between the particles a role of the thermal conduction component can be neglected at an initial stage of non-stationary heat transfer. The probable applications of the given model for research of heat transfer through a dispersion material on a vermiculite basis are discussed.

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CHARGE-DENSITY EXCITATIONS IN BILAYER GRAPHENE GRAPHENE IN HIGH MAGNETIC FIELD

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The bilayer graphene is the unique object which combines the parabolic dispersion law of quasiparticles with their chirality exhibiting Berry phase 2π . In magnetic field there is a double-degenerate zero-energy Landau level incorporating two different orbital states with the same energy. Taking into account spin and valley degeneracies, the zero-energy Landau level in a bilayer is eightfold degenerate. This one-electron structure was confirmed in experiments of integer quantized Hall effect and Shubnikov-de Haas oscillations. These properties are understood in terms of non-interacting electrons. The influence and exhibition of electron-electron interaction is the following problem. The low-lying excitations of these systems may be sensitive to interaction. Inter-Landau-level transitions in the bilayer graphene at high magnetic field have been studied. The influence and exhibition of electron-electron interaction is the following problem. The low-lying excitations of these systems may be sensitive to interaction. These transitions are the charge-density excitations (magnetoplasmons). The charge-density excitations at small momenta are considered in the frame of the Hartree-Fock approximation. The case of filling-factor $\nu \ll 1$ is considered. This filling-factor means the absence of free carriers due to doping. The presence of small asymmetry of graphene layers is included. Without magnetic field, the asymmetry gives rise to the gap in the spectrum; in the pres-

ence of the field, the asymmetry splits the eightfold degenerate zero-energy Landau level into two fourfold levels. As for monolayer graphene, there is the problem of divergency of exchange self-energy due to summation over all filled LLs. The spectrum of monolayer and bilayer graphene described by model Hamiltonian is unlimited in the top and in the bottom. This fact is physically artificial. The energy of the magnetoplasmon excitations is considered and the strong dependence of the energy on the form of the bilayer ground state is shown. In asymmetric bilayer taking into account spin we have four transitions with equal energies. Energy splitting due to asymmetry is absent, only additional shift takes place. In the case of symmetric ground state with half-filled 0 and 1 for each valley and spin there are two combined $Q_{1,2,\xi,\sigma}^+ - Q_{-2,1,\xi,\sigma}^+$ transitions splitted in energy. If this splitting would be observed it would be the evidence of Coulomb interaction in bilayer graphene.

The work is supported by the Russian Fund of Basic Research.

INVESTIGATION OF STRUCTURAL DEFECTS IN Si SUBJECTED TO HIGH PRESSURE TREATMENT

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Silicon is the most important material for electronics due to a development of relatively cheap technology for preparation of material with prescribed properties. As a result almost whole output of electronic industry is produced on the base of silicon technology. The gradual complication of electronic devices led to considerable increase of the length of connections, e.g. in a contemporary processor the common length of connections is about 12 km. This leads to slowing down the operating speed of devices. The most optimal solution of this problem is the use of optical communication between different parts of processor, which on one hand speeds up the communication and on the other hand eliminates the galvanic connection between different blocks. The main obstacle for this solution is extremely low efficiency of radiative emission in silicon due to its indirect forbidden band. Indeed, in this case the momentum conservation law requires participation in recombination process of the third particle phonon. This in turn sufficiently increase the recombination time. The only solution of this problem is the finding of the way of direct recombination of electrons and holes in silicon to increase the probability of the process at least up to the level of probability of nonradiative transitions. The intensive investigation

is proceeds in different laboratories of world. Among different approaches the most perspective is the application of interatomic transitions in transition metals inserted into the lattice of c-silicon. In particular, the use of Er enabled to obtain the effective emission in the range of 1500 nm. However, it happened that only one percent of atoms introduced in silicon participate in radiative recombination. The alternative way developed in ISSP RAS, utilize the recombination at dislocations in silicon. In this case the radiation in the range of 1530 nm arises. The investigation of the centers responsible for dislocation related luminescence revealed that they are the structural defects generated during the reconstruction of bonds in the core of dislocation. The primary task for increase the efficiency of this radiation is the search of the ways for appropriate generation of these centers, which are compatible with silicon technology. In particular, it turned out that the relaxation of structures created at the deformation of silicon under high pressure gives a considerable concentration of required centers. In this work the dynamic of generation of radiative recombination centers is studied by photoluminescence technique as a result of relaxation of silicon samples after high pressure treatment.

ON THE MICROWAVE ASSISTED SYNTHESIS OF SELENIUM NANOSTRUCTURES IN POLYMERIC COMPOSITES

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Elemental selenium, the famous old semiconductor and photoconductor, has a new birth nowadays. Its new very significant nanoproperties have been discovered. Nanoselenium has new very promising applications in nanomedicine, electronics, photonics, etc. So selenium-polypyrrole core-shell nanoparticles can be used for targeting and imaging of human cancer cells [1], and trigonal selenium nanowires—for fabrication of field effect transistors [2]. New optical materials and devices can be constructed on the base of nanoselenium. It is fast photons detectors, photonic band gap materials-photonic crystals, superlattices [3, 4]. We had researched nanocomposites of sulfur, selenium and tellurium produced in result of redox interactions at room temperatures and at thermal heating for temperatures below the temperature of destruction of the matrix polymer. Some surfactants were used by us in these preparations [5, 6]. It was very

interesting to study the formation of our nanocomposites in the field of microwave irradiation. So we have a chance to discover new phenomena in this process and to find the best way of the synthesis. These nanocomposites were prepared in the result of reactions of selenious acid with reducing agent (hydrazine-hydrate, hydroxylamine chloride) in the solution of polymer, containing one of surfactants. Last mentioned substances were from the family of oxiethylated alkylphenols. The mixture was treated in microwave oven. Obtained liquid systems contained elemental selenium and were dried on glass slides for microscopy. Films produced with this way have been studied by methods of optical and electronic microscopy, x-rays analysis, and the optical spectroscopy in UV-visible light.

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MICROWAVE SYNTHESIS OF ULTRA-NANOPOWDERS OF TUNGSTEN OXIDE

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Recently, a large amount of publications describing the fabrication of different nanomaterials using microwave radiation has emerged. It is known that the influence of the microwave radiation on the synthesis processes strongly depends on the chemical features of the compounds. For example, the synthesis of metal oxides by the decomposition of freshly precipitated hydroxides proceeds much faster than the decomposition of the corresponding salts. This can be explained by the absorption coefficient of water and hydroxyl which are present in considerable amounts in freshly precipitated hydroxides.

It is noticeably more difficult to control the absorption coefficients of crystal salts and clearly recognize the influence of the microwave field on their decomposition process. In addition, the use of microwave heating for the synthesis of individual metal oxides allows to obtain powders with a small dispersion in grain size and to a decrease of the average grain size.

The present work concentrates on the production of tungsten oxide powder from freshly precipitated tungsten acid on a carbon substrate with and without microwave heating. The influence of the duration of microwave processing on the microstructure of the obtained oxides has been determined. The freshly precipitated tungsten acid has been obtained from water solutions of ammonium tungstate (concentration 45–50 g/liter with counting from WO_3 by the addition of hydrochloric acid ($\text{pH} = 1\text{--}1.5$)). The obtained precipitates have been washed, filtered and treated by an electromagnetic field with frequency 2450 MHz and power 700 W. During precipitation tungsten acid with a monoclinic structure was obtained, subsequent drying in the electromagnetic field at temperatures not higher than 130°C leads to its decomposition into $\text{WO}_3 \cdot \text{H}_2\text{O}$. At higher temperatures, dehydration and the formation of pure tungsten oxide with a monoclinic structure have been observed.

For samples on a carbon substrate (soot), self-heating to temperatures $700\text{--}800^\circ\text{C}$ was achieved during 30 minutes and a mixture of tungsten oxide with an orthorhombic structure and soot was obtained. The obtained mixtures are suited for the synthesis of ultra-nanopowders of tungsten carbide. The specific surface of the obtained powders ranges from 20 to $100\text{ m}^2/\text{g}$ with a grain size of 50 to 200 nm, which form aggregates of about $1\text{ }\mu\text{m}$.

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NONEQUILIBRIUM RADIATION DURING IRON CLUSTERS FORMATION AT ROOM TEMPERATURE

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The nanoparticles growth from the supersaturated vapor starts with the small clusters formation, which are the initial centers of condensation. In [1] the iron nanoparticles growth due to supersaturated iron atoms condensation produced by pulse laser photolysis of $\text{Fe}(\text{CO})_5$ was investigated. To describe the iron particle size growth it was necessary to accept some values of the size and concentration of the initial iron clusters, which were unknown in fact. Direct observation of the small clusters in the experiments with supersaturated vapor condensation is extremely limited by the time and spatial resolution of the measurement system. However the formation of iron clusters is accompanied by the release of binding energy (2–4

eV per atom), therefore one can observe the radiation from excited clusters. These data could be useful to reconstruct the concentration and size of small iron clusters by kinetic modeling. The evidence of such nonequilibrium radiation from iron clusters was found in shock tube experiments [2]. In work [3] similar phenomenon of nonequilibrium excitation of C_2 radicals during carbon vapor condensation was observed.

In this work the measurements of radiation during iron clusters formation from supersaturated iron vapor were performed. The iron vapor was produced by pulse laser photolysis of $Fe(CO)_5$ in quartz reactor at room temperature. The amplitude and duration of iron clusters radiation were measured at the wavelength 633 nm. The dependences of maximum amplitude of clusters radiation on the initial concentration of iron atoms and pressures of argon or helium were found. These dependences were described in the frame of the developed kinetic model of the iron clusters growth taking into account the formation of excited iron clusters and deactivation collisions with the bath gas molecules. By the fitting the experimental data and the results of kinetic modeling the concentration of clusters Fe_2 - Fe_{10} , formed at the initial steps of the supersaturated iron vapor condensation were extracted.

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MODELLING OF WAVE INFLUENCE ON THE GASCONDENSATE SYSTEM

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For increase an economic efficiency of the resources put in mastered and reconnoitered deposits, it is necessary to develop and apply the new technologies allowing most full to use being in bowels of the earth hydrocarbon material.

The wave technologies of multiphase systems, which are, based the theory of nonlinear oscillations of multiphase systems, can find application for an intensification of technological processes in extraction of gas, including

for increase in an output of gas and a condensate. By means of cyclic wave influences, it is possible to change hydrodynamic and thermodynamic properties of process mass transfer in a layer and, thus, to promote increase in an output of a condensate during use of gas-condensate field.

In JIHT RAS the cycle of experimental and theoretical works on modeling of processes of mass transfer in two phase system (a mixture methane–n-butane) in the porous environment at conditions (pressure and temperature) of real beds is carried out. Developed software PLAST [1] of a two-phase filtration of hydrocarbon mixtures for modeling influence of acoustic waves on a bed was used.

As a result of the executed calculations the opportunity of destruction of a condensate fuse due to periodic wave influence (an interval of frequencies from 0.001 up to 100 Hz) with amplitude from 11 up to 34 atm is shown. It is shown, that time of destruction of a liquid obstruction for the set amplitude has the minimal value for the certain frequency of influence. The qualitative explanation of effect of destruction of a liquid obstruction under action of periodic influence is offered. The equations for dependences of optimum frequency and minimal time of destruction from relative amplitude of influence are received.

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**SHOCK WAVES.
DETONATION.
COMBUSTION**

**MECHANISM AND CRITERION OF STEADY
DETONATION WITHOUT CHEMICAL SPIKE**

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Recently Ashaev et al. [1] and later Utkin et al. [2] observed detonation wave profiles without a spike in several high-density explosives. Utkin et al. also traced evolution of the detonation wave structure with increasing HE density: As the density is increased, the magnitude of the chemical reaction zone spike decreases to zero and then, with a further increase of density, the pressure decay in the chemical reaction zone is replaced by its growth. Similar evolution of wave profiles also occurs with increasing pressure as found by Erskine et al. [3] in experiments with overdriven piston-supported detonations. They interpreted this finding as evidence of crossing of the product and reactant Hugoniot at elevated pressures. Alternate explanation relates observed effects with significant portion of the energy release immediately during shock compression. This assumption is not improbable but it can not be verified and can not be used in analysis and practical calculations of the detonation phenomena.

In the presentation, the mechanism by which the Chapman–Jouguet condition of steady detonation is achieved is analyzed and extended to the case when the Hugoniot of the unreacted HE may intersect the Hugoniot of the detonation products. At such relationships between EOSes the normal detonation wave with a “chemical spike” is realized for low-density HE. As the HE density increases, the relative spike amplitude should decrease, as is observed in experiments [2]. At some threshold value of the initial specific volume of the HE, the point of Chapman–Jouguet tangency reaches the point of intersection of the Hugoniot. At this point, the chemical spike of the detonation wave is transformed to a plateau. At larger density, the initiating shock wave should increase in amplitude until the pressure behind its front reaches the value P_{0c} that corresponds to the point of intersection of the Hugoniot. As the state approaches this point, the energy release process ceases to influence the evolution of the shock wave. It has been shown, there is a mechanism, which causes the pressure in the entire reaction zone to decrease or increase to the P_{0c} value. In other words,

the intersection of the Hugoniot of the unreacted HE and the Hugoniot of the detonation products determines the detonation parameters and thus replaces the Chapman–Jouguet condition for HE of high density. It may be expected that the pressure in the chemical reaction zone of such dense explosives is constant or is slightly varying. The intersection should weaken the dependence of the detonation speed upon the HE density that also was observed experimentally.

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MEASUREMENT OF SOUND VELOCITIES IN SHOCK-COMPRESSED TIN AT PRESSURES UP TO 150 GPa

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A great interest is recently shown to study of tin by theoretical as well as experimental methods. Tin has a complex phase diagram, which includes regions of some crystalline phases at high pressures.

Sound velocity is an important physical parameter, which has high sensitivity to change of substance compressibility that characterizes a phase state. Breaks in the dependence of sound velocity upon shock pressure are caused by phase transitions in shock-compressed substance. Therefore, basing on measurement of sound velocities, it is possible to reveal phase transitions (including the melting) of the substance along the Hugoniot.

In this work, measurements of sound velocities in tin are performed up to pressures of shock compression of about 150 GPa. Tin samples with initial density of 7.28 g/cm³ and purity of 99.915% were loaded with use of HE-based generators of shock waves. The samples represented disks with diameter 18 or 60 mm and different thickness. In the pressure range of 30–150 GPa, sound velocity in tin is measured by the method of over-

taking release with use of carbogal, tetrachloromethane, and bromoform as the indicator liquids. Optical gauges based on photodiode were used for recording of the luminescence of the liquid indicators. Up to shock compression pressures of about 35 GPa, sound velocity in tin is measured by the method of oncoming release with use of piezoresistive manganin gauges.

The obtained data are compared with results of calculations using a semiempirical equation of state that allows for the polymorphic transformations, melting, and evaporation effects. The multiphase equation of state presented is used to estimate temperature values on phase boundaries of tin over investigated Hugoniot pressure range.

HUGONIOT OF C₇₀ FULLERITE VIA SYNCHROTRON RADIATION TECHNIQUE

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First-time measurements of shock compressibility of C₇₀ fullerite were performed with the use of pulsed-periodical source of synchrotron radiation of the Institute of Nuclear Physics SB RAS. The starting C₇₀ specimens consisted of two crystalline phases: the phase with a hexagonal close-packed and the phase with a rhombohedral structure. The specimens were prepared by high (1 GPa) hydrostatic pressure treatment and had a density of 1.65 g/cc, a diameter of 15 mm and a thickness of 2.5-3.5 mm. Specimens were loaded by impacts of metal plates (with a diameter of 16 mm) accelerated by high explosives. Synchrotron radiation technique was used to measure the parameters of the shock-compressed fullerite. This method of measurements is based on visualization of X-T diagram of shock-wave processes by measuring a degree of attenuation of synchrotron radiation by an explored material during passage of a shock wave through this material. It was obtained that the experimental Hugoniot of C₇₀ fullerite in the explored pressure range (6.3-9.3 GPa) is allocated below the experimental Hugoniot of C₆₀ fullerite [1] on pressure-specific volume plane. The work was supported by RFBR (07-02-00625).

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GRAPHITE TRANSFORMATION IN THE DIFFERENT STRUCTURAL STATE TO THE DIAMOND-LIKE PHASE IN DEPENDENCE TO LOADING DIRECTION

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The investigation of influence of the basal plane of crystal lattice and graphite structure on parameters of polymorphous transformation of graphite to diamond was carried out. Five types of graphite with different concentration of rhombohedral phase in graphite were tested: OSCh–T1 graphite (1–3%), two types of natural graphite from the Taiga deposit with different grain sizes (5% and 25–28%), monochromator-grade graphite and colloidal graphite C1 (32%). Uniaxial shock loading of graphite sample were created by using a plane aluminum impactor accelerated by explosive facilities up to velocity of 3.3 km/s. In the experiments, VISAR laser-Doppler velocimeter was used for recording the particle velocity history of interface between the sample and LiF window. Measured transformation pressure under loading perpendicularly to axis *c* was higher and the rate of transformation was several times less than in along to axis *c*. Under loading of graphite samples with basal planes located at the 45° angle transformation pressure measured was the same, but the rate of transformation was higher. Plastic deformation of sample occurs due to displacement of basal plane disposed by 45° to loading direction relatively to each other and due to atomic displacement in basal plane graphite. Possibly, these shears along the basal plate impede transformation of graphite to diamond. It was expected, that existence of rhombohedral phase in graphite powder advance martensitic transformation of graphite to diamond, but this assumption was not confirmed. The measurements show a rise of transformation pressure with increasing of the rhombohedral phase concentrations in graphite powder, but transformation rate is not changed.

INFLUENCE OF INITIAL TEMPERATURE OF GRAPHITE ON PARAMETERS AND KINETIC TRANSFORMATIONS INTO DIAMOND AT SHOCK-WAVE LOADING

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Transformation into diamond of two types of natural graphite: graphite with initial density $\rho_0=2.08$ g/cm³ having hexagonal crystal structure, containing 5% of rhombohedral phases, and graphite with initial density $\rho_0=2.148$ g/cm³ having hexagonal crystal structure, containing 25-28% of rhombohedral phases, at shock compression was investigated. The impact loading of the graphite samples of thickness of 3.2 mm was carried out with help of aluminium plates of thickness 5 mm and accelerated up to velocity 3.33 km/s. In experiments, the structure of a shock wave at output from a sample was recorded by measurement of velocity of an interface $u_{fs}(t)$ of sample with transparent LiF “window” with laser velocimeter VISAR. Experiments were conducted at room and elevated up to 460–480°C temperatures.

Splitting of a shock wave with formation of two-wave structure on all interface velocity histories were registered, that is consequence of increase of compressibility at polymorphic transformation. Parameters behind front of the first shock wave correspond to the beginning of transformation of graphite to diamond or to diamond-like phase of high pressure. The interpretation of the data obtained was carried out with using of wide-ranges equations of state of graphite, LiF and aluminium. In particular, Hugoniot shock adiabat of graphite, LiF and aluminium have been calculated at initial temperature 470°C. Calibrating experiments for determination of correction of a constant of interferometer VISAR at high temperature were carried out.

Thus, in this work, the technique of shock-wave experiments with LiF “window” at elevated temperatures was polished and it was shown, with increase initial temperature of graphite, pressure of phase transition graphite–diamond decreases, speed of the second shock wave and speed of transformation graphite–diamond increase.

ROCK-FORMING MINERALS TRANSFORMATIONS IN CONDITIONS OF STEP-LIKE SHOCK COMPRESSION OF CRYSTAL SCHIST

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Shock-metamorphic transformations of rock-forming minerals (garnet 45–50%, biotite 40–45%, quartz 5%, feldspar 5%) in crystal schist from the Southern Urals have been studied with the use of recovery assemblies of planar geometry. The maximal shock pressures in the samples were attained upon a few reverberations of the waves between the walls of the recovery ampoule (step-like shock compression) and were equal 26, 36 and 52 GPa (see [1, 2] for details).

Different types of these rock-forming minerals transformations: mechanical (fissuring, amorphization) and chemical (bringing and carrying-out of different compounds), have been observed in the recovered samples after experimental shock loading of studied crystal schist.

Quartz and feldspar reveal the strongest transformations. Planar elements having different crystallographic orientation appear in quartz at 26 GPa already. Feldspar becomes amorphous under shock wave compression. Feldspar amorphization degree grows up with shock pressure amplitude increasing.

Biotite also reveals strong mechanical deformations which are intensive fissuring appearance and crumbling stripes forming. This mineral is partly being melted under shock wave compression. The strongest biotite melting degree is observed at 52 GPa.

Garnet transformed weaker than other rock-forming minerals. It also becomes heavily cracked under shock wave compression. Garnet fissuring degree depends on shock pressure amplitude: it becomes greater with shock pressure growth.

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MECHANISM OF ALUMINIUM HYDRIDE AlH_3 ELECTROCONDUCTIVITY AT HIGH MULTY SHOCK PRESSURES

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Aluminium hydride $\alpha\text{-AlH}_3$ (alane) is a solid with very large hydrogen content of 10.1 % by weight. Aluminium hydride is a promising additive to rocket fuels and high explosives and so need for knowledge of its properties under high pressures and temperature appears. Aluminium hydride has been intensely studied as one of the most promising materials for hydrogen storage.

The large hydrogencontent of AlH_3 leads to other interesting properties. It is well known that dense monoatomic hydrogen would be probably a room temperature superconductor. Some recent calculations put onset of metallization in solid hydrogen with the superconducting critical temperature $T_c = 225$ K at pressures 450 GPa [1]. These high pressures are far away from the current experimental limit for static pressures and low temperatures and also far away from the current experimental limit for shock pressures. There is another possibility to create a dense net of light elements which would have metallic conductivity. It was noticed [2] that “light” hydrides (such as CH_4 , SiH_4 , AlH_3 , or MgH_2) might indeed be high- T_c superconductors. Theoretical [3] and experimental [4] studies of alane AlH_3 have investigated possible metallization at high pressures along the room temperature isotherm. The results obtained are sufficiently encouraging to prompt studies of a wider range of temperatures.

In this paper, the electrical conductivity of AlH_3 has been studied under multi shock compression up to 100 GPa. The conductivity of shocked alane increases in the range up to 60-75 GPa and is about $30(\Omega \text{ cm})^{-1}$. In this region the semiconductor regime is true for shocked alane as well as for multi shocked hydrogen [5]. The conductivity of alane achieves approximately $500(\Omega \text{ cm})^{-1}$ at 80-90 GPa. The conductivity is interpreted in frames of the conception of the “dielectric catastrophe” [6], taking into consideration significant difference between electronic states of isolated molecule AlH_3 and condensed alane.

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STUDY OF SUPERCONDUCTIVITY PROPERTIES OF MAGNESIUM DIBORIDE AFTER ITS SHOCK WAVE LOADING UP TO 65 GPa

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The shock wave loading of magnesium diboride was carried out in steel ampules of planar geometry [1, 2]. Dynamic compression up to 65 GPa was reached by multi-step compression method. Magnesium diboride samples superconductivity after shock wave loading was investigated by measurement of temperature dependence of the dynamic magnetic susceptibility within temperature range of 4.2–300 K. It is shown that shock wave loading of MgB₂ samples up to 65 GPa do not change superconducting transition temperature ($T_c=38$ K). This is evidence of preservation of pristine phase of MgB₂ at present process conditions. This fact confirmed by x-ray analysis of recovered samples of magnesium diboride. It is shown that addition of alkaline-earth metals (Ca, Mg) under shock wave compression of MgB₂ decreases superconducting transition temperature. This phenomenon presumably was related to doping of magnesium diboride by alkaline-earth metals under shock wave loading.

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THEMAL CONDUCTIVITY OF INDIUM AT HIGH PRESSURE AND TEMPERATURE OF SHOCK COMPRESSION

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Results on electroconductivity and thermal conductivity of indium in a range of pressure to 27 GPa and temperatures to 1000 K are presented. Electroresistance of the indium samples at step shock compression was measured in this pressure range. The indium equation of state was constructed; on this basis indium thermodynamic parameters evolution was calculated for the shock wave experiments carried out and then the volume-temperature dependences specific electroresistance and thermal conductivity of indium were defined. It was shown that the thermal conductivity of indium does not depend on temperature, and its triple increase is caused by volume change only in the investigated pressure and temperature range.

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TEMPERATURE IN SHOCK-COMPRESSED SAMPLES AND EQUATION OF STATE OF EPOXY RESIN ED-5 AT HIGH DYNAMIC PRESSURES

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In present work, temperature measurements on principal Hugoniot of epoxy resin ED-5 have been performed in pressure range 35–70 GPa. Light emission from shock front was registered by optical pyrometer with time resolution better than 1.2 ns. Brightness temperatures were measured in spectral range 406–800 nm. Then a set of light fluxes has been approximated by Planck function with gray body model in order to determine thermodynamic temperature. Temperature decrease from 4 to 2.8 kK is found near 45–50 GPa, that may be associated with endothermic physical-chemical transformation due to decomposition of the original compound in shock waves. Obtained experimental data are used for description of

thermodynamic properties of the epoxy resin and products of its transformation in the framework of semiempirical equation of state at high dynamic pressures.

APPLICATION OF CHARGED PARTICLE BEAMS TO SHOCK-WAVE AND DETONATION STUDIES: FIRST RESULTS

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Radiographic study of matter using charged particle beams is the unique experimental technique for absolute measurements of important material characteristics of dense non-transparent objects in superhigh-speed processes.

The 800-MeV proton radiography facility for shock-wave and detonation studies of condensed matter has been developed at the ITEP Terawatt Accelerator (TWAC-ITEP). In 2008 the first dynamic explosive experiments on the registration of detonation wave structure in TNT charges were conducted. The studied samples had a density of 1.30–1.35 g/cc, a diameter of 15–20 mm and a length of 32–40 mm.

The series of pairs of radiographic images of detonating charges shot for two consecutive proton bunches with the duration of 70 ns separated by 250 ns were obtained in these experiments. Axial density profiles calculated from them show good quantitative agreement with the data on the known parameters and simulation results for the detonation of the same TNT charges in the rarefaction zone. However, the chemical reaction zone (i.e. the Von Neumann spike) failed to be registered in these experiments due to the insufficient spatial and time resolution of the present experimental arrangement. Therefore a substantial improvement of the resolution capacity of radiographic facility is needed for full-scale studies of shock wave and detonation phenomena in condensed matter. The appropriate work on its modernization and optimization is being conducted at the moment.

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**PECULIARITIES OF HIGH-RATE DEFORMATION
OF COPPER UPON CONVERGENCE OF CYLINDRICAL
CHANNELS BY ACTION OF SHOCK WAVES**

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The development of models for shear and spall strength and those for compaction of voids being formed, which will be true for a wide range of pressures, strains, strain rates and temperatures is possible. Structural changes in material occurred under large plastic deformation in shear stresses depend both on flow parameters, e.g. pressure, temperature, strain rate and the history of material deformation to the state considered.

At strain rate up to $\dot{\epsilon}_i \sim 10^5 \text{ s}^{-1}$, achieved, for instance, in Hopkinson pressure bar method and Taylor cylinder technique, the deformation process proceeds mostly due to dislocation sliding of crystallographic planes. At $\dot{\epsilon}_i > 10^7 \text{ s}^{-1}$, for example, in the front of shock waves, considerable deformation is caused by twinning and the density of dislocation reaches its maximum. The region where deformation mechanisms change places, namely, $\dot{\epsilon}_i \sim 10^5\text{--}10^7 \text{ s}^{-1}$, is still not clearly understood.

This work presents a new simple method for investigating the peculiarities of metal deformation at micro- and meso scales when the strain rate is $\dot{\epsilon}_i \sim 10^5\text{--}10^7 \text{ s}^{-1}$. A copper liner loads test copper samples pressed into copper guide rings behind which one can find a substrate made of the same material. The loading parameters, such as the intensity σ_X , and the pulse duration t are specified by the liner's thickness and speed. The loading parameters were chosen in such a way as to realize the decrease of the holes diameter and complete compaction in the recovered samples. Cylindrical holes of various diameters ($D_0 = 0.5\text{--}2 \text{ mm}$) in the test samples are produced beforehand. Coarse-grain annealed copper M1 was chosen as the subject of the study.

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DYNAMIC CHANNEL-ANGULAR PRESSING OF TITANIUM AT HIGH TEMPERATURE

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Equal-channel angular pressing (ECAP) makes it possible to deform metals by simple shear without a change in their size and shape [1]. In the Russian Federal Nuclear Center (Snezhinsk), there was suggested a dynamic version of the method of ECAP, in which pulsed sources of energy were used for the extrusion of materials through the channels [2].

Titanium samples were deformed using dynamic channel-angular pressing (DCAP) at temperature 770 K. The angle between channels was 90°. The material was deformed at a rate of 10^{-3} – 10^{-5} s⁻¹. Increasing temperature allow to avoid a cracking and adiabatic shear bands (ASB) spreading that usually occur at room temperature pressing. The result of titanium DCAP at 770 K is a microduplex structure was obtain. This structure was a dispersed mixture of small recrystallized grains and non-recrystallized fields. Size of the grains was about $(2-3) \cdot 10^{-6}$ m. The recrystallized grains arising occur by the reason of local increasing of temperature in the fields of localized deformation and it is one of the mechanisms of the strains relaxation. The recrystallized grains are grouping in the long shear bands (it is high-scale relaxation) and in the short chains/clusters (it is low-scale relaxation) located between the long shear bands. The angle between the direction of the bands and the direction of the sample is 30° that is character of the DCAP method [3]. The short chains spreads mainly along the sample longitudinal direction. TEM study show that the non-recrystallized fields of the structure consists of elongated grain (subgrain) with the size $(0.2-0.3) \cdot 10^{-6}$ m. This structure is formed by the reason of deformation and dynamic polygonization.

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MECHANICAL RESPONSE OF ULTRAFINE GRAINED METAL ALLOYS TO INFLUENCE OF SHOCK WAVES

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Experiments on plane shock waves loading of plates are widely applied to research of mechanical behavior of constructional materials at strain rates from 10^3 up to 10^6 s⁻¹. Experimental data on back surface velocity of specimens shock at known geometrical parameters usually use for estimation of strength characteristics of materials at high strain rates. In this paper we discuss the problems of numerical analysis of experiments on high velocity impact of plates to the investigation of mechanical behavior of nanostructured and ultrafine grained metal alloys. Analytical methods used for analysis of shock pulse profiles, allows to estimate the Hugoniot elastic limit, the spall strength, and the shear stress in a front of a shock wave. However, computer simulation of experiments is necessary for obtaining more full data on mechanical behavior of materials under shock wave loading. Results of computer simulation of shock pulse loading of specimens of ultrafine grained (UFG) aluminium and titanium alloys are presented. Phenomenological and micromechanical constitutive equations were used for the description of plastic flow of UFG alloys. Constitutive equations take into consideration the deformation hardening, the strain rate sensitivity and temperature sensitivity of the yield stress. Results of simulation compare with experimental time-history profiles of shock pulses in AA6063-T6, VT1-0, VT-6, Ti-6Al-4V, and Ti-6-22-22S alloys. Results of simulation testify that strain rate sensitivity of the yield stress, and the strain hardening of the investigated alloys depend from the average grains size. The strain hardening coefficient $d\sigma_s/de^p|_{\epsilon^p, T}$ depends on the grains size. The coefficient at first 1.5 percents of plastic strain sharply increases when grains size is located in the range of 1 micron to 300 nm. It is revealed, that the velocity of the elastic precursor attenuation is higher in UFG alloys, than in polycrystalline analogues. In the investigated UFG alloys fast relaxation of the elastic precursor amplitude finishes within the distance of 1 mm. The suggested model predicts the growth of plastic strain degree before beginning of mesoscale plastic flow localization and nucleation of damages of UFG metal alloys. The spall fracture is accom-

panied by the essential plastic deformations and damage nucleation and growth in the fracture zone. The effective spall strength of alloys grows with decreasing of the average grains size within submicron range.

SIMULATION OF MECHANICAL BEHAVIOR OF CERAMIC NANOCOMPOSITES UNDER SHOCK WAVE LOADINGS

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The application of the composite materials combining high electroconductivity with strength characteristics is one of directions to increase of intensity of magnetic field pulse in technical devices. The required complex of properties can be received from nanostructured composite materials with a metal matrix. The prediction of mechanical behavior of similar materials in conditions of pulse influences is complicated by deficiency of experimental data and theoretical models. In this paper the model of mechanical behavior of composite materials with the copper matrix, strengthened by nanotubes, microfibrils, and ceramic nanoparticles under intensive microsecond impulse impact is offered. Within the model's approach the relaxation of the shear stress is considered as result of structural transformations on micro- and mesoscale levels. Models of nanocomposites structures were developed on basis of the data of microscopic researches. Models were used for research of deformation and fracture processes of nanostructured composite materials on mesoscale level. Composite materials with three characteristic forms of inclusions and their concentration from 50 up to 65 % were considered. The mechanical behavior of Cu-Nb, Cu-Al₂O₃, Cu-TiB₂, Cu-CuO composites under impulse loadings with amplitudes up to 5 GPa was studied by computer simulation method. Results of simulation testify that the Hugoniot elastic limit of nanostructured composites depends on concentration of strengthening inclusions and practically does not depend on their form. The dynamic fracture of nanocomposites is preceded the inelastic strain localization and the formation of a block structure in a front of shock waves. The effective block size essentially exceeds the average size of inclusions and depends on shock wave amplitude. Block structures can be formed in the limited range of shock wave amplitudes. Formation of block structures is established at amplitudes of shock waves exceeding 1.2 σ_{HEL} (σ_{HEL} is the elastic precursor amplitude). Block structures have not been found out at the amplitudes

exceeding $\sim 3\sigma_{\text{HEL}}$. The block structure can be formed in composites with the various forms of inclusions and their chemical compound under shock wave loading. The formation of block structure at the mesoscale level of material under shock wave loading is accompanied by appearance of bimodal distribution of particle velocities, stress intensity, strain intensity, and others. The development of block structure leads to micro damage volume distribution heterogeneity. The creation of microcracks is marked on borders of blocks and was caused by displacement of blocks. The distribution of damages within material volume is formed as a result of movement of blocks behind front of a shock wave.

STRUCTURAL-SCALING TRANSITIONS IN MESODEFECT ENSEMBLES AND NONLINEAR ASPECTS OF PLASTICITY AND FAILURE IN SHOCKED SOLIDS

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Statistical theory of evolution of mesoscopic defects (microcracks, microshears) allowed us to establish new type of critical phenomena in solid with defects—structural-scaling transitions, to develop thermodynamics of solid with defects and to propose the phenomenology based on generalization of the Ginzburg-Landau theory. The key results of statistical theory and statistically based phenomenology are the establishment of two order parameters responsible for structure evolution—the defect density tensor (deformation induced by defects) and the structural scaling parameter, which reflects the scaling transition in the course of nucleation and growth of defects, and generation of characteristic collective modes of defects responsible for the relaxation (shear transformation zones—STZ) and failure (damage transformation zone—DTZ). These modes have the nature of the solitary wave and blow-up dissipative structure, provide the mechanisms of plastic relaxation and damage-failure transition and can be excited in the resonance regime in dynamically loaded and shocked materials. Dynamic, shock wave experiments and structural study supported the linkage of the evolution of these modes with material responses in large range of strain rates and allowed us to propose the interpretation of following effects:

(i) The explanation of transition from thermally activated to the steady state and overdriven shock regimes were proposed. The fourth power universality of the steady-state plastic front as the consequence of the subjection of the relaxation kinetics to the dynamics of the STZ was confirmed

both theoretically and experimentally. Experimental study of the plastic wave structure was carried out in the plate impact test for the copper and the NEW VIEW scaling analysis of the STZ distribution in the recovered specimen in the cross-section of wave propagation. High correlated distribution of STZ was established for large scale range that supported scaling law at the steady-state plastic front.

(ii) Nonlinear crack dynamics and transition from steady-state to the branching regime of crack propagation and the onset of the fragmentation dynamics as the precursor of failure wave generation were studied. The existence of two critical velocities, three characteristic regimes of crack dynamics and the role of mentioned collective modes of defects were established experimentally in the preloaded PMMA plate using the REMIX high speed framing, NEW VIEW correlation analysis of failure surface roughness. Failure wave generation was studied for the Taylor test in the fused quartz rod using high-speed framing and supported the “delayed” kinetics of failure wave generation and propagation.

(iii) The anomaly of energy absorption in fine grain materials was established and supported experimentally for fine grain titanium under cyclic and dynamic loading.

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MESODEFECT INDUCED MECHANISMS OF PLASTICITY AND FAILURE IN SHOCKED SOLIDS

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The developed statistical model of solid with mesoscopic defects allowed the formulation of phenomenological model in terms of two independent variables—the defect density tensor and structural scaling parameter and the simulation of shock wave propagation in the linkage with structural relaxation phenomena. It was established the link of the Hugoniot elastic limit with kinetics of structural transition (mathematically related to the defect density tensor) in the structural metastability area, that has generally thermally-activated character. The development of plastic front is described as the consequence of self-consistent structural (orientation) transition in microshear ensemble that is realized due to the kinetics of structural scaling parameter. The present investigation was directed to describing of the failure phenomena.

The numerical simulation of plane shock wave propagation was carried out to establish spall conditions and to propose the mechanism of damage-failure transitions described as a specific form of self-organized criticality in the ensemble of mesoscopic defects—structural-scaling transition. Characteristic features of this transition are the generation of collective modes in mesodefekt ensemble that are responsible for damage localization and transition to failure. Collective modes have the nature of self-similar solution and describe the blow-up damage localization kinetics with characteristic time (peak-up time) on the set of spatial scales. Mechanism of spall failure can be linked with resonance excitation of blow-up collective modes and has the nature of delayed failure with the delay time corresponding to the peak-time of the self-similar solution. The correlation analysis of microstructure of saved samples confirms the mentioned mechanisms.

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STRUCTURE PROPERTIES AND STRUCTURAL-SCALING TRANSITION IN THE ARMCO IRON UNDER PLATE-IMPACT LOADING

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Experimental study of material responses in large range of loading rate reveals some insight into dynamic failure and shows the linkage of solid behavior with the evolution of mesoscopic defects such as microcracks and microshears [1]. Taking into account the nature of plastic deformation and failure the key problems are related to statistics and thermodynamics of mesoscopic defects that revealed the features of non-equilibrium systems with slow dynamics. Slow dynamics is the consequence of generation of collective modes of mesodefekts with slow spatial-temporal response in the comparison to acoustic properties of materials.(elastic wave propagation). The original study was conducted to support theoretical results and constitutive relations, which describe a different scenario of damage-failure transition [2].

A setup for plate impact experiment has been developed at ICMM UB RAS to study dynamic fracture at strain rates up to 10^6 s^{-1} . Setup consists of 125 mm gas gun and measurement equipment (VISAR). Soft

recovery of a specimen allowed us to investigate structure changes caused by plate impact. All specimens were annealed during 4 hours at 800°C.

Optical microscopy and 3D profilometry were used for the investigation of the mechanisms of spall fracture at different scales. It was found that for material the is far from the spall surface Hurst exponent is close to 0.44. For material that is near the spall surface the Hurst exponent is 0.62. Taking into account that the Hurst exponent for random structure is 0.5 we can conclude, that the structure becomes more correlated near the spall surface. This can be related to the structural-scaling transition in the ensemble of mesodefects which leads to the damage-failure transition.

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NANO- AND MICROSCALE KNOCKINGS OF ROCKS IN EXPEREMENTS OF FRACTURE BY SUCCESSIVE EXPLOSIONS

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Exploration deals with the experimental study of nano- and microscale particle formation during five successive explosions at the site in the Fennoscandian granite massif near Vyborg.

The sequence of explosions and the procedure of collection of fine particles were the following. The first sample of the particles was taken from the blast cone of the first explosion. The charge for the second explosion was located in the blast cone of the first explosion. The second sample of the particles was taken from the blast cone of the second explosion. The charge for the third explosion was located in the blast cone of the second explosion, etc.

Sequential analysys of the granulometric composition of the destructed medium for each sample and its comparison with the Rozin-Rammler and Kolmogorov theoretical distributions are performed. Therefrom it is shown

that the role of multiple crushing increases with an increase in the number of explosions. However, most of splinter-type particles with sizes exceeding 40 μm are formed as a result of single-shot crushing. Within the limit of accuracy of the experiments no strength limit of the material constituting the particles has been determined.

INFLUENCE OF INTERNAL STRUCTURE ON METAL BEHAVIOR UNDER UNIFORM PULSE LOADING

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Molecular dynamics simulation of spherical convergent waves of copper samples under uniform pulse loading was carried out. Interatomic interaction was described in the framework of the embedded atom method. Interatomic interaction potentials within this approach allow describing with rather high accuracy elastic characteristics of copper, its surface properties, energies of defect formation, etc.

The influence of internal structure of samples, intensity of loading, sizes of samples on the peculiarities of solitary like wave propagation was investigated. It was shown that uniform pulse compression of spherical shape samples resulted in more degree of solitary like wave focusing in the middle of samples in the case of ideal crystal structure than in the case of disordered one. Irreversible structural changes of single-crystal sample took places at the front of solitary like wave when interatomic distances became less some threshold value.

The results of simulations showed that the solitary like wave amplitude at the middle of sample was nonlinearly connected with intensity of pulse uniform loading. Particularly, the growth of the solitary like wave amplitude in the center of sample became slower with increasing of intensity loading.

SIMULATION OF ELECTROTHERMAL PULSE DISPERSION OF A CRYSTAL-STRUCTURED METAL WIRE

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Molecular dynamics simulation of crystal copper specimen failure processes under electrothermal pulse dispersion was carried out. Interatomic interaction was described in the scope of embedded atom method. The crystalline failure character under different volume temperature distribution at the initial loading stage was studied. It was shown that in investigating temperature range high specimen speed heating as from the surface to center as in the opposite direction did not essentially change the failure character. It was obtained that the high speed electrothermal pulse action on crystal specimen could result in great increasing of its volume without discontinuity (mean interatomic distance increase not more than 10%). It could be due to less inner structure accommodation processes speed then loading one. In absence of environmental resistance the crystal specimen failure process under electrothermal pulse dispersion was accompanied by clusters and gas phase formation. The decreasing of loading intensity resulted in increasing of failure fragment size accompanied with formation of complex shape clusters.

The done calculations showed that molecular dynamics method could be effectively enough used for description of nanosize wire failure processes. Calculation results are of interest both from scientific point of view for materials failure peculiarities investigations under high speed heating and from practice point of view for optimal technology regimes determination of nanosize particles with blocked structure generation.

MOLECULAR DYNAMICS SIMULATION OF VOID GROWTH IN CRYSTALS UNDER TENSILE LOADING

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The work is devoted to study kinetics of void growth in stretched single crystals in different parts of phase diagram. High growth rates that are comparable to strain rates 10^6 s^{-1} achieved during dynamic loading are considered. Mechanisms, kinetics of void growth and stress relaxation in

crystal are analyzed by means of molecular dynamics simulation. Various conditions is taken into consideration: tension at constant strain rate, spontaneous growth of pore, growth of many voids, growth accompanied by nucleation of new voids in strongly metastable system. Typical size of the crystalline system varies from 10 to 100 nm. The results for fcc Al described within embedded atom model for interatomic interactions are presented.

Two competitive mechanisms of the void growth under tensile load are observed: lattice amorphisation around the growing pore and local shear via formation of dislocation loops. Emission of dislocations takes place near void surface owing to anisotropic distribution of shear stresses around the void. Voids act as stress concentrators even when uniform triaxial stress state is considered. Kinetics of the void growth depends on application of an additional shear stress. If crystal is in a superheated state then melting starts at junctions of dislocation loops. Amorphisation predominates in case of strong metastability at elevated temperature, when void growth rate is high.

ATOMISTIC SIMULATIONS OF DISLOCATION NUCLEATION IN Al UNDER HIGH STRAIN RATE

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The crystal becomes metastable under stretching and can be characterized by the finite lifetime. There is the limit of deformation when the lifetime equals zero, and this state is called the stability limit. We can determine the stability limit for shear deformation likewise. The maximum shear tension is determined by the theoretical shear strength. The decay of the metastable state in case of defectless crystal occurs by thermal fluctuation that results in the formation of the critical nucleus of the dislocation. Based on MD the stochastic properties of the dislocation nucleation are studied, the distributions of the lifetime are obtained. The nucleation rate is introduced by averaging of lifetimes of assemblies. Such process is important in case of the high strain rate deformations, when the nucleation of dislocations on the Frank-Read source is not enough. The comparison with theory of homogeneous nucleation is considered [1].

The second part is devoted to nucleation of dislocations on inclusions. The Frank-Read liked mechanism is observed. The dislocations nucleate in the special sites on the surface of voids and precipitates. The temperature

dependence of activation stress is obtained. The both homogeneous and heterogeneous nucleation demand rather large shear stress (1 GPa), so the main mechanism of dislocation nucleation in shock loading is Frank-Read source and the rate of formation is limited by the velocity of dislocations.

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ATOMISTIC MODELING OF SPALL FRACTURE NEAR MELTING CURVE

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The influence of melting on spall fracture at high-strain rate is studied in aluminum using large scale molecular dynamics. Simulations of tri-axial deformation, corresponding to stretching in rarefaction waves, and the following fracture is considered. A single crystal with different defects (dislocations, stacking faults, voids) and a polycrystal are modeled. There is considerable difference between behavior of the single crystal and the polycrystal near melting curve. Provided reaching the melting curve the melting starts in polycrystal at grain boundaries and voids arise in liquid phase. The single crystal behaves in a different way. Considerable overheating is observed even in the presence of stacking faults and dislocations. Melting rate depends on temperature and the fracture can start in solid or liquid phase. The comparison with the shock-wave experimental data on spall strength is carried out.

SPALL KINETICS IN LIQUIDS AT HIGH STRAIN RATES

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Kinetics of void nucleation and growth in stretched liquid is studied using the molecular dynamics (MD) method. Based on the kinetic characteristics obtained, spall strength of liquid at high strain rates is calculated. A Lennard-Jones system was chosen for the simulations as it describes well properties of simple liquids.

The rate of spontaneous phase transition is characterized by nucleation rate—an average number of voids appeared in a unit volume in a unit

time [1]. Dependence of cavity nucleation rate J on temperature and pressure was studied in the range of temperatures $T^* = 0.5 \dots 0.8$ and densities $\rho^* = 0.7 \dots 0.8$ (in reduced units). The technique used to find the nucleation rate was based on averaging lifetimes over an ensemble of independent MD runs [2]. According to the classical nucleation theory, the dependence of J on pressure and temperature should be the following:

$$J = J_0 \exp\left(-\frac{W}{kT}\right), \quad W = \frac{16\pi\gamma^3}{3(P - P')^2}. \quad (1)$$

W is the critical bubble work of formation, γ is the surface tension, P is the pressure inside liquid and P' is the vapor pressure inside the bubble. Simulations give the linear dependence of $\ln J$ on $1/P^2$ at a fixed temperature, which is consistent with the classical nucleation theory.

To study bubble growth kinetics, a spherical void of some radius was cut from the calculation cell and the time evolution of the void size was observed. Growth kinetics was studied in the range of temperatures $T^* = 0.5 \dots 0.8$ and densities $\rho^* = 0.7 \dots 0.85$ (in reduced units). The linear time dependence of bubble radii on time was obtained in simulations. Hydrodynamical approach gives different result. The inconsistency may be attributed to the small sizes of the simulated systems and short observation times. The possibility of more thorough study of growth kinetics in larger systems is discussed.

The dynamic spall strength of liquid is calculated using the nucleation-and-growth model (NAG). Deformation with a constant strain rate $\dot{\epsilon} = \dot{V}/V_0$ is considered. The result of calculations is in good agreement with the experimental data on hexane [3] and reveal weak dependence of the spall strength on the strain rate.

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TENSION FEATURES OF LIQUID AND SOLID MATTER NEAR MELTING POINT BY SHOCK WAVES

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Cavitation phenomena are a subject of research in many areas of science and technology. Study of cavitation in liquids is highly important for improving hydraulic motors, ship propellers, and other mechanical devices operating in liquids at high speeds. One possible cause of cavitation is tensile stress.

Conditions of fluid failure during homogeneous nucleation can be simulated using dynamic extension. In the present study, dynamic extension of the fluids was performed using spalling phenomena that occur in the reflection of compression pulses from the free surface of the material studied [1]. It is of interest studying fluid strain rate near melting point as it especially in this region relaxation properties of environment which can affect kinetics of destruction appears. In this work the influences of strain rate on the negative pressure have been investigated in liquids near melting point by the example of water, hexadecane, pentadecane, paraffin . The method of spall strength measurements was applied and wave profiles were registered by laser interferometer VISAR.

The abrupt dependence between the spall strength and the strain rate in water was discovered. Such type of dependence was not recorded far from freezing point. It was shown that the double metastable state of water realizes.

The double staged character of hexadecane destruction was discovered near its freezing point. This character of destruction appears only then the loading pulse is higher than threshold value of 250 MPa.

The destruction features of pentadecane were discovered near freezing point. It was found that the value of tensile strength is increasing with the rise of loading pulse amplitude, while the decrease of tensile strength with the rise of loading pulse amplitude was recorded in all previous experiments.

Paraffin was investigated in liquid and solid state. It was found that the destruction of paraffin in these two different states is almost similar.

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FRAGMENTATION MODEL OF ELASTIC MEDIA WITH DAMAGE ACCUMULATION

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Fragmentation model of elastic media with damage accumulation is considered. Supposition is made that activation of large number of micro flaws precedes macroscopic fracture of material. Distributed damage theory considers transform of elastic energy into surface energy of micro flaws. Distributed damage parameter may be considered as a measure of micro flaws surface energy [1]; it is an internal parameter which contains information about deformation history before fragmentation in implicit form. Being a part of the governing equations of continuous media [2], the kinetic equation for damage parameter has to provide non-negativity of dissipation during damage process. New form of kinetic relation is developed to satisfy this requirement. The process of macro flaws formation (from micro flaws) and fragmentation is treated as loss of hyperbolicity of the governing equations. Accounting for the micro flaws development enables one to predict basic properties of the fragmentation process such as correlation between average fragment size and tensile strength, dependence of fragmentation time delay on strain rate. The model under consideration makes it possible to obtain fragment size distribution which depends on deformation history.

The theory is applied to the problem of fracture of a rod under tension loading. Cases of quasi-static and instantaneous loading are investigated. Dependencies of fragmentation time delay and average fragment size on strain rate are obtained.

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**MODELING OF DESTRUCTION OF MATERIALS
WITH PREFERENTIAL PROPERTIES ORIENTATION
UNDER DYNAMIC LOADS**

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Last time the creation of materials with the set properties is the actual direction. Modern technologies allow optimizing strength parameters of a design for work in the certain ranges of external influences. Such optimization can be made because of impart to structure of a material the ordering, or because of material reinforcing by strengthening elements. Unfortunately, in spite of high activity of researches on creation of materials with the given properties, the developments, concerning anisotropic materials at present, is not enough. Practically, there are no data about behavior of such materials under dynamic loadings. It relates both to experimental researches, and to mathematical and computer modeling. In this work the process of deformation modeling by computer simulation and development of destruction in the monolithic and spaced barriers are investigated at high-velocity impact.

Modeling of dynamic loads is realized in three-dimensional statement by final elements method. For reception of the equations of motion for any final element the principle of possible velocities is used. Being based on the given approach, it is possible to receive the general equations of motion for elements of the continuum. In meshing of bodies are used tetrahedrons as simplex, and the uniform distribution of weight between nodes of the element is applied. For the check of correctness of the model and of the applied computer method, it have been made the comparison of numerical and experimental results.

The wide range of velocities of impact from 750 m/s to 3000 m/s is investigated. The results allow to conclude, that the algorithms of this computer modeling allow to adequately optimize properties of anisotropic materials and designs from it for work in the certain range of external influences. This material is based upon work supported by the Russian Foundation for Basic Research (RFBR) under Grant No. 06-01-00081 and programs of Presidium of the Russian Academy of Science, Project No. 9.5.

MECHANISMS OF SPALL FRACTURE OF TARGETS AT HIGH VELOCITY IMPACT

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Mathematical modelling and experimental investigation of long projectile impact was carried out on special experimental equipment including ballistics devise, track with recording means and target. The throwing of projectiles was carried out by means of powder or light-gas ballistic devices. Method of x-ray pulse technology for recording of kinetic and geometric parameters of armour-piercing elements and fragments before the target and behind it was used. It was based on using of shadow projection in two planes at fixed period for the definition of kinetic and geometric characteristics. The throwing of armour-piercing elements was made from powder or light-gas ballistic devices of various calibres. The weight of armour-piercing elements in experiences varied within the limits of 0.01–1 kg, lengthening (the ratio of length of projectile to diameter) 3–30, impact angles 0–75°, velocity of impact in a range 0.5–3.5 km/s. Projectiles were of steel and tungsten alloy. For a throwing and stabilization in flight of long projectiles with greater lengthening (10–30 calibres) separated pallets and special tail stabilizers were used. Velocity of projectiles was measured by induction gauges of velocity with accuracy 0.2%. The technique for registration of kinematics and angular parameters of armour-piercing elements and fragments in two planes by means of pulse x-ray installations has been developed. The pulse x-ray technique for registration of kinematics and angular parameters of armour-piercing elements and fragments at impact has been developed and applied. For pointed armour-piercing element of average lengthening it is shown that the sharp increase in fragments weight begins due to spall fracture of a target at velocities about 1.6 km/s and above. It is established that the angle of scattering of fragments behind a target slowly grows with growth of velocity of impact. It is shown that dependence of velocity of projectiles behind target sharply grows with growth of velocity of impact. Velocity of leading fragments behind targets of different thickness grows with growth of initial velocity of impact more smoothly.

SIMULATION OF HIGH-SPEED ORTHOGONAL CUTTING OF METALS USING FINITE ELEMENT METHOD

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Modern mechanical engineering production is characterized by using of high-strength and hard-to-machine materials, significant increase of requirements to accuracy and quality of products and considerable complication of constructive forms of machine components received by cutting. Therefore process of machining demands continuous upgrading. Now one of the most perspective direction of such upgrading is high-speed machining, at which speed of cutting makes tens and hundreds m/s, that many times exceeds speed of usual processing. It is economically advantageous at smooth machining of the workpieces having a considerable quantity of surfaces for which short time processing is necessary, frequent changes of positioning of machine units and change of tools is needed.

In this study the processes of high-speed cutting of metals are numerically investigated in two-dimensional plane strain statement using modified finite element method. The elastic-plastic model is used. Kinetic model of active type is used for numerical simulation of failure. Modeling of process of chip separation from workpiece was carried out using damage criterion of workpiece elements. The approach similar to imitating modeling of material failure of erosion type was used. As damage criterion—criterion of chip separation—threshold value of specific shear-strain energy is used.

Computations were done for speeds of cutting from 1 up to 200 m/s. The sizes of a working part of the tool: length of the top side was 1.25 mm, lateral—3.5 mm, a rake angle—6, a clearance angle—6. The machined steel workpiece had a thickness of 5 mm; depth of cutting—1 mm. A material of processed workpiece—steel St3, a material of a working part of the tool—cubic boron nitride.

It is established, that character of distribution of contour lines of specific shear-strain energy and temperatures at high-speed cutting is the same, as well as at speeds of cutting of an order of 1 m/s, and qualitative different in a mode can arise owing to melting of a material of workpiece which occurs only in a narrow layer contacted to the tool. Computations show, that gradient changes of specific volume of cracks before a tool are expressed much more strongly, than changes of shear-strain energy or temperature, therefore it is preferable to use threshold value of specific volume of cracks as criterion of chip separation.

This work was supported by the Russian Foundation for Basic Research (projects 07-08-00037, 08-08-12055).

**NUMERICAL STUDY OF VISCOUS SHOCK WAVE
BEHAVIOUR IN THE REGIONS OF AMBIGUOUS
REPRESENTATION OF THE SHOCK WAVE
DISCONTINUITY**

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Shock wave behaviour in the regions of ambiguous representation of the shock wave discontinuity is studied numerically in the framework of initial value problem for the compressible Navier-Stokes equations with initial data corresponding to the perturbed shock wave. The modification of the model equation of state [1]

$$e(p, \rho) = (1 - \exp(-p^2) + \varepsilon p^2 \rho^{-1})(4 - \exp(-(4 - \rho^{-1})^2))$$

is used which admits various types of shock wave instabilities. The modified version retains all advantages of the original equation of state and permits to overcome computational problems characteristic for it at high values of pressure.

Convergence of the solution to the self-similar limit is considered. Shock waves corresponding to the linear instability conditions $L < -1$ or $L > 1 + 2M$ are found to be not observed. The behavior of shock waves that correspond to the Hugoniot region of their ambiguous representation containing the segment with the fulfilled linear instability condition $L > 1 + 2M$ is studied in one- and multidimensional formulations. In one-dimensional calculations shock wave splits into two shocks or a shock and rarefaction wave propagating in opposite directions, either (in stability region) remains unchanged. The solution choice depends on shock wave parameters (i.e. Hugoniot point) as well as on the disturbance type and intensity. Multidimensional 2D and 3D modeling of the behavior of the periodically disturbed shock wave has shown the formation of a cellular detonation-like front structure with finite value perturbation amplitude not increasing and not decreasing in time. The existence of such structure is explained by switching of local shock parameters between admissible types of the break-up configurations.

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NUMERICAL SIMULATION OF CONVERGING SHOCK WAVES IN THERMODYNAMICALLY NON-IDEAL MEDIA

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Converging shock waves are an essential tool in high energy physics. The problem of their stability in an ideal media has been studied for along time both theoretically and experimentally, but the influence of the strong thermodynamic non-ideality at high degree of compression on this problem remains unclear. The admissibility of the linear theory of the plane shock wave stability in the process of converging shock waves focusing is not evident.

Neutrally stable (according to D'yakov-Kontorovich criterion [1, 2]) converging shock waves are investigated. Equation of state [3] is used in the calculations. The choice is motivated by presence of extensive neutral stability regions on Hugoniot of the dense Mg plasma predicted on the basis of Thomas-Fermi model. The converging shock wave is initiated by instantaneous energy release in a spherical layer with onset of small amplitude initial perturbations.

Numerical simulation is conducted using the total variation diminishing (TVD) finite difference scheme and Glaister's type approximate Riemann solver.

Numerical simulation has shown that the fulfillment of the neutral stability criterion (1) does not affect significantly on the behavior of the shock wave in the process of converging, (2) the flow behind the converging shock wave is essentially non-uniform: there are large spatial fluctuations of flow parameters. The fluctuations originate from small amplitude perturbations of initial data.

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THE CASCADE MECHANISM IN FREE SHEAR FLOWS

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Physical model of the cascade mechanism of development of instability in free shear flows is proposed. The model is based on the results of numerical simulations of instable flows development of an ideal compressible gas. The main ideas of the proposed theory are stated as follows: the onset of instability begins with the formation of large vortices. It is shown that the evolution of the cascade depends on the interaction between a shear flow and large-scale vortices.

EXAMINATION OF COLLISION OF JETS WITH ULTRAHIGH VELOCITIES USING VARIOUS EQUATIONS OF STATE

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The problem of hypervelocity symmetric collision of two infinity jets from dissimilar condensed materials is considered. The main characteristics of the flow, namely, maximal values of pressures, temperatures and densities behind detached shocks and on the interface between two substances and also the shock wave and penetration velocities are determined during rigorous treatment of the flow along the center line of symmetry that is one of streamlines. Complete thermodynamics is described by introducing the general calorific equation of state (ES) for a condensed matter and, in addition, the thermodynamic identities for determination of temperature. Besides, the Bernoulli integral, which connects the state parameters behind the wave fronts and at the stagnation point, and the shock and continuation conditions are implied. As a result, the system of 12 integero-algebraic and differential equations as a general mathematical model is derived. In the cases of the Mie-Grüneisen and Tillotson ES, one is based on experimental date regarding Hugoniot curves and another does the theoretical wide-diapasonic ES, the model is simplified. With the first ES, calculations of the characteristics pointed in dependence on the collision speed (1–20 km/s) were carried out for many pairs of substances and the results were compared with ones for incompressible liquids. For both ES the calculation are performed up to 50 and more km s for the

pairs of iron-iron and granite-granite and the differences between the results in dependence on the collision velocity were estimated. Along with comparison of isentropes and Hugoniot curves, such estimations allow us to reveal the contribution of the ES specific character to solving the representative problem. And, if one of the ES is taken as a standard one, for another non-standard ES the comparison gives a domain of applicability placed into the state space and, may be, that gives some expansion of this applicability like in the case considered.

EXTENSION OF ACOUSTIC RIEMANN SOLVER FOR ELASTIC BODY ON CASE OF RIEMANN INVARIANTS JUMP ON CONTACT DISCONTINUITY

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The acoustic (or linearized) Riemann solver [1] proposed for elastic body works well and provides fast solution with out iterations in a case of smooth distributions of matter properties (density, elastic modules, sound speeds) but does not work when the properties change significantly across contact discontinuity. In this case an iterative procedure is usually used. Noniterative procedure for solution of Riemann problem with arbitrary jump of properties on boundary separating regions is developed. Acoustic assumption is used on both sides of contact discontinuity except the boundary. The proposed solver is naturally extended on case of different models used separately for left and right sides of contact discontinuity in a Riemann problem.

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PARALLEL IMPLEMENTATION OF SMOOTHED PARTICLE HYDRODYNAMICS

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Smoothed particle hydrodynamics (SPH) is a method of computer simulation in continuous media mechanics. Like all Lagrangian particle methods, one especially suited to hydrodynamic problems which have large empty regions and moving boundaries. SPH used to solve different spacial problems with free surfaces and erasing effect [1]. But there are limits to use SPH in simulation on one-processor machines. The lack of processing power is an obstacle in modeling systems with high spacial resolution, which is determined by an amount of particles used in simulation. Thus, we cannot discover an important local effects in hydrodynamic flows. There are some interesting phenomenon, what can be seen with high spacial resolution: initiating of erasing processes, collapsing of pores, appearing of discontinuity of medium etc. Modeling of such effects requires an effective parallel implementation of SPH.

To use a cluster computer in this case is the only solution. Creating, testing and using of code for parallel computer was a subject of this work. The program was successfully tested against the shock-tube problems, which are the popular test [2] for SPH codes because the exact solutions are available.

The method of segmentation of the calculation area, called a domen decomposition [3], allows to reduce a volume of a data passing between computers in a cluster and provides an evenness of load regardless of spacial configuration of the calculation area. This technique also has great advantage against the fixed partitioning, where regions ascribed to the processors are constant along calculation time. We realized this segmentation method to make SPH code parallel.

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NUMERICAL MODELING OF TRANSIENT TEMPERATURE FIELDS IN BLANKET OF HEAVY ION FUSION REACTOR CHAMBER

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In this work time evolution of unsteady temperature field in blanket of hypothetical fast ignition heavy ion fusion (FIHIF) [1] reactor chamber during one power pulse period is considered.

Work is based on solution of one-dimensional equations of solid state mechanics subject to the equation of thermal conductivity. The system is supplemented with the model of convection, which describes the flux of the coolant in blanket of FIHIF reactor chamber. The results showing that the temperature of walls does not exceed certain value when reactor works in suggested frequency mode (500 msec between microexplosions) are obtained.

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METHOD OF CLUSTER DYNAMICS FOR SIMULATION OF DYNAMIC PROCESSES OF CONTINUUM MECHANICS

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The method of cluster dynamics (CDM) [1], one of the variants of particle method, has been developing in VNIIEF for the past years. The method of cluster dynamics consists of the following: continuum mechanics equations are substituted for equations of motion of distinguished units (clusters); the solution of equations of cluster motion is similar to molecular dynamics methods; the choice of cluster interaction model is based on real equations of state of simulated material.

The basic advantage of the method is the possibility to calculate the physical processes in a wide range of spatial scales (from micrometer to tens of centimeters) due to the choice of the required structural cluster.

The other advantage of the method is the possibility to simulate the processes associated with large deformations and continuity violation of the material (dispersion, jet separation, mixing). The possibility of numerical implementation in standard molecular dynamics programs is also one of the advantages of the method, as well as the possibility to combine CDM method with the existed grid gas-dynamic techniques to develop hybrid simulation methods. CDM method is of high reliability, computational stability and does not require interference in computation.

Described here is the construction technique for cluster (potential) interaction models corresponding to real equations of state of material by the example of certain metals. Given here are computational results of certain material properties with derived potentials. The numerical simulation of shock wave arrival at profiled plate surface and high-velocity target penetration was carried out with CDM method potentials. The computational results are compared with experimental data and computational results using other techniques. The simulation results of shock wave loading and penetration show that CDM method allows the reproduction of full-scale experiment results.

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1D GAS-DYNAMIC SIMULATION OF SHOCK-WAVE PROCESSES VIA INTERNET USING DIFFERENT MODELS OF EQUATION OF STATE

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We present a web-interface, which allows one to perform 1-dimensional gas-dynamic simulation of typical shock-wave processes via the Internet using the database on shock-wave experiments. In this interface a user can supply initial conditions, control the process of simulation and make a treatment of the results. Up to seven objects can take part in the experiment; for every object a substance, its initial position and velocity, equation of state and destruction pressure should be defined. The simulation itself is based upon the Eulerian second order Godunov approach. To start computations, the user also has to set the final time, grid “coarseness” and the number of moments in which the output of necessary parameters

will take place, including initial and final. Additionally, the user can define several Lagrangian markers to trace the state of matter at a given initial coordinate. At the end of simulation the user can analyze the profiles of different values at different times or at points with the specified coordinates of Lagrangian markers both as charts and in textual form. If necessary the simulation can be repeated with modified parameters. The main advantage of this system is the possibility to use in simulation all equations of state available in the database (more than 130). This system will be useful for specialists studying properties of matter at high pressures and temperatures. It is available freely via addresses <http://teos.ficp.ac.ru/rusbank/>, <http://www.ihed.ras.ru/rusbank/>. This work has been doing under the RFBR financial support, grant 07-07-00406-a.

**THE TECTONIC PROCESSES CAUSED BY FALLINGS
OF LARGE SPACE BODIES (ACCORDING
TO GEOLOGICAL DATA)**

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Tectonic consequences of fallings of large asteroids and comets on the Earth surface are almost uninvestigated theoretically. It is known that the energy of a falling body consisting of iron and iron-stony material utilizes essentially by the formation of a crater. Such craters are absent in the cases of comet fallings. It is clear that there is another mechanism of energy dissipation for comets.

Calculations show that fragile nuclei of comets disintegrate in the atmosphere of the Earth. As a consequence a supersonic jet arises. It consists of evaporated comet's substance and shock-heated air and does not form a crater. The geological data testify that in this case the specific pressure wave occurs in the lithosphere. This wave heats up rocks of the Earth's crust and mantle. Further this energy is consumed in tectonic and magmatic processes.

Some typical geological phenomena and structures arising on continents and at oceans as the result of these processes are discussed in the report.

SYNCHROTRON DIAGNOSTICS THE DENSITY DISTRIBUTION AT THE DETONATION FRONT

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The most important problem at creation and adjustment of a new experimental technique is the statement of its correctness and accuracy of results, received with its help.

Criterion of reliability of results of experiments can be reception and comparison of the data about detonation process with the help various, including internal non-perturbed techniques. The concurrence of results received with the help of different methods, is of powerful arguments for the benefit of their correctness.

The method, offered us, of definition of parameters of a detonation before and after a plane Chapman-Jouguet is based on measurement transmitted synchrotron radiation from the accelerator VEPP-3 (Institute of nuclear physics SB RAS). Using calibration of the detector, on measurement transmitted radiation the distribution of density is reconstructed. In the report the results of measurement of distribution of density are given at a detonation of cylindrical charges HE of TNT, RDX and their alloys. As the diameter of charges, which could be exploded in the explosive chamber, was equal 15 mm, the detonation front has curvature, which influence should be taken into account. The important research problem is the attestation of a correctness of a new method by test on known HE and estimation of accuracy of measurements, which can be realized with its help.

DENSITY EVOLUTION DURING THE INITIATION OF DETONATION IN POROUS PETN

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The paper will present obtained experimental density distribution during transition from combustion to detonation in porous high explosives. The method of reconstruction density distribution rests on x-raying charge of HEs by synchrotron radiation.

The spatial density distribution $\rho(r, z, t)$ has been determined for cylindrical charges of porous PETN. Solving the inverse problem of density reconstruction bases on using a priori information of structure of the arising flow. This has made it possible to increase the accuracy of density reconstruction.

HIGH EXPLOSIVES EXAMINATION BY HIGH-RESOLUTION X-RAY COMPUTED TOMOGRAPHY ON THE VEPP-3 SYNCHROTRON RADIATION

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High-resolution x-ray computed tomography (HRXCT) is a technology ideally applicable to a wide range of materials investigations. It is an express non-destructive method to produce 3D images corresponding to series of slice projections through a sample. In the present study, HRXCT was applied to high explosives samples with the use of synchrotron radiation from the VEPP-3 storage ring (Novosibirsk, Russia), at the station “x-ray microscopy and tomography”. Comparative analysis of internal structure was carried out for different samples including pure hexogen, TNT and their alloys. In order to efficiently increase the spatial resolution of the method, x-ray magnification system (Bragg magnifier) was used. The “Bragg magnifier” is based on the diffraction from an asymmetrically cut crystal. Bragg diffraction from an asymmetrically cut crystal produces one-dimensional magnification. Two asymmetrically cut crystals reflecting in mutually perpendicular directions gave a uniform two-dimension magnification. Bragg magnifiers with magnification factor 20 allow one to achieve 2-3 mkm spatial resolution in the registered images. 3D models of the samples reveal clearly the spatial relationships between different components of high explosive and their surroundings. This gives clues to the control of high explosive production. This study confirms the high efficiency of HRXCT method to recover the information on internal structure of the high explosives samples.

ACTION OF THE WATER CONTENT ON THE SCATTERING DYNAMICS OF DETONATION PRODUCTS OF WATER-CONTAINING EXPLOSIVES

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In circuits of an alternating current of 50 Hz, explosive switches are used for emergency switching-off of sections of a circuit. These sections can accumulate an energy up to 10 MJ. In this case the basic function of explosive switches becomes the dissipation of a significant amount of energy at low power, in the course of a rather long (about 20 millisecond) time. Conversion of this energy to the energy of an elastic strain of the breakers construction is limited by the mechanical characteristics of the constructional materials (the conversion of 1 MJ leads to elastic stress of 1 GPa). Therefore it is necessary to minimize the energy of the explosive payload, as well as to perform the removal of the excess energy to the environment. Earlier [1], transformer oil was offered as arc quenching medium of explosive switches for commutation of the 50 Hz circuits. The arc quenching properties of the oil are known for a long time and are used in oil switches. However, the dump of pressure from the volume of oil-containing explosive switches can cause the formation of the oil drops—air mixture. In the high-energy environment, the ignition of this mix is very probable. The combustion of the mix is accompanied by the significant (up to 35 MJ/kg) energy release. It is possible to spend a part of excess energy for evaporation of some amount of water. Power consumption of this phase transition is about 400 kJ/kg. We experimentally studied the peculiarities of scattering of detonation products of water–RDX powder (GOST 20395-74) mixture versus the amount of additive water. These experiments and some estimations are giving representation about the probable role of water in the chemistry of detonation decomposition and about the character of water evaporation in the course of our experiments. The estimations were made with the use of the technique [2, 3]. The experiments were performed with the use of high-speed digital chamber Cordin 222-16.

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PHENOMENA OF ENERGY FOCUSING IN EXPLOSIVE SYSTEMS, WHICH INCLUDE HIGH MODULUS ELASTIC ELEMENTS

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The phenomenon of energy focusing in explosive systems, which include high modulus elastic elements made from self-bounded silicon carbide, presented earlier, is experimentally investigated. The phenomenon was observed in a passive HE charge of cast TG 40/60 without cumulative shape under shock wave loading by explosion of an active HE charge through water after preliminary compression by a leading wave in silicon carbide insert. The phenomenon manifested itself as a hole in identification steel specimen with depth of about 10 mm and diameter of about 5 mm. Identification steel specimen was mounted for detect presence or absence of detonation in passive HE charge. The surface of specimen had typical temper colours that demonstrated presence of high temperatures.

In the given work results of experiments on studying of conditions of implementation of this phenomenon for SEP HE (plastic HE on the basis of PETN) and Composition B HE (analog TG 40/60) are presented. For each HE a number of experiments has been executed at various length of silicon carbide insert. Presence or absence of a hole in the steel specimen was determined. Also a number of optical registrations of process in framing mode with record step of 1 mcs have been executed. Digital video camera SHIMADZU HPV-1 was used for optical registration.

Results of experiments testify that the phenomenon is reproduced both for SEP, and for Composition B. Thus, focusing process is observed in conditions close to critical conditions of transfer of a detonation from active to a passive HE charge. Strong influence on results benefits accuracy of assemblage. Besides on process of detonation transfer from active to a passive HE charge strong influence benefits air bubbles and clearances between elements of fastening and HE charges which in case of the big thickness of elements of fastening lead to channel effect.

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INFLUENCE OF THE SHOCK WAVE IMPACT ON THE COMBUSTION REGIMES

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Contemporary problems in the field of combustion physics are devoted to examine nonstationary and transient combustion regimes in gaseous explosive mixtures. One of these problems is a design of methods of deflagration-to-detonation transition (DDT) control. This requires the sensibility of the combustion process to extrinsic factors have to be examined. Most vividly example of the extrinsic factor is the shock wave impact. Under certain physical conditions such an impact causes acceleration of DDT [1]. The shock-flame interaction launches non-linear gasdynamic processes. The evolution of these non-linear processes greatly affects the development of flame structure. As a result the flame structure is highly perturbed and DDT occurs [2].

This paper examines the shock-flame interaction phenomena in hydrogen bearing combustible mixtures in confined volumes (channels and tubes). The method of examination is the computer modeling. The solver is based on a two-dimensional model of hydrogen bearing mixture combustion. This model includes the gas dynamic transport of viscous gas, the hydrogen oxidation kinetics, multi-component diffusion, and heat conduction. For multi-component mixture and combustion products the equations of the real gas state were used. The reduced model of chemical kinetics describes process sufficiently detail. Such approach differs from approaches of a majority of the contemporary researchers who usually use the simplest one-step reaction models described by the Arrhenius kinetics. This approach allows to consider the interaction of hydrodynamic and chemical factors more accurate. In addition the various mixture compositions and various shock waves are examined.

Paper's results give relatively detailed description of the shock-flame interaction in confined volumes. Depending on shock wave and flame characteristics DDT may take place in two fundamentally different cases: DDT may occur in the shock wave itself or in the shock reflected from the wall. These characteristics are related mainly to the dynamics of flame and shock wave (velocities, shape etc.). In both variants, as the shock interacts with

the flame surface, the non-linear gasdynamic effects are triggered by the curvature of the flame. These effects are more intensive than the flame front instability (Darrieus-Landau instability). The highly perturbed flame is generated. Besides the pressure increase plays its role. And as a result DDT takes place earlier than in absence of any extrinsic factors. In the variant when DDT occurs during the first interaction with the flame the retonation wave interacts with the perturbed surface once again and generates one more detonation.

This paper enlarges the contemporary conceptions related to the problem of shock-flame interaction.

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COMBUSTION OF EXPLOSIVE MIXTURES OF VARIOUS COMPOSITION

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A topical problem concerning flame acceleration and deflagration-to-detonation transition (DDT) in real gaseous explosives is examined using numerical simulation. The aim of such investigation is to understand mechanisms and to propose methods of DDT control. One of these mechanisms is a deformation and acceleration of the flame due to the hydrodynamic instability of the flame front—the Darrieus-Landau instability (DLI) [1]. Most vividly DLI is observed in the flames that propagate in channels and tubes with smooth walls [2]. In such conditions the deformation of the flame front is developed as the result of the interaction between the flame and the boundary layer near the walls. Under certain physical and chemical conditions the complicated wrinkled flame structure can be generated [3]. Wrinkled flame is defined by the presence of deep folds in its structure. Conditions of detonation formation can develop in the folds.

The paper examines scenario of the DLI evolution in hydrogen bearing combustible mixtures in confined volumes (channels and tubes). The main problem of the research is connected with interaction of hydrodynamic and chemical factors. The main objective of this paper is to study interrelation of hydrodynamic and chemical factors and to provide insight into relation

between the mixture composition and the DLI evolution. All the results are received by methods of numerical simulations and in agreement with the experimental studies. The solver is based on a two-dimensional model of hydrogen bearing mixture combustion. This model includes the gas dynamic transport of viscous gas, the hydrogen oxidation kinetics, multi-component diffusion, and heat conduction. For multi-component mixture and combustion products the equations of the real gas state were used. The reduced model of chemical kinetics includes nine reactions. Such approach differs from approaches of a majority of the contemporary researchers who usually use the simplest one-step reaction models described by the Arrhenius kinetics.

Paper's results are related to the flame propagation dynamics in the hydrogen-oxygen and hydrogen-air mixtures. It is shown that various combustion modes are realized depending on the mixture composition. In the hydrogen-air mixture, perturbation caused by flame-boundary interaction develops into the DLI structure elongated along the channel axis. In this case the permanent acceleration mode is formed; however, DDT, if possible, takes place at distances about 2–3 meters. In the hydrogen-oxygen mixture the flame structure is rather different from the hydrogen-air mixture flame; similarly to the previous case it is elongated along the axis, but the shape is more complicated and has deep folds near the axis. The cold hydrogen-oxygen mixture turns to be blocked out in a layer between flame surfaces. Due to heat transfer from the reaction area the layer temperature increases, "hot spots" that can become centers of detonation initiation are formed.

In addition to this the authors examine flame evolution in hydrogen-oxygen mixtures with deviation from the stoichiometry. Comparison of the dynamics shows that the oxygen concentration is more important factor that affects the flame evolution than the concentration of other components (hydrogen and nitrogen).

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THE STATISTICAL CORRELATED PARAMETERS OF AXIALLY TURBULIZED MEDIUM INSIDE COMBUSTION CHAMBER UNDER MOVEABLE PISTON

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Axially-symmetrical turbulence being natural generalization of homogeneous isotropic case are progressing in problems with one detailed direction, as for instance flow into compression chamber of piston engine. Experimental and theoretical investigations have started at the middle of last century. And its are being high continued to present day [1], [2], [3].

The numerical simulation results of air-ethanol gas mixture dynamic into combustion chamber of piston engine have been introduced. For numerical simulation the two-dimensional model of combustion of ethanol-air mixture was used. The gas dynamic transport of viscous gas, oxidation kinetics of ethanol, multicomponent diffusion and heat conduction [4] were included to this model. For multicomponent mixture and combustion products the equations of state for real gases [5] were used. Instead of direct calculations of turbulent pulsations the series of the similar computations were carried out. They distinct with weak perturbation of initial conditions. Here the instantaneous speed distinct from ensemble-averaged speed distribution were used as turbulence pulsations. The statistical properties of turbulized medium induced by piston movement were described in terms of integral correlated scales of speed distribution. The effect of piston placement and speed to correlated parameters was considered. Variations of correlated characteristics under ignition and during combustion of gas mixture were investigated. The qualitative conformity (quantitative for some parameters) of computational modeling results and results of physical measurements [3] was obtained.

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HIGH PRESSURE INFLUENCE ON VELOCITY OF MONOMOLECULAR REACTION

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There is a whole number of phenomena based on influence of nearby molecules on a formation process of activated complex (AC). For example, braking or accelerating influence of high pressure at monomolecular reaction, braking effect of the solid state at the reaction velocity, or explosive accelerate reactions in “high pressure plus shift” conditions. These effects are used for an explanation of reaction mechanisms and should be taken into account in detonation processes and thermal decompositions of solid power-intensive compounds.

Since characteristic times of intramolecular processes are about 10^{-13} c and times of intermolecular moving are $\sim 10^{-8}$ – 10^{-10} c, the AC formation in dense molecular surrounding should be consider as thermodynamic non-equilibrium process.

We suggest the simple model of braking effect of high pressure. Lets consider that the reaction takes place in a stationary molecular surrounding. So, if near the molecule there is a cavity with a size more than AC size, than reaction will go with constant k_0 ; in the absence of such a cavity the reaction will not go on. The possibility of formation this cavity with required size could be estimated in the model of “free volume” from the state equation.

Given that crystal matter has more dense packing in comparison with liquids, it has less possibility than liquids of cavities formations with sizes larger or equal than size of AC. That is the reason of braking speed rate of chemical reaction in crystal as compared with liquids. An accelerating influence of high pressure occurs because of deformation of molecule along reaction coordinate till formation of AC. In the time of reaction the molecular surrounding is fix, so, it leads to square dependence of $\ln(k_p)$. In geterolytical reactions there is an additional mechanism of medium polarization owing to AC dipolar momentum. The peculiarity of this polarization is the small time of AC existence. So, for estimations we should consider an electronic polarization, while orientation polarization occurs only for field of particles with long life time. One more type of deformation—plastic deformation—leads to defects formation and amount of defects is proportional to the value of deformation. In the case of high pressure the energy which

arise from destruction of these defects could accelerate the reaction in orders.

ENERGY EXCHANGE IN SHOCK WAVES PROPAGATING IN HELIUM CONTAINING A SMALL CONCENTRATION OF $\text{Mo}(\text{CO})_6$

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The kinetic peculiarities of chemical transformations in the relaxation zone of shock wave propagating in helium, containing a small concentration of heavy molecules $\text{Mo}(\text{CO})_6$, were investigated experimentally and numerically.

The experiments were carried out in the incident shock waves with Mach numbers $M = 2.4\text{--}3.5$ under conditions when the free paths between collisions $\text{Mo}(\text{CO})_6 + \text{Mo}(\text{CO})_6$, were of the order $10^{-4}\text{--}10^{-5}$ less than free paths between collisions $\text{He} + \text{Mo}(\text{CO})_6$ [1]. The data on the distributions of concentrations of radiating states and charged particles in the shock wave relaxation zone are obtained by means of multi-channel emission spectroscopy and electrostatic probe located in a flow core.

The numerical simulation was carried by the use of CHEMKIN II code. The thermodynamic part of simulations is based on the data of the $\text{Mo}\text{--}\text{CO}$ bond energy in the $\text{Mo}(\text{CO})_6^+$ ion, given by [2], while evaluations of rate constants correlate with ones for the like processes during $\text{Fe}(\text{CO})_5$ dissociation, represented in details in [3]. The distributions of $\text{Mo}(\text{CO})_6$ dissociation products and small clusters of Mo atoms forming later, were evaluated. The results of simulation are compared with the experimental data. The role of energy exchange processes in SW front was shown to be important to describe the experimental data otherwise the frequency of Mo recombinative collisions have to exceed the gas kinetics frequencies essentially.

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ON AIR COMPRESSION WITH THE HELP OF DETONATION

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One of the greatest milestones in the history of aviation was the creation of gas turbine jet engine. Lots of improvements has been proposed and done to push its performance to the limits. The thing that makes one being stunned at least no less than the engine itself is the industry needed to create these sophisticated mechanisms.

However, the concept of turbine jet engine cannot be improved further to achieve greater thrust while having lower fuel consumption rate. In 1940 Y.B. Zel'dovich showed that thermodynamic efficiency of fuel combustion at detonation regime is greater than at deflagration regimes [1]. This theoretical result gave rise to numerous studies of possibility of creation and utilization of a detonation engine for aviation needs [2]. Advantages of detonation engines are design simplicity, low fuel consumption, operation range from zero up to supersonic velocities, high specific impulse [3].

Currently, development and application of Pulse Detonation Engines (PDE) faces at least to problems: possibility of air intake directly from the atmosphere and severe vibrations. It has been proposed to use a turbine compressor for air intake, as is in the case of turbojet engines [4]. Note that the turbine compressor is a very complex device which requires the use of high-precision equipment and modern materials for manufacture.

In this paper, a new PDE concept is suggested for the first time; according to this concept, the compression of oxidizer at zero velocity ($M = 0$) is performed without involving a compressor. Overcoming of vibration problem is an intrinsic feature of the concept.

The possibility of performing the oxidizer compression by a piston moving under the effect of detonation and shock waves was investigated. For this purpose, a numerical simulation of PDE according to the new concept was performed.

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**EXPERIMENTAL INVESTIGATION OF ACOUSTIC
INFLUENCE ON THE IGNITION
OF OXYGEN-HYDROGEN MIXTURE**

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Control of gaseous mixtures ignition is topic of interest in current state of combustion investigations. While investigating of detonation formation in non premixed components [1] the strong influence of acoustics on the detonation onset point was found. A number of numerical investigations [1] had shown that acoustics affects heat and mass transfer of intermediate combustion products in gases. These phenomena are governing at the stage of ignition. These observations suggest that acoustic disturbances could interfere with the gas ignition zone and affect combustion development.

In present work the experiments were carried out on specially developed setup included detonation tube, acoustic generator and spark system, which allows adjustment of spark energy. Detonation tube is equipped with pressure transducers and light gauges for ignition and combustion diagnostics.

As measure of acoustic action, minimum energy of igniting spark was gaged. The dependence of minimum energy of ignition spark from frequency and amplitude of acoustic wave was experimentally obtained. Also the experiments were carried out under different initial pressures from 1 bar and lower.

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INHIBITION OF SPONTANEOUS DECOMPOSITION OF ACETYLENE BY HYDROCARBON AND HYDROGEN BY INITIAL PRESSURE 1–2.5 bar. AN EXPERIMENTAL INVESTIGATION

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Subject was experimental definition of lower dilution limits of acetylene by propane-butane mixture and hydrogen at which the self-ignition of acetylene is not observed by initial pressure 1–2.5 bar.

Mixtures of acetylene with both oxygen and air are characterized by:

1. A high heat of combustion (gas-welding and torch cutting).
2. The smaller detonation cell size (0.1 mm) (increase the efficiency of detonation, devices including a detonation engine).
3. Monopropellant mixtures are widely studied (binary fuel mixtures remains still unclear).

It appears attractive to use a binary mixtures of combustible gas with inhibitor, such a gas causes hardly any change in the overall thermal effect of reaction with oxidizer.

Experimental setup included a tube (detonation chamber and measuring section), spark gap, vacuum pump, ball cock, pressure transducers, photodiodes. Pressure of mixtures was 1–2.5 bar. Ball cock separated detonation chamber and measuring section. It was opened just after filling the chambers by mixtures. Contact surface moved and stopped.

Minimal addition of propane-butane mixture for inhibition of acetylene decomposition by 1 bar was 7% of inhibitor. Minimal addition of hydrogen for inhibition of acetylene decomposition by 1 bar was 12% of inhibitor. If initial pressure of mixture increases, then minimal concentrations of inhibitors for inhibition of self-decomposition of acetylene increases too. Minimal addition of propane-butane mixture for inhibition of acetylene decomposition by 2.5 bar was 16% of inhibitor. Minimal addition of hydrogen for inhibition of acetylene decomposition by 2.5 bar was 39% of inhibitor.

Comparison of thermodynamic analysis and experimental data showed that the reason of the inhibition of acetylene is governed by both heat desorption and chemical-kinetic mechanism.

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SOLUTION FOR A PRACTICAL PROBLEM IN HYDROGEN SAFETY PROGRAM

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In this paper an important problem on hydrogen safety is being tackled, namely, possible dangerous situation that might happen during storage and usage of highly pressurized hydrogen. Results of a robust numerical modelling are shown. Based on the results, a new concept for a pressure release valve nozzle design has been proposed.

Recently, lots of interest towards hydrogen as a possible alternative type of fuel emerged. At normal conditions hydrogen density is low, thus this is advantageous to store hydrogen only under high pressure. Vessels that can withstand up to 1000 atm pressure has been reported lately. However, highly pressurized hydrogen might be very dangerous to handle because of its properties: broad concentration limits and high speed of sound. In this connection an investigation on what possible accidents can occur at storage and usage of highly pressurized hydrogen becomes of a great importance.

Throughout the world data has been collected on accidents involving ignition of hydrogen at spontaneous depressurization of vessels at high pressure [1]. According to the data, ignition causes like flame, hot surface, collision, friction spark are responsible for only 15% of all incidents. For the rest 85% the cause remained unknown. Recent investigations revealed that the main mechanism in charge was diffusion self-ignition ([2, 3, 4]).

In this work a 3D numerical modelling of a hydrogen jet behavior at its release in atmosphere has been done. Initial and boundary conditions that are sufficient for suppression of hydrogen diffusion self-ignition has been obtained.

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PHYSICS AND MODELLING OF UNDER-EXPANDED JETS AND HYDROGEN DISPERSION IN ATMOSPHERE

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The hydrogen is seen as an energy carrier for clean transport and fuel cell application within the affordable and sustainable energy supply chain. The pressure of onboard hydrogen storage in early-market vehicles already reaches 700 bar. Such high storage pressures make accidental hydrogen release and dispersion a potentially hazardous scenario. This paper describes the modelling of under-expanded hydrogen jets and modelling of its dispersion in atmosphere at large scales. The following is presented:

- A novel notional nozzle model that takes into account non-ideal behaviour of hydrogen at high pressures through the Abel-Nobel equation of state. Similar to the approach by Birch et al. [1] the developed model is based on the assumption of uniform sonic flow through notional nozzle. However, the model includes the energy conservation equation. This approach avoids formally supersonic velocities in the notional nozzle as in the model of Schefer et al. [2] that is important to decrease computational error during application of CFD tools for numerical simulations of hydrogen dispersion from under-expanded jets at large scales.

- A model for blowdown dynamics at adiabatic expansion of hydrogen from high pressure vessel to the atmosphere. Transient character of hydrogen discharge from a storage with changing in time pressure and temperature within the vessel results in the variation of the notional nozzle diameter, velocity and density of hydrogen at the notional nozzle. Accurate simulation of hydrogen dispersion and flammable mixture envelope is important for risk assessment of hydrogen technologies.

- Intercomparison of the blowdown characteristics in a limit of adiabatic and isothermal walls. The heat transfer plays an important role in the hydrogen blowdown dynamics [2]. The effect of heat transfer on the blowdown dynamics is estimated and conclusions are compared to published results [2].

- Effect of pressure losses on the blowdown dynamics. Large pressure gradients and release velocity during blowdown phenomenon imply significant pressure losses, which, in due course, should lead to decrease in a mass flow rate. A model for local losses is presented and the effect of release manifold design on the pressure losses and mass release rate is anal-

ysed. Comparison between simplified engineering method for prediction of losses' effect on mass flow rate and CFD predictions is given.

- Validation of CFD model to simulate hydrogen blowdown from a variable diameter notional nozzle against experimental data by Shell and HSL [3]. The model includes time dependent volumetric source terms for momentum, energy and hydrogen mass to avoid simulations with variable geometry at the inflow boundary and surroundings. The applicability limits of this method are demonstrated.

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DETONATION WAVE OF CONDENSATION

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A principally new phenomenon—formation of detonation wave driven by the condensation of supersaturated vapor is for the first time observed. Highly supersaturated carbon vapor was formed at the thermal decay of unstable carbon suboxide $C_3O_2 \rightarrow C + 2CO$ behind a shock wave in the mixtures containing 10 ÷ 30% C_3O_2 in Ar. This reaction was followed by the fast growth of condensed carbon particles. Previous experiments [1, 2] have shown that the integral heat release of complete transformation: $C_3O_2 \rightarrow CO + \text{carbon nanoparticles}$ is rather high (≈ 120 kJ/mol) and comparable with the combustion of hydrogen-air mixtures (≈ 140 kJ/mol). An important peculiarity of this process is that a bottleneck of condensed particle growth is the reaction of carbon vapor formation, exponentially accelerating with the temperature [3].

Analyses of kinetics of a heat release in the given conditions [4] and the calculations by one-dimensional detonation theory have shown that in the mixture 10% C_3O_2 +Ar the insufficient heat release resulting in regime of “overdriven detonation”. In the mixture 20% C_3O_2 +Ar a very good coincidence of measured values of pressure and wave velocity with calculated

Chapman-Jouguet parameters has been attained. In more rich mixture 30% C_3O_2+Ar an excess heat release caused the slowing down of the effective condensation rate and regime of “underdriven detonation” has been observed.

The important practical application of this issue is the new understanding of a role of condensation processes in detonation of gaseous fuels yielding condensed products.

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MONTE-CARLO AND KINETICS MODELING OF NONEQUILIBRIUM PROCESSES IN SHOCK WAVE FRONT

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The complex of nonequilibrium processes resulting in the peaks of radiation and free electrons concentration, experimentally observed in the front of weak shock waves in inert gases with small admixture of heavy iron pentacarbonyl molecules $Fe(CO)_5$ (IPC) [1], is studied.

A non-stationary statistical Monte-Carlo modeling [2] of molecular velocities distribution function in shock wave in helium containing an admixture of IPC was performed. The goal of modeling was the simulations of distribution functions of relative velocities of pair collisions in the region of translation relaxation of shock wave (considered energies run up to 5–7 eV) and an analysis of high-energies collisions hypothesis convenience to explain a nature of observed non-equilibrium effects in shock waves.

Calculated distributions of collisions of IPC molecules with helium did not show noticeable deviations from equilibrium values, while the excess of pair collisions between IPC molecules for high relative velocities in the mixtures containing 100 ppm of IPC amounted to a factor of 10^{14} . How-

ever, to estimate the real contribution of such collisions in observed non-equilibrium phenomena one should consider their effective frequency (still extremely low) and a dependence of inelastic interaction cross-section on collision energy. For most systems probabilities of non-elastic transitions in collisions with energy above 3 eV do not exceed 10^{-4} – 10^{-5} [3, 4]. Thus, performed estimations have shown that intensive non-equilibrium effects, observed in [1], could not be explained in such approach and predominantly originated by the exothermic processes of iron clusters growth.

For analysis of kinetics of excited and ionized iron clusters formation behind the shock wave front a numerical modeling was performed using developed detailed kinetic scheme. The results of calculations are in a good agreement with the experimental observations.

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THE APPLICATION OF ARAS AND SHOCK WAVE TECHNIQUE FOR INVESTIGATION OF SMALL IRON CLUSTERS FORMATION IN DIFFERENT GAS-DILUTERS

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One of the most informative methods to study the metal cluster growth is a pyrolysis of metal carbonyls ($\text{Fe}(\text{CO})_5$, $\text{Mo}(\text{CO})_6$ etc.) behind shock waves. For accessing more information about the process of particles formation it is necessary to perform the extensive research of cluster growth mechanisms depending on initial molecules source and ambient conditions. Up to now the influence of kind of carrier gas on constant rate of particle growth was neglected in all-known mechanisms of particles formation.

In this work the combination of shock-tube techniques and atomic resonance absorption spectroscopy (ARAS) were used for investigation of kinetic of formation of small iron clusters from iron atoms produced during iron pentacarbonyl ($\text{Fe}(\text{CO})_5$) pyrolysis behind shock wave. Very high

sensitivity of ARAS method allowed to study the extra small initial concentrations of $\text{Fe}(\text{CO})_5$ ($10^{12} - 10^{14} \text{ cm}^{-3}$). In these conditions the influence of interference reactions could be neglected and due to that an analysis of kinetics of iron atoms formation and consumption in recombination processes is essentially simplified.

In the course of this work the high vacuum shock tube “NEFRIT” was completely re-equipped with evacuation up to $2 \cdot 10^{-6}$ mbar. The leakage and desorption from the walls were not more than $2 \cdot 10^{-5}$ mbar/min. The method of ARAS on Fe atoms at wavelengths 248.3 and 271.9 nm was realized with the space-time resolution about of 5 μs . The calibration dependence of iron atom concentration on absorption signal was obtained in wide range of iron concentrations (10^{12} – 10^{14} cm^{-3}). As a result the experimental dependences of iron cluster growth rate on temperature in the mixtures containing 2–10 ppm Fe in Ar and He at the pressures 0.3–0.5 bar have been measured.

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CHARGING OF CARBON NANOPARTICLES FORMED DURING SHOCK WAVE PYROLYSIS OF C_3O_2

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In this work the kinetics of charging of carbon nanoparticles, formed at pyrolysis of C_3O_2 behind shock waves was investigated. A process of particle charging was registered by means of high-sensitivity electric probes [1]. Experiments behind the reflected shock waves at temperatures from 2000 to 3500 K in the mixtures (0–2)% C_3O_2 in argon were carried out. A considerable decrease of concentration of free electrons, arising at thermal ionization of a natural impurity of sodium, in the presence of carbon nanoparticles is revealed. In a mixture of 2% C_3O_2 in argon a final concentration of negatively charged particles of plasma was approximately at 100 times less than in pure argon. It is shown that characteristic time of charging of carbon nanoparticles does not depend on their concentration and decreases with the temperature rise from 400 to 40 μs .

Modeling kinetics of charging of carbon particles was carried out taking into account a step-by-step ionization of sodium and subsequent recombination of free electrons and ions on a surface of the particles [2]. Both the experimental and modeling results show that the final concentration of the

charged particles in most cases is much more higher, than free electrons concentration. This fact means that electrostatic properties of gas-particle mixtures are completely determined by the charged particles.

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COMPRESSION OF AIR BEHIND THE PISTON DRIVEN BY DETONATION: EXPERIMENTAL INVESTIGATION

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Compression of air for technological applications are usually realized by turbine or piston compressors. Typical driver of compressor device provides constant force. Current work is devoted to compression of air behind the piston driven by detonation wave and to dynamics of piston movement. Investigation of detonation formation and propagation in the tube with moving back wall is also the subject of this investigation. Mutual influence of high-pressure combustion, piston displacement under the pressure difference and its own inertia, pressure waves in the volume behind the piston is subject of the consideration. Previous our estimations [1] were made numerically and shown the dependences of pressure behind the piston on the piston mass and frequency of detonation pulses repetition. Numerical model contained solution of gasdynamic equations, detailed chemistry of combustion and mechanical kinetic simulation of piston displacement. The report will present experimental study conducted on detonation tube equipped with pressure transducers, light gauges and detectors of piston displacement. Dependences of compression on the length of detonation tube will be presented. Observations in compression of air behind the piston driven by detonation wave and dynamics of piston movement will be described in the report.

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EXPERIMENTAL INVESTIGATION OF HYDROGEN SELF-IGNITION AT THE DISCHARGE INTO AIR

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Utilization of hydrogen as a prospective fuel is developing very actively. However, because of wide concentration limits of hydrogen ignition and high speed of sound the development of hydrogen energetics is concerned with research in hydrogen safety. Hydrogen energetics requires kinetic information on hydrogen ignition and detonation at different conditions.

In the paper experimental data on fundamental constants of chemical kinetics of hydrogen oxidation in air under high pressure will be presented. The motive of this work was the lack of knowledge on kinetics scheme under pressure over 10 bar and temperature less then 700-800 K. At these conditions the differences between experimental and calculated values of ignition delay time were about 1000 times. [1]

The paper describes experimental investigation of hydrogen self-ignition at the discharge into air. Dependence of ignition delay time behind the shock wave front at the initial pressure up to 150 bar are obtained.

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NUMERICAL INVESTIGATION OF MECHANISMS OF ACETYLENE SPONTANEOUS SELF-DECOMPOSITION

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Chemical reactions in gases with heat release at high pressure depend both on initial conditions and duration of an affection. Depending on this duration some reactive state of gaseous system may be established with passing over a transient state. It was shown [1] that mechanism of prevention of explosive decomposition of acetylene at initial pressure 1 bar has not only thermal effect but the chain one too.

The numerical investigation of explosive decomposition of acetylene is carried out by diluting it with a household gas (propane-butane) and

hydrogen. Shock wave loading was used to compress acetylene-inhibitor mixture and to avoid a flame propagation “from layer to layer” by heat transmission.

The main thermodynamic parameters and initial conditions were determined from experiments. Simulation of inhibition of acetylene decomposition with hydrogen has been carried out with using a scheme of the second order of accuracy.

Kinetic mechanisms were investigated numerically at initial pressure range from 1 to 4 bar. It has been shown that the first strongly depends on the pressure. The chain mechanism of inhibition of acetylene was found to be governable one not only at atmospheric pressure, but at higher pressure.

Minimal limits of bulk concentration of propane-butane mixture and hydrogen are obtained, at which no spontaneous decomposition of acetylene occurs.

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THE CYLINDRICAL AND SPHERICAL FAST INTENSE COMPRESSION OF IDEAL GAS WITH THE ADIABATIC EXPONENTS FROM 1.2 TO 3

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The problem on the cylindrical ($\nu = 2$) and spherical ($\nu = 3$) fast intense compression (FIC) of the perfect gas is considered. The term “fast” means that the duration of the compression is much less than transit time of a sound wave through initial cylindrical or spherical space, and the term “intense” is understood as simultaneous obtainment of arbitrary high density and temperature. The fast compression begins on an intense shock wave (SW), imploding to the center or the axis of symmetry (further to CS). At approach SW to CS this flow is described by Guderley selfsimilar solution with unlimited growth of temperature, pressure and speed in CS and finite increase in density both for imploding, and for reflected SW (after reflection SW in CS density is equal to zero, pressure is finite, and temperature and speed of sound are infinite). Problem on FIC includes Guderley problem (GP) which complete solution for $\nu = 2$ and $\nu = 3$ is obtained for the adiabatic exponents γ from 1.2 to 3. At the solution of GP the selfsimilarity exponent $n = n(\nu, \gamma)$ is determined and in the plane of

dimensionless “speed of gas—square of speed of sound” the integral curve is plotted. The curve, having passed through the singular point (SP) on “the sound parabola” (SPSP) and having undergone a shock corresponding to the reflected SW, is over at the infinite SP (ISP). If r is distance to CS, $t = 0$ at the moment of reach of SW and overtaking it “special” C^- -characteristic, corresponding to SPSP, in CS, then on rt -diagram the axle of time $t > 0$ corresponds to ISP. SPSP at γ from 1 to $\gamma_* \approx 1.9$ at $\nu = 2$ and to $\gamma_* \approx 1.86$ at $\nu = 3$ is a saddle, and at greater γ it is a node.

For obtaining an arbitrary large increase in density the centered compression wave (CW) with focus in CS is attached to the special C^- -characteristic at $t = 0$. Beyond of a small vicinity of the focus of CW the trajectory of a piston realizing the compression is calculated by the method of characteristics. As well as for any CW, such calculation begins on focus in CS. In such focus some of parameters (trivially, pressure, temperature and speed of gas) are infinite. Therefore the calculation by the method of characteristics is preceded with derivation of the analytical solution, valid in small vicinity of CS. For $\gamma < \gamma_*$ in the infinitesimal vicinity of CS this solution gives small additives to the Guderley solution, and at $\gamma > 2.3$ for $\nu = 2$ and $\gamma > 2.2$ for $\nu = 3$ —on the contrary, even in a small vicinity of CS pressure, temperature and speed of gas, determined in Guderley solution, being infinite quantities, are small in comparison with the additives induced by focusing C^- -characteristics. Solutions with CW which focuses on the special C^- -characteristic or reflected SW are obtained, at that at arbitrary small r . There is a problem on decay of arbitrary discontinuity at focusing on reflected SW as a result of its interaction with a bundle of compression waves. The solution of this problem has shown, that to CS always propagates formed at the decay SW. As opposed to it, the wave propagating to the right from the corresponding contact discontinuity can be both SW and a rarefaction CW. For γ which are close to 1 the first opportunity is realized and for γ which are close to 3 the second one is realized. Values γ of “transition” are determined by symmetry of the problem (parameter ν) and intensity of a bundle of compression waves.

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NUMERICAL SIMULATION OF DYNAMICS OF VISCOUS LIQUID DROPS ENSEMBLE IN A GRAVITATIONAL FIELD

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The complexity of the description both single drops dynamics and the ensemble of interacting viscous liquid drops in the external force field (gravitational, electromagnetic) is caused by necessity to solve a nonlinear system of Navier-Stokes equations with boundary conditions on the free surface, changing its position in space and time. The main characteristics of hydrodynamic processes are closely connected by evolution of free surface.

Unlike the model [1] built using adaptive-grid numerical method and describing the dynamics of a single drop oscillations the model developed on the basis of level-function method describes nonlinear oscillations of drop and the processes of fragmentation and merging of droplets. Navier-Stokes equations written in variable “velocity-pressure” on a rectangular staggered grid in a cylindrical coordinate system with the symmetry of the angle are solved by the method of splitting of physical processes [2] (projection method). For the time discretization of derivatives third-order accuracy Runge-Kutt scheme is used, for discretization of diffusion terms central-difference schemes of second-order accuracy are used, for convective terms finite-difference schemes of high resolution (ENO-schemes third order accuracy) for obtaining non-oscillation solutions at the boundary between two phase are used.

Non-oscillation solutions for 2-phase medium with a characteristic attitude of phases densities $< 10^{-3}$ and $Re < 1000$ are obtained. Capabilities of developed method are shown by the example of solving the problem of falling drops from capillary (droplet detachment from the capillary, formation sphere of Plato, flight, collision with a flat surface, oscillations at the surface and spreading). Comparison of the simulation results with well-known numerical models and experimental data show satisfactory agreement for phases and form droplets.

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BIOCONVERSION: POWER TECHNOLOGICAL COMPLEXES

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Russia has huge reserves of plant energy stuff (logging waste, wood, pulp and paper industry, peat, crop residues), but, except for the incineration of wood and peat in household stoves, this potential still little used. In today's domestic prices for traditional energy resources only aggregate technologies of organic raw materials sold in power technological complexes economically justifiable in Russia can be. Such systems should provide a virtually complete recycling plant material, in addition to producing basic products—heat and electric power—by-products demanded in the market.

In the Laboratory of energy saving problems of JIHT RAS experimentally and theoretically justified the aggregate technology of vegetable raw materials (wood, peat), which provides a high-gas and by-products: activated carbon, pyrocarbon, metallurgical coke, technical hydrogen. Depending on the type of feedstock and the market the technology may shift towards the preferred production of certain products.

A basic scheme of industrial technology is developed, major elements of which are reactor-gasifier with two-stage gasification, pyrocarbon's reactor, power unit based on gas-piston engine. Elements of the scheme have been tested in laboratory facilities and bench testing. Technoeconomic evaluation showed that under certain conditions (raw materials base, good logistics, regimes and the consumption of energy, etc.), investment attractiveness of a potential project is high enough.

STUDY OF PYROCARBON FORMATION IN THE BINARY MIXTURES OF METHANE AND ITS GOMOLOGUES

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The results of experimental and theoretical study of pyrocarbon formation on the surface of the porous carbon material in the process of heterogeneous pyrolysis of binary mixtures of methane, propane and butane are presented.

The experimental data on the rate of pyrocarbon formation in the flow of methane, propane and butane in the temperature range 850–1050°C and in the flow of binary mixtures of methane-propane, methane-butane at the temperature 1000°C are received. Charcoal is used as a porous carbon material. Analysis of the experimental data is based on the using the model of randomly located pores for description of porous material structure and on the rate constant of heterogeneous pyrolysis of methane known from the literature [1]. As a result the magnitudes of the activation energies and the rate constants of pyrocarbon formation in the flow of propane and butane are determined.

To describe the process of pyrocarbon formation in mixtures of paraffin hydrocarbons the mathematical model is developed. In the model the double-stage scheme of pyrocarbon formation proposed in [2] is used. According to this scheme, the rate of pyrocarbon formation is characterized by the generation rate of nucleus of crystallites and by the rate of their growth. As a result, the rate of pyrocarbon formation in binary mixtures is not additive in relation to the rates of pyrocarbon formation in individual gases. Application of the developed model along with the experimental data gives opportunity to determine the ratio between the rate constants of nucleus generation and the rate constants of crystallite growth for methane, propane and butane. These data make it possible to carry out the calculation of pyrocarbon formation velocity for any fraction of heavy hydrocarbons (propane or butane) in methane. This work is done with support of RFBR (grant number 06-08-00543-a).

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HIGH-CALORIFIC GAS MIXTURES PRODUCED BY PYROLYSIS OF PEAT

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The results of experimental investigations of composition and quantity of gas evolving during pyrolysis of peat in the temperature range 200–1000°C are presented. It is shown that at the temperatures above 500°C the content of carbon dioxide in the escaping gas mixture significantly decreases while the content of combustible gases (methane, carbon monoxide, hydrogen) increases. As a result the calorific efficiency of the gas mixture rises. The total output of gaseous products is 0.34 nm³ per kg of the original dry product, and the specific caloricity is equal to 11.7 MJ/nm³. It is important to note that the maximum specific caloricity of a gas produced in the gasification process does not exceed 5.8 MJ/nm³. Extraction of pyrolysis gases evolving in the temperature range 550–1000°C, of course, leads to a significant increase in caloricity of gas mixture to 15.85 MJ/nm³, but the gas output will decrease and will be equal to 0.20 nm³ per kg of the original dry product.

Increasing the fractional conversion of the feedstock into high-calorific gas can be achieved by means of high-temperature (~1000°C) processing of liquid fraction escaping during carbonization of peat in the temperature range 200–550°C. On the base of the composition measurements of gas mixture produced by thermal processing of liquid fraction, it is shown that one can get 1.42 nm³ gas with specific caloricity 12.08 MJ/nm³ per kg of the original dry product. So the total calorific value of the gas will be more than 80% of the calorific value of the feedstock. The findings can be used as a basis for the development of modern high-performance technology of the thermal processing of peat. This work is done with support of RFBR (grant number 07-08-12309).

NUMERICAL MODELING OF SEVERE ACCIDENTAL EMISSION'S CONSEQUENCES IN INDUSTRY

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Explosions, detonation processes, combustion, emergency destruction of large vessels under pressure lead to emission of considerable volumes of hazardous substances. Propagation of dangerous substances accompanies with catastrophic consequences (with fatalities and injury of the staff, ecological problems etc.). It defines necessity simulation of probable accidents on a design stage of industrial objects. One of the dangerous effects of emergency emissions is connected with possibility of drift of clouds on the considerable distances which size depends on properties of substances, emission and environment conditions. For the analysis of accident the TOXI+ software has been developed by us in STC "Industrial Safety". Developed TOXI+ software provides calculations with gas emissions of any density. Our model takes into account a possibility of drop-gaseous mixtures formation with effective density more than air ("heavy gas"). The majority of severe accident emissions on typical chemically dangerous manufactures actually has happens with formation of heavy gas emissions. The reasons of heavy gas formation are high molecular weight of the substances or low temperatures and presence of drop inclusions in gas emission. TOXI+ considers evaporation of a liquid and emission cloud drift by a wind. Initial simulation parameters include many properties of accident for example suggested method includes four initial temperatures (inside equipment, surface of spill, surrounded area and environment air). The type of surface is defined by 30 different surface roughnesses which are available for choose. There are 21 included hazardous substances (typical for oil-gas industry). Presence of the built-in matter database allows supply the operative prediction of cloud expansion. In this work results we present results of simulation for 3 accidents. (1) 09.12.1970, Port Hudson (USA, Missouri). As a result of pipe line with liquid propane destruction, there was emission and propane-air cloud formation. The amount of propane emission was about 60–70 tons. After ignition the combustion transited into the detonation regime. (2) 13.07.1973, Potchefstroom (South Africa). This accident is characterized by the greatest quantity of victims on objects with ammonia for all history. After destruction of the tank with liquid ammonia, the 38 tons were released. (3) 06.01.2005, Graniteville (USA, South Carolina). In

the result of two trains collision on railway station the 82 tons of chlorine were released.

INFLUENCE OF SPECTRAL STRUCTURE OF AEROSOL PARTICLES IN AN ATMOSPHERE ON A DEGREE OF ABSORPTION OF ELECTROMAGNETIC RADIATION

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For practical researches and theoretical calculations of influence of spectral structure of aerosol particles in an atmosphere on a degree of absorption of electromagnetic radiation it is necessary to know properties of aerosol formations: physical, chemical and spectral structure of particles. Thus with other things being equal the spectral structure of aerosol particles on the size determines a degree of absorption of electromagnetic radiation of various ranges.

For estimations of characteristics of environment experiments with creation of artificial aerosols and definition of their parameters have been lead. In total it has been created three kinds of aerosols—an aerosol water the pair, received waters, an aerosol, received at burning a smoke candle and an aerosol, at burning rubber.

It is known, that the water fog is effective means of protection against all kinds of optico-electronic means in a spectral range 0.2–14 microns. Till now numerous attempts of creation of a fog with the help of undermining of water suffered failures. Attempts of mechanical and pneumatic dispersion of water also have terminated in failure since it was not possible to spray water till diameter of drops 5–15 microns.

Us experimentally, by undermining, water has been transformed into a fog and in drops as a result of influence of high temperature and short dynamic impacts. Experiments on research of characteristics of the aerosol cloud consisting from of drops of water were carried out in field conditions on research range GU “VGI”.

Characteristics of dispersion, easing and absorption of lengths of waves 8–14 microns for volume with concentration of particles of 1–3 cm are counted with use by experimentally certain function of distribution of particles in the sizes $f(r)$. This distribution of water particles is lognormal. Calculations have been lead at value of average geometrical radius r_0 equal 5.6 microns.

The executed experiments by definition of spectral structure have shown a real opportunity of measurement of distribution of particles of an aerosol on their size, educated by water drops and firm particles.

PERIODIC ORBITS IN ATOMIC-ION SYSTEMS

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The role of the periodic orbits in quantum physics has been discussed in the literature since Bohr (see, for example, references in the review [1]). In following this question is considered for spherically symmetric potentials.

Research of the bound interacting fermion system (free atoms and ions, plasma, metal clusters, nuclei) using the density functional method reduces to the single-particle states in a self-consistent potential. In spherical approximation the self-consistent attractive potential can be assigned to one of the two possible groups [2]: 1) finite at zero point (potentials in spherical clusters and nuclei) and 2) having Coulomb singularity at zero point (intra-atomic potentials). The group specificity appears in the gradient, oscillating and shell effects.

To calculate the semiclassical particle density distribution and thermodynamical properties of the system it is enough to know the particle classical motion characteristics only for the energy equal to the chemical potential μ . In particular, radial action $S_\mu(l)$ for a particle with energy μ and orbital momentum l contains all the necessary information for the shell effects description. The shell effects are connected with the periodic orbits and result, for example, in the magic numbers of metal cluster mass spectra and in the irregular dependence of atomic properties on the atomic number.

In small clusters there are two important periodic orbits: the particle having a zero orbital momentum $l = 0$ traverses the centre along the linear orbit, and the particle with the highest possible orbital momentum $l = l_\mu$ moves along the circular orbit. In the clusters having a hard potential the k -angle ($k = 3, 4, 5$) closed orbits appear when cluster size increases [3]. Oscillations with beats in the experimental sodium cluster mass spectra are the result of triangular and square orbits interference. In the large soft potential clusters the five-point-star orbit makes the main contribution [4] that appears in the different, similar to sine, oscillations in the aluminium cluster mass spectra.

It is shown, that cluster situation can't come true in the atomic systems under any atomic number. There are always only two periodic orbits which

appear in the measurable quantities: a linear motion in the s -state of the particle which reflects from the centre and a circular movement with the maximum orbital momentum $l = l_\mu$, the latter contribution being dominant [5].

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QUASIZONES AND RESONANCES IN THE SELFCONSISTENT FIELD MODELS OF DENSE PLASMA

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In the quasizone model the spectrum of the high density plasma is described by using a so-called quasizone. This is an energy band which allows to treat bound states for inner electrons, free states for continuum and intermediate electron states with energy close to zero, including resonances, in the same manner. The quasizone appears due to the special boundary conditions for wave functions—quasi-periodical conditions in mean spherical approximation [1]. In this case the electron wave function is presented as an expansion over spherical harmonics. There is only one harmonic for every bound state, several for weakly bound states and an infinite number of terms for the free states. Using the quasizone model and local density approximation for electron exchange and correlation effects it is possible to obtain energy spectrum, equation of state (EOS) and photon absorption coefficients in a wide range of plasma temperatures and densities. The detailed comparison with other approaches such as average atom model of B.Rozsnyai [2], D.Liberman model (Inferno) [3] and EOSTA model [4] is fulfilled. In the last two models the resonance states are included that is very important in calculations of the equation of state. It is shown, that the quasizone model (and models including resonances) allows to obtain smooth pressure ionization curves at high densities. The cold and Hugoniot curves are in a good agreement with experiment.

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EQUATIONS OF STATE FOR COPPER, SILVER AND GOLD

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Results of theoretical calculations and experimental measurements of the equation of state (EOS) at extreme conditions are discussed and applied to Cu, Ag and Au. It is pointed out that the available high pressure and temperature information covers a broad range of the phase diagram, but only irregularly and, as a rule, is not thermodynamically complete; its generalization can be done only in the form of a thermodynamically complete EOS. A multi-phase EOS model is presented, accounting for solid, liquid, gas, and plasma states, as well as two-phase regions of melting and evaporation. The thermodynamic properties and phase diagrams are calculated with the use of this model. Theoretical calculations of thermodynamic properties of the solid, liquid, and plasma phases, and of the critical point, are compared with results of static and dynamic experiments. The analysis deals with thermodynamic properties of solid metal at $T = 0$ and 298 K from different band-structure theories, static compression experiments in diamond anvil cells, and the information obtained in isentropic-compression and shock-wave experiments. Thermodynamic data in the liquid state, resulting from traditional thermophysical measurements, “exploding wire” experiments, and evaluations of the critical point are presented. Numerous shock-wave experiments have been done to measure shock adiabats of crystal and porous samples, release isentropes, and sound speed in shocked metal. These data are analyzed in a self-consistent manner together with all other available data at high pressure.

The model’s results are shown for the principal shock adiabat, the high-pressure melting and evaporation regions and the critical point. The present EOS describes with high accuracy and reliability the complete set of available information.

STRUCTURE OF BETA-BRASS CuZn AT HIGH PRESSURE TO 90 GPa

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The copper-zinc system is a classic example of an alloy system displaying a sequence of phases along an alloy composition, called Hume-Rothery phases. The crystal structure of these phases is determined by electron concentration (that is the number of valence electrons per atom), and the lowering of the electronic energy is considered the key factor for the structure stabilization [1]. Using powder x-ray diffraction we study the beta-phase of CuZn in its bcc phase in the pressure range up to 90 GPa and find a transformation to a modulated trigonal structure at around 40 GPa. We analyze the structural distortion of the bcc phase CuZn by looking at the configuration of the Brillouin zone of the bcc and the trigonal structures and their interaction with the Fermi surface. We demonstrate that the stabilization of the complex high-pressure structure can be explained with the Hume-Rothery effect [2].

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THERMAL EXCITATION OF ELECTRONS AND APPLICABILITY BOUNDARY OF PSEUDOPOTENTIAL APPROACHES

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In this work, we compare the contribution of electrons in thermodynamic functions of substances at different densities (higher than normal density) and electron temperatures. One of the methods, FP-LMTO [1] (complex of programs LMTART [2] modified similar to the way described in [3]) describes all electrons in the framework of the density functional theory. The other approach, VASP [4] uses the most exact pseudopotential among others—the ultra-soft pseudopotential [5] also in the context of the

density functional theory. The obtained results are compared with each other and with the equation of state calculations [6, 7]. We think that such a comparison is informative and allows us to improve the thermodynamic description of matter.

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THERMODYNAMICS OF ELECTRONS IN METALS UNDER FEMTOSECOND IRRADIATION

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Thermodynamic properties of electrons are important under strongly non-equilibrium conditions of femtosecond laser irradiation. Usually free electrons in metals are considered as independent and one uses the equation of state of ideal Fermi-gas. In order to approximately take into account the interaction between electrons one could use more realistic expression for the density of states of electrons in metals. In this work we use the results of first-principle calculations of a density of states of Ag and Au and derive a simple thermodynamic model for the description of influence of d-electrons of these metals. We consider heat capacity, isothermal sound velocity, and electron-phonon coupling constant and note significant distinction of these values from the ideal Fermi-gas model as it was stated earlier [1]. The constructed equation of state is supposed to be used in hydrodynamic simulation of femtosecond irradiation experiments.

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AB INITIO MODELING OF METALS WITH HOT ELECTRON SUBSYSTEM

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The description of the electron-ion relaxation in condensed phase of real substances with excited electrons is currently an actual theoretical problem that has no general methods of solution in the framework of quantum molecular dynamics. As a tool of analysis of the electron-phonon interaction in solid phase the finite-temperature density functional theory is applied. The phonon dispersion and the electron DOS studies are carried out for the two-temperature system “cold lattice–hot electrons”. The analysis was performed of the influence of electron temperature on stability of simple and d-metals (Al, Au and Ni). The results point to the substantial redistribution of electron densities and change of the interionic interaction at electron temperatures above 2–3 eV.

THE CRITICAL POINTS OF SEVERAL METALS DETERMINED ON THE BASIS OF THEIR CONNECTION WITH UNIT COMPRESSIBILITY LINE (ZENO-LINE) PARAMETERS

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The critical parameters of several metals were determined on the basis of the low temperature binodal measurements and their connection with the line of unit compressibility factor. (Below this line is referred as to Zeno-line, $Z = P/\rho T = 1$ is the compressibility factor, P is the pressure, T is the temperature, ρ is the particle density.) For a wide class of substances this line is the straight line in the density-temperature plane. Zeno-line is also the tangent line to the liquid branch of binodal at $T \rightarrow 0$ in this plane. These facts allow us to construct general expression for the coexistence curve liquid-vapor (liquid branch), which is transformed into the Zeno-line at low temperatures. This expression depends on the four parameters, which were determined by the condition of minimum deviation of calculated and experimental binodals. The analysis of a large number of experimental data for non-metallic substances [1] (Ar, Ne, CO₂, O₂, CH₄ and others) and metals (Hg, alkali metals) [2] with known critical parame-

ters and coexistence curves have shown good agreement between calculated and measured binodals. At that time we find that two factors are weakly dependent on the substance sort. These factors are $\rho_c/\rho_B + T_c/T_B$ and $(\rho_c T_c - P_c)/(\rho_B T_B)$, where subscript c refers to the critical point parameters, subscript B refers to the Zeno-line parameters. Thus, these factors can be considered as the correspondence relations. Another classification parameter is the compressibility factor at the critical point. It defines the binodal opening. The less this factor is, the more the binodal opening is. We showed that the compressibility factor at the critical point for classical substances $Z_c \leq 0.32$. Hg and quantum substances (H_2 , He^4 , He^3) belong to another group where $Z_c \geq 0.37$. At this time the binodal opening for quantum liquids is defined by effective compressibility factor $Z^* = Z_c(1 + aB_1)$, where a is some constant, B_1 is the de Boer parameter. We applied the technique in hand to found the critical parameters of several metals (Al, Cu, W, U, Zr), located at high temperatures inaccessible for measurements. Our critical parameters were compared with estimates of other researchers.

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PHASE TRANSITIONS IN METAL CLUSTERS

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We compare the properties of dielectric and metal clusters in a range of the phase transition that is connected with change of the cluster configuration state. Though the configuration degree of freedom is separated from oscillation (thermal) degrees of freedom at low temperatures, nevertheless, the oscillation degrees of freedom give a remarkable contribution to the transition entropy Coexistence of phases [1] for small clusters consisting of a number of atoms below 100 relate also to metal clusters. Separation of the liquid and solid aggregate states in dynamic evaluations of Lennard-Jones clusters allows us to find the temperature dependence of the entropy jump for the phase transition near the melting point. The method of PES (potential energy surface) [2, 3] that is productive for the analysis the properties of dielectric clusters and is suitable also for metal clusters until a

thermal electron energy is small and electron transitions are not essential in phase transitions. It is shown that in contrast to dielectric clusters, where the configuration of atoms for the liquid aggregate state varies weakly with cluster heating, the liquid aggregate state of metal clusters includes many atomic configurations and this configuration mixture depends on the temperature. Nevertheless, though the calculated structure of the solid state of metal atoms depend on used interaction potentials, for all the metal clusters the solid aggregate state exist and it separated from the liquid state by an energetic gap. The contribution to the entropy jump in metal clusters is larger than that for liquid clusters. An additional phenomenon for large metal clusters consisting of hundreds and more atoms, is different temperatures of melting and solidification [4, 5]. This fact is determined by competition of the decahedral and icosahedral cluster structures and also by large times of melting and solidification.

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EOS AND CHEMICAL COMPOSITION IN THE SUN THROUGH THE HELIOSEISMOLOGY

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Advantages of the helioseismology give a new look on physics of the Sun. Evolution of the radial profiles of elemental abundances is the main point of the stellar structure modeling. The principle structure parameters, like helium abundance and entropy of the solar envelope, have been revised with helioseismic tracers. These results essentially based on detailed model an equation of state, while the most recent one is SAHA-S. Expanded version of the EOS allows finding abundances of heavy elements and estimating the Coulomb effect with inverted profile of the adiabatic exponent in the solar envelope.

ELEMENT DIFFUSION DURING EVOLUTION OF THE SUN

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Element diffusion changes the solar chemical composition during evolution. The main effect, barodiffusion, is element segregation due to the force of gravity. Thermal and concentration diffusion are less remarkable, but also considered. The diffusion leads to hydrogen enrichment in the solar envelope and settling of heavier elements towards the solar core. As a result, the Sun convective envelope lost 3.5% of the initial helium abundance and 0.14% of heavier elements (in mass). Additionally, effects of partial ionization and photo-levitation are considered.

NUMERICAL INVESTIGATION OF NUCLEATION IN THE FIRST-ORDER PHASE TRANSITIONS

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First-order phase transitions are prevalent in nature and technique but nucleation kinetics (it's generation kinetics of new phase minimal volumes) was studied with insufficient thoroughness [1, 2]. Nucleuses number evolution is described by analogy with gases kinetic theory. In the issue we have infinite system of ordinary different equations [3]. Using of continuous function of nucleuses dimensions distribution leads to Fokker-Plank equation (it is named Frenkel-Zeldovich equation [4, 5] if we consider nucleation problem). It is known that nucleation problem solution [4] included quasi-equilibrium distribution of precritical dimensions nucleuses is applied for unhurried processes [1].

In present work nucleation different models is considered. Appropriate mathematical problems (they are system of ordinary different equations [3], Fokker-Plank equation and quasi- equilibrium solution [4] of nucleation problem) are solved by numerical methods. Using of implicit finite-difference schemes allows reaching of quasi- stationary nucleation regimes.

Comparison results of different nucleation models solutions are presented. Workability regions of these models are determined.

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OPTICAL VIBRATIONS OF HYDROGEN IN DISORDERED PALLADIUM-GOLD ALLOYS

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In the fcc lattice of palladium, hydrogen occupies octahedral interstitial positions with cubic symmetry. One could therefore expect that in dilute solid H solutions in Pd the fundamental band of optical H vibrations should be reduced to a narrow line of 3-fold degenerate, non-interacting isotropic local oscillators. A few attempts to test this assumption by inelastic neutron scattering (INS) gave ambiguous results due to the very small limiting hydrogen concentration, $x_{max} \leq 0.001$, of the PdH_x solutions at low temperatures [1, 2]. We increased x_{max} by alloying Pd with 20 at% Au and studied disordered Pd_{0.8}Au_{0.2}H_x solutions with concentrations varying from $x = 0.03$ to 0.74. The samples were prepared at hydrogen pressures from 1 bar to 75 kbar.

According to ¹⁹⁷Au Mössbauer studies in [3], hydrogen atoms in the Pd_{0.8}Au_{0.2}H_x solutions with $x \leq (0.8)^6 \approx 0.26$ can only occupy interstices having no Au neighbours. This abates the effect of H-Au interactions in the solutions with lower H concentrations and effectively prevents hydrogen clustering at low temperatures. Our INS investigation at 5K (IN1-BeF spectrometer, ILL, Grenoble) showed that the fundamental optical H band in both concentrated and dilute Pd_{0.8}Au_{0.2}H_x solutions consists of a sharp peak with a broad shoulder towards higher energies. The shoulder shows no tendency to vanish with decreasing H concentration and amounts to approximately 0.44 integral intensity of the main peak in all studied samples. The optical band in infinitely diluted H solutions in Pd should therefore consist of a peak with a pronounced shoulder too.

The shoulder is similar to that observed in palladium hydrides and usually ascribed to strong long-range H-H interactions [4, 5]. As the shoulder

cannot result from H-H interactions in the dilute solutions, other explanations are discussed in the present paper.

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VIBRATIONAL PROPERTIES OF HYDROGEN IMPURITY IN HIGH-PRESSURE PALLADIUM DEUTERIDE

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Local vibrations of a light-atom defect chemically identical to heavy atoms of the host lattice were experimentally studied only once in ref. [1], in which a solid solution of 3.7 at.% H in PdD_{0.6} was investigated by inelastic neutron scattering (INS). The experiment demonstrated the occurrence of a local-mode peak shifted beyond the band of optical vibrations of the D atoms, but no other details of H or D vibrations could be seen because the INS spectrum was broadened due to the non-stoichiometric composition of the deuteride.

Homogeneous samples of stoichiometric PdD and PdH can only be prepared at high pressures. The present work reports on an INS study of three PdD_{1-x}H_x powder samples with $x = 0.05, 0.07$ and 0.09 synthesised in a deuterium-hydrogen atmosphere at $P = 50$ kbar and $T = 600$ K. The samples were prepared at ISSP RAS and studied with the IN1-Bef neutron spectrometer at the Institute Laue-Langevin in Grenoble.

An analysis of the collected INS spectra allowed us to obtain the vibrational spectrum of pure stoichiometric PdD and to isolate the contribution from the H impurity. The latter proved to have a rather unexpected profile. In particular, it showed a negative scattering intensity in the energy range of the main peak of D optical vibrations, and the width of the local-mode peak showed no tendency to vanish with decreasing H concentration in the deuteride.

To ascertain the origin of such an unusual profile, we have also calculated the lattice dynamics for PdD_{1-x}H_x crystals with $x = 0.5, 0.25$ and 0.125 using the Born-von Kàrmàn model with the force constants taken

from [2]. The model successfully reproduced the main features of the H contribution to the INS spectra of the studied samples. The most intriguing negative scattering intensity in the range of the main D optical peak was shown to result from the reduction in the density of states of D vibrations due to the increase in the energy of vibrations of those D atoms that were located near the atoms of H impurity and were partly involved in their motions.

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DYNAMIC CRITICAL BEHAVIOUR OF HEISENBERG MODEL WITH STRONG EASY PLANE ANISOTROPY

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In a modern physics of the condensed state a greater interest arouses study of metal magnetic superlattices. Experimental investigations of such systems encounter the significant difficulties, therefore recently the methods of computational physics have been applied for their studying. In particular, by means of methods of numerical experiment was investigated a static critical behaviour of magnetic superlattices Fe/V. Also it is interesting to investigate the dynamic critical behaviour of magnetic superlattices, which remains unstudied absolutely till now.

We try to apply procedures of critical dynamics investigation of magnetic superlattice Fe₂/V₁₃. We offer a microscopic model of this superlattice where the magnet moments of iron atoms are ordered in plane XY, and the Hamiltonian of such system represents the modified 3D XY-model. As a rule, as a numerical research technique for spin dynamics of magnetic systems is used the method of the molecular (spin) dynamics which is based on the solution of equations of spins motion in a local magnetic field. However in case of magnetic superlattices this method is failure to use directly because of dimensionality misfit of spins.

In this case, for investigation of similar systems offered the special procedure based on a use of 3D Heisenberg model with strong anisotropy of an exchange constant in a z direction. The Hamiltonian of such model is analogous to the Hamiltonian of classical 3D Heisenberg model with one exception: interaction of spin z projections is equal to zero. Lack of

interaction of spins z projections leads to emersion of the strong anisotropy in plane XY that allows to suppose similar character in a behaviour of the such model with classical 3D XY-model.

The approach based on sharing of a Monte-Carlo method and a method of the molecular dynamics is applied to investigate the critical dynamics of Heisenberg models with strong anisotropy. The analysis of the obtained data shown, that Heisenberg model with the strong anisotropy of easy plane type describes both static, and dynamic critical behaviour 3D XY-models and its various alternatives well enough, what allows to use the observed model for study of critical dynamics of magnetic superlattices.

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MAGNETIC ORDERING IN MODEL OF SUPERLATTICE Fe/V WITH THE NEGATIVE INTERLAYER EXCHANGE INTERACTION

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The manipulation by interlayer exchange coupling, magnetoresistance and other magnetic properties of the multilayers via hydrogen adsorption in the non-magnetic layers allows creation of the structures, where the continuous transition from 3-dimensional toward 2-dimension magnetism can be realized experimentally. For simulation of magnetic phase transition in multilayers we suggested a model of superlattice Fe/V. Superlattice Fe/V represents structure where there is an alternation of magnetic (Fe) and nonmagnetic (V) layers. In superlattice Fe/V inside monolayers of iron exchange interaction J_{\parallel} ferromagnetic interaction (an intralayer interaction). Also there is an interaction J_{\perp} between 'iron' layers through layers of vanadium (an interlayer interaction).

One of techniques for modeling and investigations of such superlattices is the Monte-Carlo method. In the given work the iron-vanadium model of a superlattice is offered and results of investigation of magnetic phase transition of this model are resulted by a method of Monte-Carlo. The Hamiltonian of a superlattice model could be presented as

$$H = -\frac{1}{2} \sum_{i,j} J_{\parallel} (S_i^x S_j^x + S_i^y S_j^y) - \frac{1}{2} \sum_{i,k} J_{\perp} (S_i^x S_k^x + S_i^y S_k^y) - m_0 H_0 \sum_i S_i^x, \quad (1)$$

where the first sum took into account an exchange interaction of every iron atoms with all nearest neighbours inside a layer with the exchange interaction J_{\parallel} , the second sum was the contribution to a Hamiltonian of interaction of iron atoms through vanadium layers with an interaction parameter J_{\perp} , H_0 is magnetic field, S were magnetic moments of atoms Fe.

We have calculated spontaneous magnetization, susceptibility and specific heat as functions of the temperature, magnetic field and exchange parameters. In model with two and three layers of iron ($\text{Fe}_2/\text{V}_n/\text{Fe}_3$) are found two maximums of a heat capacity at small values of a relation of interlayer and intralayer exchanges. Temperature dependences of thermodynamic values testify to presence in model of a superlattice $\text{Fe}_2/\text{V}_n/\text{Fe}_3$ of two phase transitions.

The investigation is supported by the Russian Foundation for Basic Research (project N 07-02-00194).

DIMENSIONAL DEPENDENCE OF SURFACE ENERGY OF IONIC DIELECTRIC OF THE NANODIMENSIONAL SCALE

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Essential changes of ionic dielectrics properties of nanodimensional scale, caused by physical features of separate particles, occur at the reduction of sizes of the latter to 100 nanometers. The effects observed in this case explain the influence of the surface on the properties of a crystal. The analysis of physical and chemical properties nanosystems shows, that in this range there is a conditional transitive area of the sizes above which it is possible to speak about the presence of properties of a massive firm body and below which particles possess typical for macromolecules signs.

In ionic dielectrics of the nanodimensional scale all features of superficial conditions are clearly shown as systems the share of superficial atoms can reach several tens percent in such systems. Besides that the, developed surface influences on the lattice and electronic subsystems of the particles, strongly changing the spectra of various excitements, sensitive to the change of symmetry and boundary conditions.

The surface contribution to full thermodynamic potential is noted in the form $4\pi r^2 \sigma$ [1], where b numerical factor considering a deviation of a crystal form from a spherical one.

At transition from the massive condition to nanodimensional the contribution of a surface into free energy increases, and, hence, it is necessary to consider dimensional dependence of surface energy. In the existing models energy is calculated without dimensional dependence.

Dependence of surface energy on the size of a crystal in our model is registered in the form of [2]:

$$\sigma(r) = \sigma_{\infty} \left(1 - \frac{2\delta}{r} \right), \quad (1)$$

where σ_{∞} corresponds to an infinite surface; $\delta = r_e - r$, r_e —radius of equimolecular surfaces.

The necessity of the account of the described dimensional dependence is proved to be true by the fact, that for nanocrystals the specific contribution of superficial energy makes up not less than 30% of full thermodynamic potential [1].

The role of the surface energy for nanodimensional systems is found much more essential, than for the massive objects which properties are basically defined by volume contributions to thermodynamic potential. For nanoparticles the size of the surface contribution is comparable by its size with the volume contribution to the energy of the system that causes unique properties of similar objects.

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EQUATION OF STATE FOR COMPRESSED INERT GASES

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We construct the equation state for argon, krypton, xenon in the range of high pressures until they are dielectrics. At low temperatures they have polycrystal structure [1], and individual clusters-domains in macroscopic compressed inert gases have the face-centered cubic crystal structure at low pressures and hexagonal structure at higher ones. Interaction the system of repelling inert gas atoms is determined by exchange interaction between neighboring atoms due to overlapping of the wave functions of valence electrons. Since this interaction is concentrated mostly near the axis joined interacting atoms, the interaction has the pairwise character, and the total energy of the atomic system may be constructed as a result of pair interactions. The pair interaction potential in a repulsed range with the interaction energy below 1 eV was measured on the basis of elastic scattering of an atomic beam with keV-energies on small angles. We use below the pair interaction potential of inert gas atoms in the case of Ar, Kr and Xe measured in [2, 3, 4, 5].

The pressure in a system of repelling atoms is expressed through the pair interaction of neighboring atoms on the basis of the virial theorem [1, 6], and the connection between the volume per atom and the average distance between neighboring atoms we take in the form [7]. As a result we construct the equation of state as the dependence of the compressed gas on the volume per atom. In the range of pressures below 100 GPa the equation of state with using different pair interaction potentials is compared with experimental data [8, 9].

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HIGH-PRESSURE HYDROGEN HYDRATES

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The occurrence of hydrogen hydrate phases C_1 and C_2 has for the first time been revealed in the high-pressure optical and x-ray studies on the H_2 - H_2O system by Vos et al. [1]. A rhombohedral hydrate (C_1 -phase) described as H-filled ice II with a tentative H_2/H_2O molecular ratio of $X = 1/6$ was shown to form at room temperature and hydrogen pressures above 7.5 kbar, and the formation of another hydrate (C_2 -phase) with a cubic diamond-like H_2O sublattice and $X = 1/1$ was observed at 23 kbar. The occurrence of clathrate hydrate phase stable at hydrogen pressures from 1 to 3.6 kbar was first deduced from the behaviour of the melting curve of H_2O ices [2]. Further neutron diffraction studies showed [3, 4] that this phase has a cubic clathrate structure of the *s*II type with the concentration of the H_2 guest-molecules varying with pressure and temperature from $X = 32/136 \approx 0.235$ to $48/136 \approx 0.353$ [4].

Using volumetric technique, we have studied the transformations and compositions of the hydrogen hydrate phases at pressures up to 5 kbar and temperatures from -36 to $+20^\circ C$. The investigated T - P interval encloses two triple points of phase equilibria among the condensed phases. The clathrate hydrate phase *s*II is shown to be in equilibrium with the low-pressure hexagonal ice I_h and the liquid phase L at $P = 1.07$ kbar and $T = -10^\circ C$. The triple point of the $L + C_1 + s$ II equilibrium is localized at $P = 3.6$ kbar and $T = 1^\circ C$.

According to our volumetric results, the minimum hydrogen content of the *s*II phase is as low as $X \approx 0.200$ along the line of the *s*II $\rightarrow I_h$ transition. Our neutron diffraction investigation showed [5] that $X \approx 0.200$ is the concentration limit of the mechanical stability of the *s*II hydrate.

The H_2/H_2O ratio of this hydrate increases with pressure and reaches $X = 0.207$ at the $L + I_h + sII$ triple point and $X = 0.32$ at the $L + C_1 + sII$ point. The hydrogen content of the C_1 hydrate near the $L + C_1 + sII$ point is close to $X = 0.1$.

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THERMODYNAMIC CHARACTERISTICS OF METALS WITH BASIS ON HARTREE–FOCK–SLATER MODEL

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Some results of modeling of the semiempirical wide-range equation of state of metals, based on the modified Hartree–Fock–Slater model, are presented. The Helmholtz free energy potential is considered of two parts, electronic and ionic components, each of which is divided into cold and thermal energies. The electronic cold component is combined with the ionic cold and thermal contributions in one, that is represented as the analytical formulae with the coefficients, adjusted for the best agreement with experimental data. Thermal electronic component is calculated on the basis of modified Hartree–Fock–Slater model for matter with given temperature and density [1]. At the same time the calculation of discrete, zonal and continuous energy spectrum is performed. The calculated thermodynamic characteristics of aluminum on the Hugoniot of samples with different initial porosities are presented in comparison with experimental data available at high energy densities.

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**ELECTRICAL PROPERTIES OF COPPER
CHALCOGENIDES CuInAsS_3 , CuInAsSe_3 AND CuInSbS_3
AT LOW TEMPERATURES AND HIGH PRESSURES**

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The abstract concerns investigation of the electrical properties of CuInAsS_3 , CuInAsSe_3 and CuInSbS_3 in the temperature range of 78–450 K at pressures 15–45 GPa by the method of impedance spectroscopy. The compounds crystallize in a tetragonal structure. The cell parameters are closed to parameters of CuInSe_2 and CuInS_2 [1] and vary with the atom radius value of V and VI elements.

High pressures have been generated in the cell with synthetic carbonado-type diamond anvils of the “rounded cone-plane” type.

The impedance measurements in the frequency interval of 1–200 kHz were carried out to separate the bulk sample properties (high-frequency part) from the properties at electrode/sample interface (low-frequency part). The temperature dependences of conductivity and permittivity are typical of ionic conductors and semiconductors. In the compound CuInAsSe_3 the maximum on temperature dependence of permittivity was observed in the range 170–220 K and in the same temperature range the change of activation energy was found out. The maximum on temperature dependence of the permittivity in CuInAsSe_3 can be connected to the existence in the material of pyroelectric properties. The similar behavior of the electric characteristics in the ferroelectric CuSnAsSe_3 had been observed [2].

The analysis of hodographs and pressure dependences of the tangent of dielectric losses angle and resistance allowed to conclude that there are noticeable changes of electrical characteristics of the compounds CuInAsS_3 and CuInAsSe_3 at pressures 34–37 GPa. The changes can be connected to the phase transitions at these pressures.

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**CATION CONDUCTANCE OF THE SOME GLASSES
IN SYSTEM Cu-Ag-Ge-As-Se**

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The abstract is devoted to research of the influence of nonstoichiometry and doping on electrical properties of ionic conductor AgGeAsSe_3 [1]. New chalcogenides with general formula $\text{Cu}_{1-x}\text{Ag}_x\text{GeAsSe}_3$, $x = 0.5-0.9$, have been obtained from compound AgGeAsSe_3 by replacement of a part of Ag atoms by Cu atoms. x-ray powder diffraction patterns of compounds are typical for glasses of the systems Ag-Ge-As-S and Ag-Ge-As-Se [2].

The electrical properties of synthesized compounds were investigated by a method of impedance spectroscopy at temperatures 78–400 K with use investigated-analyzer of impedance RLC-2000 in the range of frequencies 1–200 kHz. Impedance measurements were carried out to separate the bulk sample properties (high-frequency part) from the properties at electrode/sample interface (low-frequency part). The boundary frequency increased with the increase of temperature. At the fixed frequencies exceeding boundary the measurements of temperature dependences of conductivity and permittivity were carry out. These dependences are typical for ionic conductors. At 200 kHz the conductivity of a compound with $x = 0.9$ is 0.12 mS/m at 300 K and 6.4 $\mu\text{S}/\text{m}$ at 78 K.

The temperature ranges where the ionic transfer starts is 150–170 K [1], 190–230 K and 225–235 K for compounds $\text{Cu}_{1-x}\text{Ag}_x\text{GeAsSe}_3$ with $x = 1, 0.9$ and 0.8 accordingly. The parts of the ionic conductivity component for a compounds with $x = 0.9$ and 0.8 are not less than 0.9 and 0.48 accordingly. The replacement of a part of silver atoms in the compound AgGeAsSe_3 on copper atoms in a compounds under study results in following: the decrease of the total conductivity and of ionic component of the conductivity, the substantial increase of a relaxation times, the increase of the temperature for the onset of the ionic transport, the decrease of the activation energy.

The researches were supported in part by RFBR grant No. 06-02-16492.

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**THE SIZE EFFECTS OF THE METALLIZATION
PRESSURE OF ALKALI-HALIDE CRYSTALS WITH
SMALL DIMENSIONS**

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Transition of the dielectric into a metallized state occurs when the degree of crystal compression ensures the equality of the thermodynamic potentials of both phases [1].

Here, in order to calculate the pressure of an omni-directional compression at which the dielectric is expected to be metallized, we use an electron-statistical model in the formalism of the density-functional method [2]. We proceed from the model of an ideal crystal lattice with a CsCl-type structure (B2 structure) consisting of unlike point charges [2]. The temperature is assumed to be absolute zero.

The thermodynamic potential of the dielectric phase of an ion crystal is written in the form:

$$G_{B_i} = \sum_{k=1}^7 N_k^{(i)} U_k^{(i)}(a_k^{(i)} R^{(i)}) - V^{(i)} \frac{\partial}{\partial V^{(i)}} \left[\sum_{k=1}^7 N_k^{(i)} U_k^{(i)}(a_k^{(i)} R^{(i)}) \right] - \frac{\alpha_\mu^{(i)}}{R^{(i)}} + 2\pi r^2 k n_0(hkl) \sum_i \left(\beta^{(i)} - 1 \right) W_\infty^{(i)}, \quad (1)$$

where $\alpha_\mu^{(i)} = 1.76268$ is the Madelung constant of the B2-structure and $U_k^{(i)}(a_k^{(i)} R^{(i)})$ is the potential of the interaction of ion pairs, obtained by a self-consistent calculation within the framework of the theory of an inhomogeneous electron gas [2].

At a zero external pressure, a structure of the NaCl-type (B1) is stable. As the pressure increase and the polymorphic transition point is attained, a phase transition to a structure of the CsCl-type (B2) takes place. Within a small vicinity of the metallization pressure p_{met} the thermodynamic potentials of the dielectric and metallization phase are equal, and, with a further rise in the pressure, the metallization phase becomes more stable. In the further analysis, phase 1 refers to a dielectric phase with the CsCl-type structure and phase 2 is a metallized crystal state. It was assumed in the calculation that the surface of phase 1 bounded by a (110) face with a minimal surface-energy value. Its thermodynamic potential was calculated using formula (1) for $T = 0$ K. The thermodynamic potential

of the metallization phase is calculated using the Gombas model [1] (for bulk part), which satisfactorily describes the properties of alkali metals, and the “jelly” model [1, 2] (for calculating the surface contribution to the potential).

We obtained the metallization pressures for several alkali halide crystal.

In study of the pressure of a polymorphic transformation as a function of crystal size, the anomalous behavior of LiF was discovered [1]: in contrast to other alkali-halide crystals, as the size of a LiF crystal diminishes, the pressure polymorphic transformation decreases rather than rises. This is explained by the fact that this compound in the B2-structure (a CsCl-type lattice) has a lower surface energy than in the B1-structure (a NaCl-type lattice). Therefore, taking account the surface contribution to the thermodynamic potential of the crystal “promotes” the phase transition by reducing the pressure of the polymorphic transformation. However, during the insulator-metal transition, the LiF crystal behaves similarly to other alkali-halide compounds; i.e., the metallization pressure increases with a decrease in the sample size.

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PHASE TRANSITION DIELECTRIC–METAL IN MASSIVE ALKALI-HALIDE CRYSTALS IN THE CONDITIONS OF HYDROSTATIC COMPRESSION

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Structure like NaCl (B1) is stable for ionic crystals when outer pressure is equal to zero. Then, after achieving polymorphous transformation point phase transition is carried out to the structure like CsCl (B2-structure). And as for small metallization pressure vicinity p_m thermodynamic potential of dielectric and metalized phases are equal. By further increase of pressure metalized phase becomes more stable. Within the limits of functional destiny method calculation of comprehensive compression pressure was carried out. Supposition of even distribution of electronic gas in the first place is suitable for alkali metals. According to this model simplest metals have a lattice built of statistically positive metal ions and evenly

distributed electronic gas of valent electrons conductance. Gombash [1] model is used for the calculation of thermodynamic potentials of metalized phase and it describes alkali metals properties. Ionic crystal dielectric phase model is expounded in work [2]. It leads to metallization of dielectric. Minimizing thermodynamic potentials of both phases determined by metallization pressure for a number of alkali-halide crystals. Metallization pressure is calculated for massive alkali halide crystals with 0 K temperature.

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**THE THIRD, MOLECULAR, FORM
OF CARBON—FULLERENES, FULLERITES
AND FULLERIDES. PRE-HISTORY, DISCOVERY
AND PHYSICAL PROPERTIES**

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A brief review is being done on the pre-history [1–3] and discovery [4] of fullerenes that make the third, molecular form of carbon. Higher and smaller fullerenes. A family of fullerenes. The elaboration of methods for the production, separation and deep purification of fullerenes in quantities enough for growing crystals of macroscopic sizes [5]. Fullerites and fullerides. Superconductivity of fullerides. Intermolecular forces in fullerites. The Girifalco potential is presented for eight orientationally disordered phases of fullerites from C₂₈ to C₉₆ and its generalization is made for the interactions between the different fullerene molecules, C_m and C_n. The thermodynamic properties of the high-temperature modifications of a family of the fullerites, from C₃₆ up to the C₉₆, calculated [6] in equilibrium with their saturated vapors on the basis of the correlative method of the unsymmetrized self-consistent field that enables one to take into account the strong anharmonicity of the lattice vibrations, are discussed. The calculations were accomplished up to the temperature of loss of stability (spinodal point) T_s . The behavior of some characteristics is considered in their dependence on the number of atoms in the molecule.

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INVESTIGATION OF THE LIQUID CARBON: NEW APPROACH AND FUNDAMENTAL RESULTS

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The main results of the experimental studies of liquid carbon during the past five years are reviewed in this work. We consider methods for determining the melting temperature of graphite, carbon vapor pressure, pressure p_{tp} in the triple point of liquid carbon, contact angle (liquid carbon (LC)–graphite) and anisotropy of the graphite various edges wetting by liquid, numerical values of the variables are presented here too.

Crystallization (at speeds 10^6 K/s) of metastable non-graphite tetragonal and linear-chain forms from LC conserved under normal conditions has been considered. Registration of the laser induced periodical surface structures (LIPSS) was the evidence of graphite melting.

In this work we discuss the features of plasto-elastic deformation of graphite at high temperatures. Screw dislocations generate non-finished growth steps that result in the growth of graphite from the vapor. Step morphology analysis gave an opportunity to find difference between the mechanisms vapor-solid and vapor-liquid-solid.

We also considered growth capability of new carbon structures, such as carbon nanotubes, carbon ribs, graphene-like structures, and atomic-smooth surfaces of graphite from high pressure ($p \geq p_{tp}$) vapor. Produced structures are compared with the forms known to be the result of natural metamorphism and alternative synthesis methods. Feasible fields of application of the received results and structures are under consideration.

STRUCTURE OF NON-GRAPHITE CARBON PHASES QUENCHED FROM LIQUID CARBON

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Liquid carbon structure near the triple point (TP) solid-liquid-vapor is not experimentally investigated virtually. In experiments at $p < 400$ MPa the density of the liquid carbon (LC) was observed to be about 1.2 g/cm^3 [1] (e.g. graphite density 2.25 g/cm^3). MD-simulations indicate that liquid carbon of such density should have mainly carbene-like short-range order [2]. Experimentally revealed that low density LC has mainly conjugated bonds between carbon atoms[3].

This paper focuses primarily on investigation of the structure of non-graphite carbon phases (NGCP), quenched from LC. It is known that ultraspeed quenching ($V \approx 10^{13}$ K/s) results in amorphous structure [4], while quasi-equilibrium chilling results in hexagonal graphite equilibrium structure. Crystal structure of NGCP is supposed to be the result of high-velocity quenching ($V = 10^5 - 10^8$ K/s) under the condition of such phases critical nuclei presence. Earlier high-velocity quenching ($V = 10^6 - 10^8$ K/s) phases of monoclinic and cubic systems with a stability under normal conditions were obtained from ethylene plasma.

In this work the required quenching velocity ($V \sim 10^6$ K/s) was obtained using HOPG sample pulse laser ($\lambda = 1.06 \mu\text{m}$) heating in the helium chamber with the pressure $p > p_{TP}$. Generation of the laser induced periodical ($\delta \approx \lambda$) surface structure (LIPSS) in the crater, formed after pulse laser heating was the evidence of the liquid phase presence. NGCP's structure in the crater surface area was investigated with Raman scattering, microdiffraction and energy dispersive spectrometry. Quenched carbon was revealed to have high temperature treatment hybrid glass-like carbon (GLC) structure with inclusions of crystal chaoit and body-centered cubic (bcc) array of C8, which is denser than a diamond. Earlier hybrid phases of GLC and C8 as possible forms of LC crystallization were not considered.

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DETERMINATION OF THE CONTACT ANGLE: LIQUID CARBON AND GRAPHITE

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The contact angle Θ data characterizing the wetting of graphite by liquid carbon turned out to be absent. This paper focuses primarily on the definition of the Θ using sessile drop method [1].

This method is based on the determination of the drop form lying on the structural supporting material. The conditions of the drop formation on the atomic-smooth graphite layer (001) have been considered in [2]. Since it seems to be impossible to investigate liquid carbon drop in-situ, frozen drop profile data were used. Profile of such drops (15–60 nm in diameter) was determined with atom-force microscope Veeco diMultimode V using cantilever FESP (tip ROC ≤ 10 nm). Drop profile image array analysis showed that all drops have spherical shapes and for small drop, when it can be considered a part of a sphere, parameter Θ can be determined by formula

$$\tan \frac{\Theta}{2} = \frac{h}{r},$$

where h is the height and r is the radius of the drop base [1].

The mean value $\Theta=(21\pm 5)^\circ$ of twenty drop data array was determined in case of amorphous carbon final state, while in case of graphite final state (graphite density 2.25 g/cm^3) there was made shrinkage correction: $\Theta=(39\pm 8)^\circ$. Frozen drop shrinkage was taken into account under the assumption of the drop spherical shape with constant mass and radius of the base. The calculated data indicate low lyophilic behavior of the carbon surface (with respect to LC) and are in good agreement with data for germanium ($\Theta=30^\circ$). Large value of Θ was colligated with the Ge crystal cross-linked structure.

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VAPOR-CRYSTAL AND VAPOR-LIQUID-CRYSTAL GRAPHITE GROWTH MECHANISMS

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In the present work we discuss the difference in the manifestation of graphite stepwise growth mechanisms vapor-liquid-crystal (VLC) and vapor-crystal (VC). Step-ended terraces with attached growing units were formed under the conditions of such growth.

VC: no drops are observed and terraces are covered with multiple screw dislocations. Dislocation formation is the result of the interaction of the solid growth steps among themselves or the steps with solid particles, adsorbed on steps.

VLC: growth occurs through a liquid drop on the growth steps and terraces remain atomic smooth. Collisions of wetted steps or steps with solid particles are not accompanied by the formation of defects.

Extended position derived from atomic-force microscopy research of the graphite layer-spiral vicinal growth hillock (VGH) resulted from HOPG samples pulse laser heating in the helium high-pressure chamber. After heating typical thermo-deformation surface topography and VGH were observed on the periphery of the crater. According to Frank theory VGH formation is known to be the result of the plastic deformation of the non-finished growth step. The step, being surrounded by supersaturated vapor, produces VGH growth initiation on the periphery of the crater where the maximum of the overcooling exists. The VLC mechanism manifestations on VGH were observed under $p_{He} = 11.2$ MPa, while the VC mechanism manifestations—at $p_{He} = 9$ MPa.

DEVELOPMENT OF PROCEDURES AND AN EXPERIMENTAL STUDY OF PHASE TRANSFORMATIONS ON THE SURFACE OF GRAPHITE AT TEMPERATURES UP TO 3.3 kK

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It is known that the methods of productions of the nanostructural formations may be accepted as the basis for their classification. This requires

the concentration of primary attention in development and creation of the methods of effective production and investigation of the structural states of the different classes of the nanophase.

The methods of production of the nanostructures are quite diverse. For obtaining the carbonic nanotubes the some other procedures may be regarded as quite promising. The famous method of synthesis of nanotubes is based on the using of an arc discharge with the graphite electrodes. The other methods are the ablation of graphite with the aid of the laser irradiation in an atmosphere of buffer gas and the catalytic decomposition of hydrocarbons on the surface of metallic catalyst.

In this work the combined method is proposed to use for the generation of the nanostructures of carbon. During the first stage the usual volume heating of the sample by direct current is used to obtain the temperatures about 3 kK. On the second stage the further heating of the carbon surface is provided by the arc discharge. The considered procedure allows using advantage of the combination of low-temperature Joule heating and high-temperature arc discharge. In addition it proposes to use preliminary treatment of the samples by the electron and proton beams having energy about 50–100 keV.

The Joule heating of cylindrical samples with a diameter of 3 mm was provided in a atmosphere of argon at a pressure 30–90 kPa. The time of holding of samples at a temperature of 2.5–3 kK was about 10–300 min. The structural analysis of surface after the heating showed the presence of the nano-dimensional phases of diamond and carbyne.

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PHYSICAL SYNTHESIS OF CARBINE. THERMODYNAMIC BACKGROUND, CHALLENGES, AND RESULTS

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The thermodynamic background of the physical synthesis of carbine consists in the carbon phase diagram where the phase states are defined by the carbon heating and cooling rates. According to that phase diagram, the carbine synthesis may be produced by the carbon vapor condensation on a substrate within the temperature range of about 3200 to 3700 K; by the liquid carbon crystallization within the temperature range of about 3800

to 4600 K and within the pressure range of 1 to 100 atm, respectively. The main challenge in the way of the carbide production from the liquid carbon phase under the local heating by the laser ray, the electron beam, etc. of the initial carbon-graphite material is the heterogeneous crystallization that should cause the carbide production within the melt zone. On the base of the carbon phase diagram and with account for the characteristic time intervals of the phase transitions, the carbide production methods may be developed that are absent in the nature. Different research teams when trying to physically synthesize the carbide obtain a number of such modifications.

THERMODYNAMICALLY NON-EQUILIBRIUM MATERIAL

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To develop the materials where the particle dimensions are comparable to and even less than the correlation scale of the energy and particle transfer in the microscopic materials is one of the main problems now. The ultra-disperse particle UDP creation is aimed at this problem solution. That is, the thermodynamic state of individual UDPs should, by definition, differ essentially from the thermodynamic equilibrium state of the substance from which these particles are produced. The thermodynamic non-equilibrium of the UDPs is supposed to govern, to a large extent, the physical properties of the compact materials CM made of these UDPs. Yet, the method of the CM production from the UDPs pressing provides the thermal and the electric contacts between the particles composing of one and the same chemical substance; yet, it neutralizes the non-equilibrium peculiar to the separate particles. The present work reports on synthesis of two- and three-component composite metallic particles of about 100 nm in diameter. The three-component particles and the compact material produced at this base show a number of properties that are evidence of the fact that the thermodynamic equilibrium is not realized in this material. The arbitrary in time fluctuations of the compact material electric resistance is the most interesting above property. The resistance fluctuation distribution against its averaged value is close to the Gauss one.

SYNTHESIS OF THE NEW CARBON MODIFICATION BY QUENCHING CARBON VAPOR AND CONDENSED PARTICLES IN ARGON ATMOSPHERE

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The phase state of carbon-graphite materials versus their heating and cooling rate and sufficiently long-time phase transitions for liquid carbon→carbine and carbine→graphite allow to obtain new modifications of carbon. These modifications are quenched liquid carbon or carbine with partially or fully preserved structure. The present work is the first where the cooling rate of carbon vapor (the evaporated material is graphite) and condensed particles in argon under pressure of 1 atm was carried out on the level of 10^6 K/c and carbon nanoparticles with physical and chemical properties different from graphite were obtained. Particularly, the typical example of such a mismatch of properties is the thermal decomposition kinetics of obtained samples. The decomposition reaction was investigated by the derivatography analysis in the atmosphere of nitrogen or air. The material revealed the significant mass loss under conditions of analysis. The insignificant mass loss was observed at the temperature range of 100–300°C (the conversion level was no more than 0.15). It was obviously connected with the desorption of substances adsorbed by material, for example, with the desorption of water. In the oxidation atmosphere the material started to react with oxygen at the temperature up to 500°C. Then, the mass of the sample was stable. In this relation the material behaves as carbon black oxidizing at the temperature above 450°C. Apparently, that was the only difference between carbon black and the investigated material. The decomposition of carbon material in the inert atmosphere at the temperature higher than 500°C was the most interesting fact. This is unlike the most pure carbon materials. Probably, this fact was connected either with the presence of heteroatoms in macromolecules of the substance or with the major part of the relatively weak single carbon-carbon bonds generated along with the triple bond in the alpha-carbine molecule.

STATE EQUATION OF KRYPTON AND XENON ON THE GRAPHITE SURFACE

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A krypton monolayer, based on the graphite surface, is of interest as a two dimensional system with wide variety of surface structures and phase transitions between them [1], [2].

We have obtained a state equation of krypton and xenon on the graphite surface by means of the method utilizing the radial distribution function $f(r)$ satisfying the equation

$$\beta P = \frac{1}{v} - \frac{\pi\beta}{2v^2} \int_0^\infty f(r) \frac{du(r)}{dr} r^2 dr, \quad (1)$$

where $u(r)$ is an interatomic potential, $\beta = 1/kT$, T is the absolute system temperature, $v = V/N$ is the volume per particle, N is the number of particles, k is the Boltzman constant.

The radial distribution function $f(r)$ has been found by the method of molecular dynamics for different values of the system density. Inserting the obtained radial function into the equation above we obtain the state equation, which can be approximated by the Van der Waals expression

$$\left(P + \frac{a}{v^2}\right)(v - b) = \frac{kT}{\varepsilon}, \quad (2)$$

where the pressure is given in the units of $P_0 = \varepsilon/l^2$, l is the characteristic size, which in our case is equal to $l = 1 \text{ \AA}$. Parameters a and b are defined by fitting the results of computer simulation with equation for $f(r)$ given above. This gives the values $a = 6.33 \text{ \AA}^4$, $b = 6.41 \text{ \AA}^2$. The corresponding critical temperature of krypton monolayer is equal to $T = 48.3 \pm 0.5 K$.

The temperature interval has been found within which the phase commensurate with the substrate is realized: $\sqrt{3} \times \sqrt{3} R 30^0$. The dependence of internal energy on temperature (i.e. the thermal state equation) has been calculated.

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SCALING MODELS OF THE SATURATION PRESSURE IN THE CRITICAL REGION: POSSIBILITIES AND LIMITS

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Theoretical models of properties, F = (the pressure, P_s , the densities, ρ_l , ρ_g , the order parameter, f_s , the coexistence curve diameter, f_d) are analyzed in the work, among them equations suggested by Landau, 1972, Anisimov, 1990, Abdulagatov, 2007, et al. They are taken to compare with reliable experimental data of several substances (HFC 134a, HFC 143a, HFC 236ea, H₂O, NH₃, alcohols). One more analytical form of F is considered. It has a combined structure with scaling and regular parts

$$F(\tau, D, B) = F(\tau, D, B)_{scale} + F(\tau, B)_{reg}. \quad (1)$$

This Model of P_s is written as

$$\ln(P_s/P_c) = B_1\tau^{(2-\alpha)} + B_2\tau^{(2-\alpha+\Delta)} + B_3\tau^{(2-\alpha+2\Delta)} + \\ B_4\tau + B_5\tau^5 + B_6\tau^7 + B_7\tau^9. \quad (2)$$

here $D = (\alpha, \Delta, T_c, P_c)$ —critical characteristics, $\tau = 1 - T/T_c$ —a relative distance of T from the critical temperature, T_c , B —amplitudes. Model is got by the authors [1]. The degree laws of the scaling theory were taken into account to express F_{scale} . Adjustable coefficients, B , D , of the Model (1, 2) have to be determined by fitting F to the input data sets those are formed in the temperature interval from the triple point T_{tr} up to the critical value T_c and include reliable experimental results. Criteria, S1, S2, Sc, are taken into account: S1 represents a RMS deviation of measured F_{exp} values from F_{scale} in the critical region, $\tau=(0 \dots 0.1)$, S2 represents a RMS deviation of measured data from P_s (2). A compromise criterion Sc is chosen as a middle value of S1 and S2. A routine is elaborated to calculate coefficients B and characteristics D of the Model.

Our tests have shown that it is possible to find an optimal realization, $F_{opt} = f(D_{opt}, B_{opt}, \tau)$, and to reduce a start value of Sc. The combined Models of P_s are built for HFC 134a, HFC 143a, HFC 236ea, H₂O, NH₃ and alcohols. Calculated results correlate with the measured data in acceptable limits of an experimental accuracy in the interval ($T_{tr} \dots T_c$). A characteristic, $D_{opt} = \alpha$, is placed not far from theoretical value. A computer code (ThermoData Engine NIST/TRC) was implemented to test

the input data sets and calculated thermodynamic properties of the substances.

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PECULIARITY OF SURFACE MELTING OF Al AND Fe AT HIGH PRESSURE

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We present the results of molecular dynamic simulation of the surface melting of Fe and Al at the contact with Ar at high pressure. This report focuses on the role that premelting plays in the surface melting of metals. This phenomenon is studied for melting in vacuum generally. It is not enough information on premelting at contact to other substance. The surface atoms make a transition to disordered state although temperature of system still corresponds to the crystal phase. In such condition the surface layer possesses characteristics of a liquid. In particular property of fluidity is occurred, and the surface gets ability to be deformed [1]. The temperature interval of premelting of Fe is comparable in magnitude with the difference between the melting temperature obtained as a result of shock and static measurements [2].

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DENSITY FLUCTUATIONS AND THE KINETIC SPINODAL IN A SIMPLE LIQUID

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A key property of a particular substance is its phases' stability boundaries. Estimations of the position of the spinodal were performed via various experimental and theoretical approaches. In this work an effect of the thermodynamical density fluctuations on the position of the liquid-vapor spinodal is discussed in the case of simple liquid.

Regularities appearing in the fluctuation spectra of Lennard-Jones liquid during an advancement to the stability boundaries are investigated through an analysis of molecular dynamics simulation data. A method of dynamical structure factor calculation based on molecular dynamics trajectory processing is developed [1]. The results for calculations of density fluctuations spectra in various stable and metastable liquid states are presented. It is shown that for long waves there is a peak in the spectrum at certain value of frequency ω_s , that is corresponding to the speed of long-wave collective oscillations of particles (in other words, speed of sound) [2]. Dispersion relations for sound waves are plotted. The results show that these relations exist only for long waves. A break of dispersion curves in transition to short waves is due to the decay of wave on density fluctuations, sizes of which l are of the same order (or maybe one order less) than the wavelength [3]. An analysis of the results shows that sizes of density inhomogeneities grow up with an increase of metastability. Therewith, the critical nucleus size r_{cr} decreases. This fact allows to assume that in advancement to the metastable area a state is achieved, at which the characteristic size of density fluctuations becomes equal to the critical nucleus size. We can expect that this state corresponds to the kinetic spinodal because nucleation frequency subject to this proviso is actually the frequency of particle oscillations in liquid. On the basis of this hypothesis location of the kinetic liquid-vapor spinodal on the phase diagram of Lennard-Jones system is determined.

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MODELLING OF METHANE HYDRATES USING MOLECULAR DYNAMICS

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Methane hydrates are the crystalline structures formed by water and methane with methane concentration hundreds times higher than it is in a water solution. These compounds are considered as a perspective fuel source that by some estimations can give two times more energy than other fossil fuels [1].

In this work we study the equation of state and mechanical properties of sI methane hydrate structure. The model of a cubic unit cell of the sI structure was created that consists of two dodecahedrons (5^{12}) and 6 tetrakaidecahedrons ($5^{12}6^2$) with shared faces and O atoms are placed in vertexes. The SPC/E and TIP4P potentials were used for water and a united-atom potential was chosen for methane molecule [2]. The range of temperatures and pressures resulting in a spontaneous decay of the sI structure were determined. The kinetics of the decay process was described.

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MOLECULAR DYNAMICS SIMULATION OF THE ELECTROCHEMICAL INTERFACE BETWEEN GRAPHITE SURFACE AND IONIC LIQUID [BMIM][PF₆]

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Electrochemical supercapacitors have received much attention due to their possible application as high-power energy-storage devices utilized in portable electronics, electric vehicles, fuel cell based power plants. Ionic liquids (ILs) are now considered as an alternative electrolyte for supercapacitors, since they exhibit wide electrochemical windows, high thermal stability and low melting points.

An operating efficiency of supercapacitors is greatly influenced by the molecular structure of the electrode/electrolyte interface. However, an electrical double layer in ILs has not yet adequately explored. To enhance the performance of supercapacitors it is necessary to understand the ILs behavior at the interface.

A major goal of this research was to investigate the double layer in ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate [BMIM][PF₆] at the graphite surface by the molecular dynamics simulation.

A classical force field for the [BMIM][PF₆] has been developed and successfully tested against experimental data. The structure of the double layer in [BMIM][PF₆] near a basal plane of graphite was investigated for the first time. The variations of the relative mass density, volume charge density and concentrations of different atoms along the normal to the graphite surface have been determined.

The influence of the electrode (graphite surface) potential on the volume charge density and electric potential profiles in an electrolyte was studied.

The simulation shows that ionic liquid has well-ordered layering structure at the surface. It has been established that in the event of an uncharged surface the imidazolium ring in the [BMIM]⁺ cation tends to be arranged in parallel to the graphite surface at a distance of 0.35 nm. The [PF₆]⁻ anion in the first adsorption layer is so oriented that phosphorus atom is at a distance of 4.2 nm from the surface and triplets of fluorine atoms form two planes parallel to the graphite surface.

We would like to acknowledge the Joint Supercomputer Center of RAS for the computational resources placed at our disposal.

EXPERIMENTAL STUDY OF THERMODYNAMIC PROPERTIES OF CONSTRUCTION MATERIALS WITH THE METHOD OF SUBSECOND RESISTIVE HEATING

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High-speed (subsecond) resistive heating is an effective instrument for study thermodynamic, optical and electrical properties of electroconductive materials. Strict mathematic model of this process have to register the power of radiation losses from sample surface. In this paper the method of experimental getting the emittance (emissivity factor) using two phases of thermal history is described. It is possible to find the numerical values

of emittance and their changes with time in conduction of correct temperature measure. The difficult of this purpose is the changing of the sample properties in the process of high-speed heating (10^3 – 10^5 K/s) and following cooling of the sample.

The results of studied properties of technical titanium (VT1-0) are presented in this paper. There is analysis of the obtained data of temperature dependence of the heat capacity, electroconductivity, emissivity factor and enthalpy in this paper.

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USE OF PHYSICAL MODELS FOR EXPERIMENTAL RATINGS OF PROTECTIVE PROPERTIES OF ENGINEERING

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The physical models of radiating fields are widely used in various areas of scientific researches, including for an experimental rating of protective properties of mobile engineering from penetrating radiations influencing engineering in extreme situations (at nuclear explosions or radiating failures) [1].

It is known [2], that radiation at the certain levels of influence can cause damage of the electronic equipment or irradiation of crew over allowable norms which are taking place inside mobile engineering. First of all it concerns to military engineering, and also to engineering used for liquidation of consequences of radiating failures on nuclear objects. Before acceptance in operation samples of this engineering are tested to influence of gamma-ray and neutron radiations. Thus the technical protective characteristics of a tested sample are estimated. Most correctly protective properties of engineering can be estimated by an experimental way in modelling fields

of radiations research reactors on fast neutrons, the physical processes and parameters of radiations in which are similar to processes at nuclear explosions or radiating failures.

Controllable parameters of radiations in a modelling field are the power and angular characteristics, and also relation of a doze of neutrons to a doze of gamma radiation in places of realization of tests. At reproduction of these parameters in a modelling field the results of tests can be transferred on conditions of influence of radiations at an extreme situation without adjusting factors.

In the present work the physical model of formation of a field of radiation of nuclear explosion on open district with use mobile research reactors PRIZ is considered. The parameters of radiations in a modelling field and algorithm of definition of the technical protective characteristics of tested engineering are analyzed.

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MODELING INTERFACIAL PHENOMENA IN MULTICOMPONENT MIXTURES USING GRADIENT TERMS INTRODUCED IN FREE ENERGY

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A method to model dynamics of multiphase multicomponent liquid mixtures, called density functional method, is considered. According to this approach, state of the mixture is described by continuous fields of component molar densities, while interfacial boundaries are smoothed. In order to describe interfacial static and dynamic phenomena including surface tension, specific free energy is assumed to be a function of not only component molar densities, but also of their gradients. In this way free energy becomes a functional of component density fields. Introduction of gradient terms allows one to account for non-local contributions to the energy, which depends not only on mixture composition in the point, but on the composition in the neighborhood as well. Gradient terms are significant only inside boundary regions between liquid phases, thus representing the interfacial energy. From the variational principle for the free energy, an expression for static stress tensor in a medium with variable

composition is derived. This static stress tensor is then supplemented by the Navier-Stokes viscous stress tensor, and the total stress tensor is put into the momentum balance equation. Also, the generalized Fick's law for diffusion fluxes is used to close the model. Some numerical results and comparison with experimental data are presented.

**WIGNER REPRESENTATION OF QUANTUM
MECHANICS AND CONDUCTIVITY OF DENSE
HYDROGEN PLASMA**

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Combining both molecular dynamics and Monte Carlo methods for solving the integral Wigner-Liouville equation we calculate the temporal momentum-momentum correlation functions and their frequency-domain Fourier transforms. Alternatively, at low temperature we use the density functional theory and the Greenwood formula to obtain frequency-dependent electrical conductivity. In the canonical ensemble at finite temperature for weakly coupled plasmas the obtained numerical results agree well with the Drude approximation. The growth of coupling parameter results in strong deviation of the frequency dependent conductivity and permittivity from low density and high temperature approximations. In particular, slowly-damping oscillations on the momentum-momentum temporary correlation functions can be observed, and the transparency window appears on the dependencies of electrical conductivity on frequency.

**PLASMA POLARIZATION IN MASSIVE ASTROPHYSICAL
OBJECTS**

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We discuss macroscopic plasma polarization created in massive astrophysical bodies by gravitation and other inertial forces. It creates quasi-stationary electrostatic field of the same order (counted per one proton) as the force, which gives rise to this polarization, in particular gravitation. This effect was established long ago by Pannekoek and Rosseland (1922-1924) for the case of ideal, isothermal and non-degenerated plasma in outer layers of a star. Their approach based on solution of several separate (“individual”) equations of hydrostatic equilibrium for partial pressures for each species of particles. This approach was extrapolated later (see for

example, Bilsten et al.) on dense and degenerated interiors of compact stars. Present work presumes non-correctness of this extrapolation. We consider generalized multi-component density functional approach combined with simplified local densities approximation for separate densities of positive and negative charged species. The resulting extremum condition for thermodynamic potential corresponds to equivalent condition for generalized (electro-)chemical potential and/or condition of equilibrium for all the forces acting on the charged particles. In this latter form new non-traditional “non-ideality force” due to strong Coulomb non-ideality is added to two traditionally competing forces: gravitational and electrostatic ones. Present approach leads to final expression for average electrostatic field, which does not restricted by condition of ideal and non-degenerated plasmas. Presently the effect of non-isothermality, magnetic field influence and relativistic effects are not taken into account. The resulting formula in present work reproduces two known limiting cases: for degenerated and non-degenerated ideal gas and leads to additional effects. The most interesting sequences of these effects on structure, thermo- and hydrodynamics of a star are under discussion.

DIAGNOSTICS OF DENSE COULOMB SYSTEMS VIA TRANSPORT AND OPTICAL PROPERTIES

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Transport and optical properties of Coulomb systems are described by the dielectric function, which is related to correlation functions such as density-density, current-current, or force-force correlation functions [1]. Therefore, deduction of plasma parameters from such quantities as the reflectivity, absorption, thermoelectric properties or spectral line shapes is investigated. We will compare theoretical calculations and experimental results. Central quantity of interest is the free electron density since it can't be measured directly but is crucial for the plasma properties.

For the evaluation of equilibrium auto-correlation functions at arbitrary coupling strength we can apply MD simulation techniques for classical systems. Using pseudopotentials in order to mimic quantum effects, correlation functions are evaluated for bulk systems and finite clusters [2, 3]. We find a more structured frequency spectrum of plasma correlations in

clusters indicating several collective modes. Size effects have been found for the damping of plasma oscillations [3, 4].

Alternatively, analytical calculations for quantum systems can be performed in the weak coupling region. The dynamical collision frequency for bulk systems is evaluated in different approximations systematically and consistently by including strong collisions, dynamical screening, electron-electron interactions and effects due to partial ionization in the plasma state [1]. Good agreement is found with MD simulations [2].

Using the concept of dynamical collision frequency, the influence of collisions on different optical and transport properties such as absorption and reflection in plasmas, Thomson scattering, static and dynamic conductivity has been considered. In particular we will reconsider the dc-conductivity in inert gases [5] and, in this context, discuss the so-called Coulomb contribution [6].

We also investigated the influence of the plasma environment on spectral line shapes [7, 8]. The features of x-ray spectral lines are relevant for diagnostics of warm dense matter. Hence, K-line profiles have been investigated by irradiation of solid targets with intense ultra-short pulse laser beams [9, 10]. The emitted K-spectra of sparsely ionized radiators can be used to determine plasma parameters and fields of target regions beneath the laser created hot plasma layer.

In conclusion, improving the RPA dielectric function, collisions prove to be of relevance in strongly coupled plasmas. In the context of the analysis of experiments, those can be seen as diagnostic tools for the free electron density in plasma systems. Further work is necessary for a more consistent description of frequency dependent properties of partially ionized plasmas.

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THE ANGULAR DEPENDENCE OF S- AND P-POLARIZED REFLECTIVITIES OF EXPLOSIVELY DRIVEN DENSE PLASMA

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The investigation of properties of the electronic subsystem in a strongly correlated plasma remains an ongoing problem in the physics of high density energy. The analysis of the response of dense plasma to electromagnetic waves of moderate intensity, e.g. via transport properties, can be used as a tool to investigate the validity of the physical models describing the behavior of matter under extreme conditions, high temperatures and pressures. However, to interpret correctly the results of reflectivity measurements it is necessary to know parameters of a transitive plasma layer. Angular dependence of s- and p-polarized reflectivities at several wavelengths can be used in the integration of Maxwell equations to construct the spatial profile of the density of charge carriers.

The results of first experiments on reflectivity of polarized light on explosively driven dense xenon plasma is presented. The study of polarized reflectivity properties of plasma was accomplished using laser light of wavelength $\lambda_{prob.} = 1064$ nm and at incident angles $\theta = 0 - 40$ degrees. With density $\rho = 2.7$ g/cm³, pressures $P = 10.5$ 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 $\Gamma = 2.0$) were present. To measure the dense xenon plasma polarized reflectivity coefficient, the pulsed Y₃Al₅O₁₂:Nd³⁺-laser system and four-channel high-speed polarimeter have been used. 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 [1]. The integration of Maxwell equations was based on an interpolation formula for dc conductivity, obtained from a systematic quantum statistical treatment of different limiting cases.

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DYNAMICAL COLLISION FREQUENCY IN WARM DENSE MATTER

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The dynamical collision frequency is the central quantity for calculating the dielectric function in warm dense matter. In particular, we are interested in static transport properties, e.g. dc-conductivity, and optical properties, e.g. reflectivity [1]. The description over a wide parameter region of the plasma's temperature, density, ionization degree and frequency is subject of current research.

Based on a generalized linear response theory, the dynamical collision frequency has been calculated in different approximations. Within the Gould-deWitt approach, dynamical screening and strong collisions have been taken into account [2, 3].

We discuss interpolational expressions for the dynamical collision frequency from its respective limiting cases over a wide parameter range and present exemplary results for optical frequencies.

Additionally, we compare the influence of these approximations on the dielectric function with expressions, that result from a treatment of collisions with the help of kinetic theory [4].

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EMISSION SPECTRA RESEARCH OF THE PLASMA MIX

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The report contains comparison results of modelling plasma mix emission spectra (aluminium with tungsten addition) with the experimental measurements obtained in TRINITY on Angara-5-1. As a loading of installation the aluminium with various percentage of tungsten wire array was used. In the measurements liners with cylindrical and cone configuration were used. Measurements were carried out with the crystal spectrograph. As a detector, the x-ray CCD was used. The current through the liner was about 3–5 MA. The analysis of comparison results of plasma mix emission spectra were carried out in high-energy region 1400–2600 eV. The codes THERMOS and BELINE were used for computation of nonLTE emission spectra on the basis of the nuclear data obtained by the package FAC. The selfconsistent solution for an optically thick plasma layer was obtained by iterations as a result of consecutive refinement of the level equations for ion concentrations and equation of radiation transport. The calculations were carried out on the super computer MVS-100K of the Interdepartmental supercomputer center of RAS. Emission of a homogeneous cylindrical layer of the plasma mix with radius 0.1 cm was considered at electronic temperatures 300–700 eV and density 0.01–0.03 1/cm³.

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EXTRA EUV EMISSION FROM THE XENON IONS

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Well known, that the EUV emission at 13.5 nm substantially can be achieved from 5p-4d resonant transitions in Xe XI. After it was found that the set of satellites in highly charged Xe XVII–Xe XXXI ions may also contribute to the emission under certain conditions. Highly charged Xe ions have a high ionization potential in comparison with plasma temperature in most cases of experiment and acquisition of such ions by thermal heating is on very low population level. Discharge and laser produced plasmas that are used in EUV sources often have nonequilibrium electron distributions

with fast (high energy) electrons. Before it was shown that the presence of the fast electrons in different types of plasma like discharge, solar, laser etc at small relative concentrations (0.5–2%) even may have a significant influence on the ionic compound and line intensities. Results of kinetic modeling demonstrated high sensitivity of ionization degree state to the accuracy of the used cross-sections of impact processes.

In the report fast electrons influence on the level populations and the line emission within highly charged Xe ions is considered. Nonmaxwellian electron distribution by the energy, found out by adding of fast electrons used for calculations of impact processes rates on the basis of Hartree-Fock-Slater (HFS) quantum-statistical model. The calculation approach for the rates of inelastic electron-ion interaction processes with arbitrary electron distribution function based on the distorted waves approximation with the using of numerical and semiclassical wave functions for discrete and continuous spectra calculated in self-consistent HFS potential. It is shown that Extra EUV emission at 135Å may be achieved from the highly charged Xe ions under the fast electron interaction.

CROSSOVER BETWEEN EXCITED ATOMS AND FREE ELECTRONS

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The self-consistent fluctuation approach is developed to bridge the smooth crossover from the plasma waves to pair fluctuations, and finally to excited atoms (stabilized pair fluctuations) in the electron spectrum of strongly coupled plasmas. The approach is based on the joint description of free and weakly bound electron states. Existence of two problems is emphasized. The first one is a well-known restriction of the number of atomic excited states. Another one is to present an idea of the smooth crossover from bound pair electron-ion excited states to collective excitations of free electrons. The fluctuation approach is developed to study the spectrum domain intermediate between low-lying excited atoms and free electron continuous energy levels. The molecular dynamics method (MMD) is applied to study the plasma model since the method is able to distinguish all kinds of fluctuations. The electron-ion interaction is described by the temperature-independent cutoff Coulomb potential. The diagnostics of pair electron-ion fluctuations is developed. The concept of pair fluctuations elucidates the smooth vanishing of atomic states near the

ionization limit. The approach suggested removes the artificial break of the electron state density at the ionization limit: atomic state density divergent at the negative energy side and free electron state density starting from zero density at the positive energy side.

The following effects are discovered with the help of the MMD. The smooth but steep restriction of pair fluctuation density is obtained which could explain the restriction of excited atom contribution to the atomic partition sum. The energy domain adjoining to the ionization limit (a “gap”) is found out where the pair fluctuation density is close to zero, contrary to the monotonous Coulomb, and Plank-Larkin approximations for the excited atom density. The area of plasma nonidealities is discovered where there are neither excited atoms nor pair fluctuations. Maxwellian distribution of free electrons turns out to be non-shifted with respect to the ionization limit of the isolated atom.

The important advantage of the fluctuation approach is that it does not use any separate concepts of the partial number densities, e.g. of free and bound electrons as in chemical model. Such quantities are not physical ones since they do not correspond to any quantum operator. The fluctuation approach deals with the various energy, time and other distributions over the total number of electrons.

DESCRIPTION OF RECOMBINATION IN STRONGLY COUPLED PLASMAS

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The goal of this works is to study the rate of collisional recombination in non-equilibrium nondegenerate nonideal plasmas. The results are obtained by molecular dynamics (MD) simulations including the simulation technique to distinguish electron-ion pairs corresponding to the quasiclassical bound states.

Rate of recombination in ideal plasma can describe ratio

$$K_e = C(Z)e^{10}m^{-1/2}n_e^2n_iT^{-9/2},$$

where $C(Z) \sim Z^3$ and coefficient C is independent from temperature and pressure of plasma. In strongly coupled plasmas this ratio is not describe rate of recombination on plasma. But it can describe it if coefficient C consider how function of temperature and concentration of plasma.

Dependences of rate of recombination on various plasma parameters such as nonideality, ion charge and distribution of particle in plasma are obtained. It is found that coefficient C decrease monotonous with growth of nonideality of plasma. Moreover coefficient C decrease fast than power of $-9/2$ in strong nonideality plasma. As a result of this depend of rate collision recombination on nonideality is not monotonous.

At the area of small value of nonideality parameter coefficient C is constant. But dependence of coefficient C from nonideality undergo sharp bend when nonideality increasing. And coefficient C decrease in area of strong nonideality plasma according to exponential low. In the second exponentially vanishing region recombination rate describe approximation $K_e = K_0 Z^3 \Gamma^{9/2} \exp(-a\Gamma) \exp(-bZ\Gamma)$ where the coefficients K , a , b are calculated from results of MD simulation.

The presences of two parts of dependence of coefficient C from nonideality indicate changing mechanism of recombination in strong nonideality plasma. By analysis lifetime distribution proof that in the second area process of recombination does not describe Fokker-Plank model. At this area it is result of single electron collision near ion. Such changing recombination mechanism in the area of strong nonideality plasma is conditioned increasing area of many-particle fluctuations with growth of parameter of plasma nonideality.

INFLUENCE OF PAIR FLUCTUATIONS ON THE EQUATION OF STATE OF NONIDEAL PLASMAS

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The given work is devoted research of influence of pair fluctuations on the equation of state of equilibrium nondegenerate singly charged nonideal plasmas at various values of parameters of nonideality $\Gamma = 0.1 - 2$. The classical method of molecular dynamics is applied. As potential of electron-ion interaction it is used the coulomb potential which has been cut off on U_0 . Calculation of a total pressure of system of the charged particles is carried out at various values of Γ and U_0 . At values of $\Gamma < 0.4$ results of calculation well enough co-ordinates with expression for dependence of pressure on the density, received within the circular approximation, and practically do not depend from U_0 . At values of $\Gamma > 0.4$ reduction of value of a total pressure is observed at increase of U_0 . By consideration of dependence of a total pressure from $\Gamma = 0.1-0.55$ it was revealed nonmonotonic

behavior of the given dependence in area owing to what fluctuations of values of pressure have been analyzed and function of distribution of pressure is constructed at various values of Γ . By comparison of the received functions of distribution to normal distribution it was revealed that in certain area of values of appreciable distinction, and the given range of Γ is observed depended from U_0 . At values of Γ being out of the given area function of distribution of pressure co-ordinates with the normal distribution. Dependence of the compression modulus on Γ has been considered at the fixed value of U_0 in a range of $\Gamma \in (0.1, 0.6)$. At values of $\Gamma > 0.4$ appreciable dependence of the compression modulus on U_0 is observed. The approached allocation of contributions of subsystems of pair fluctuations and free particles was carried out (Lankin, Norman, (2008)). It is shown that dependence of pressure of a subsystem of pair fluctuations from Γ is described by the equation of state of ideal gas and does not depend from U_0 . The increase in the contribution of pressure of a subsystem of pair fluctuations in a total pressure is observed at increase in depth of a potential hole. Pressure of a free subsystem in the field of small $\Gamma_1 < 0.5$ co-ordinates with expression for dependence of pressure on the density, received within the circular approximation. By comparison of function of distribution of pressure of the free subsystem to normal distribution the appreciable divergence in the fixed area of values which are not dependent on parameter U_0 , unlike a total pressure of system was observed. Comparison of results to the results received within the limits of physical and chemical models of plasma is carried out.

HIGH-TEMPERATURE AND LOW-TEMPERATURE CHEMICAL MODELS OF DENSE METAL VAPOR PLASMA

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In the present study for advance in the region of low temperatures and high densities the chemical models of dense metal vapor plasma are developed. In addition to electrons, atoms and various ion species Al^{l+} where $l = 1, 2, 3$ considered in paper [1], we added molecules and molecular ions (high temperature variant for aluminum) and also neutral and charged clusters with number of atoms up to 6, thus multi-charged ions not considered (low temperature variant). To take into account a charge-charge interaction in multi-charged plasma, the approaches used in the literature were analyzed and as a result other expressions than in work [1] are

used [2]. Charge-neutral interaction is considered and take into account the short-range influence on virial correction, calculated by Likalter [3] for ion-atom interaction in quasiclassical limit. Wigner approximation is used for low-speed electron scattering by atoms. The available in the literature data have been used for calculation of oscillation and rotation partition functions of clusters. The models are used for calculation of caloric and thermal equations of state and plasma composition. This calculation allowed to analyzed the charge composition of cesium and aluminum plasma with use of low temperature variant of model. Dependence of a resistivity of plasma on internal energy was calculated using Frost's interpolation formula, the received caloric EOS and various approximations for transport cross-sections calculation. The satisfactory agreement with experimental data is received and the important role of molecules, molecular ions and clusters of aluminum in an initial phase of heating is shown.

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THE CALCULATION OF THE TRANSPORT COEFFICIENTS OF NOBLE GASES UNDER HIGH PRESSURE

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Electronic transport coefficients of noble gases under high pressures can rise in several orders with respect to their ordinary value and can reach almost metallic state. This effect is analogous to the phenomena observed in metals in the vicinity of the critical point, which is known as dielectric-metal transition. This transition occurs because of the pressure ionization in both cases. It gives rise to a steep increase in the free electron density, which in turn results in a large increase in the electrical conductivity and other coefficients.

There are many experimental and theoretical works studying these coefficients. Nevertheless some questions concerning theoretical description and interpretation of the measurements data are still open. In particular the question about change of ionization degree with the pressure are still open. Consequently, different ionization mechanisms are possible, which can produce contradictive results. Here is example of such contradiction. Recently, new experimental data have appeared [1, 2] where partial ionization of noble gases was reached by shock compression. In [2] two numerical codes were applied to describe the results of the measurements (correspondingly SAHA IV [3] and COMPTRA04 [4]). Both codes are based on so-called generalized chemical models and have been successfully tested for many other substances. But calculated and measured conductivity for the experiments in hand can differ in two times [2]. In this work we try to apply different theories to the calculation of the transport coefficients of noble gases. The results of calculations were compared with available experiments and calculations of other authors.

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NUMERICAL SIMULATION OF CLUSTER MAGNETRON DISCHARGE PLASMA

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Present work is devoted to investigation of the processes involving atoms and clusters occur in magnetron discharge plasma [1] in the frame of computer simulation. We have developed the mathematical model describing processes which are of importance for the efficient using of the magnetron discharge as a cluster generator.

There is a gap near cathode where magnetic trap for slow electrons obtains because of the presence of the magnetic field. Discharge ions are pulled in this gap because of the ambipolar diffusion. Therefore elec-

tric conduction of this region arises and almost all discharge current goes through this gap. Discharge ions bombard cathode after acceleration into this region of high electric conductivity and it causes to efficient sputtering of the cathode material because of high ion energy (on the order of 100 eV). Then sputtered atoms lose its energy due to scattering on the buffer gas atoms. Atomic motion becomes to be random after value of an atomic energy reaches a thermal value as a result of diffusion, and free metal atoms can be lost due to escaping on the chamber walls and as a result of an attachment to cathode. Thus there is cathode material atomic gas and cluster generation sets in when the certain conditions are satisfied. There are two types of the competitive processes involving clusters, namely growth due to attachment of the atoms to the cluster surface and also due to collisions between cluster with subsequent joining and evaporation. There is a buffer gas flow for extracting clusters from aggregation area and for cluster guiding to deposition chamber for further application.

All peculiarities of the processes described above (exclude coagulation and evaporation which are not very important for typical experimental conditions [2]) are taken into account and our model simulates evolution of cluster magnetron plasma by numerical calculations of the appropriate equations for cylindrical geometry of the magnetron chamber. We suggest a number of offers for optimization both design of the chamber and discharge parameters on the basis of obtained results. These suggestions allow to increase cluster generation efficiency.

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VELOCITIES COEFFICIENTS FOR EXCITATION AND DEEXCITATION AT COLLISIONS BETWEEN RYDBERG ATOMS AND SLOW ELECTRONS

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We have compared theoretical and experimental data for velocities coefficients at temperature 300–1000 K. Theoretical data from article [1] and experimental data from [2] have a difference about two times at 300–1000 K. We have made conclusion that theory from article [1] not correct for recombination processes in ultracold plasma. In our work we have

suggested formulas based on expansion of excitation cross-section at value electron energy equal transition energy. Half-empirical expressions for excitation cross-section from article [3] have used. Values of velocities coefficients for slow electrons have calculated. These values several times less then values based on extrapolation from high temperature region.

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KINETICS OF TRANSITIONS BETWEEN RYDBERG STATES IN LOW TEMPERATURE PLASMA

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Present work is devoted the analysis of kinetics of transitions between Rydberg states in excited atom.

We consider the process of stepwise atom ionization in a dense ionized gas and at low electron temperatures. Then radiative processes involving excited atoms are not important, and atom ionization results from many successive transition between atom excited states in collisions with electrons. In analyzing stepwise ionization as kinetics of excited atom states and the detailed opposite process of three body electron-ion recombination BKW scheme was used [1].

The rate constant of the process of three body electron-ion recombination at low electron temperatures has the form (Thomson formula) [2]

$$\alpha = A \frac{e^{10}}{m_e^{1/2} T_e^{9/2}}. \quad (1)$$

In present work coefficient A is determined on the basis of the classical rate constants of inelastic collisions involving electrons and a highly excited (Rydberg) atoms. A standard classical method of computer simulation is used for evaluation of the inelastic cross section in electron collisions with Rydberg atom [3].

In this work the coefficient of diffusion of electron in power space of atom was also calculated. It is possible to present $D(E)$ in the form

$$D(E) = \frac{1}{2} \frac{d\langle \Delta E^2 \rangle}{dt} = \frac{1}{2} \sum_m (E_m - E)^2 w(E, E_m). \quad (2)$$

The rate constant $w(E, E_m)$ present in the form

$$w(E, E_m) = N_e \langle v \sigma(E, E_m) \rangle = N_e \int_0^\infty \sqrt{\frac{2\varepsilon}{m_e}} \sqrt{\varepsilon} f(\varepsilon) \sigma(E, E_m) d\varepsilon, \quad (3)$$

where $\sigma(E, E_m)$ —cross section of inelastic transition from a state with energy E in a state with energy E_m , $f(\varepsilon)$ —electron distribution function.

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REFLECTION EFFICIENCY OF TWO-DIMENSIONAL SQUARE SYMMETRY UNMAGNETIZED PLASMA PHOTONIC CRYSTALS IN MICROWAVE WAVELENGTH RANGE

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Photonic crystals are known as structures which exhibit many unique features, in particular, in optical physics. Such structures can be used for passive and active devices development based on intense energy fluxes. In this report we theoretically study microwaves reflection from plasma photonic crystals (PPC) newly proposed as one- and two-dimensional (2D) structures. Theoretical calculation was supported by experimental investigation of the plasma parameters, dielectric permittivity measurements. Let a plane E-polarized em wave be incident from dielectric medium ε_1 at an angle α on an L thick slab of a 2D PPC consisting of $m = 1, 2, \dots, N$ rows of cylindrical plasma columns with radius ρ and dielectric permittivity ε . The columns constitute a square lattice with the constant Λ . Energy flux density of the microwave field reflected from a PPC slab ($N = 20$), we calculate on the basis of the matrix Riccati equation technique. The relative permittivity of the non-magnetized plasma at microwave frequency is assumed to be given by Appleton equation. With the average electron density from 10^8 to 10^{11} cm^{-3} and the electron temperature $T = 1.5$ eV, the real (imaginary) part of the plasma permittivity ranges from 0.9 (0) to 0.48 (0.14). Reflection spectra of a 2D PPC slab were evaluated in

the case of non-absorptive plasma columns with simultaneous variation of columns radius and lattice period at the fixed filling fraction, $f = \pi(\rho/\Lambda)^2 = 0.5$, of volume occupied by columns (per unit length). It is shown, the lower is the plasma dielectric constant the higher is the reflection efficiency. Note, purely real value of the dielectric constant excludes microwave energy absorption in PPC. From the other hand, our computations illustrate significant reflection efficiency reduction due to the wave energy absorption in 2D PPC plasma columns. Besides, a shift of spectra maximum is caused by small magnitude (in order of 0.01) of the imaginary part of the dielectric permittivity. For plasma parameters investigation the plasma flux (500 mm in dia) with density about 10^{12} cm^{-3} was generated at atmospheric pressure in air. The measured value of imaginary part at permittivity was about 0.01.

RESONANT CHARGE EXCHANGE INVOLVING NITROGEN AND OXYGEN

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Recently [1, 2] we evaluate the electron terms and average cross sections of resonant charge exchange when colliding ion and atom are found in the ground electron state and the cross section is averaged over momenta and their projections for colliding particles. We now spread these evaluations for excited states with a more accurate calculations the exchange ion-atom interaction.

Colliding pair	Number of terms	Excitation energy, eV
$O^+(^4S) - O(^3P)$	72	0
$O^+(^2D) - O(^3P)$	180	3.32
$O^+(^2P) - O(^3P)$	108	5.02
$O^+(^2D) - O(^1D)$	100	5.29
$O^+(^2P) - O(^1D)$	60	6.28
$O^+(^2P) - O(^1S)$	12	9.21

We evaluate electron terms of molecular ions in a range of distances between nuclei that determine the cross section of resonant charge exchange at energies starting from thermal energies up to 1 eV. The energy range for electron terms of interacting ion and atom with a nonexcited electron shell is divided in 6 separate diapasons in the case of large distances between particles. In particular, the number of degenerate terms and energy inter-

actions for ion- atom interactions with shells $O(2p^2) - O(2p^3)$ is given in Table. The principle role in ion-atom interactions that is that is of importance for the resonant charge exchange process is the exchange ion-atom interaction potential whose accuracy is determined by the accuracy of the asymptotic coefficient for atomic wave function. We find this value in the standard method [3, 4] by corporation of the asymptotic wave function with that form numerical calculation. In turn, numerical wave function of valence electrons in the atom are determined on the based of the computer code created in Physical institute RAS. The value of these coefficients depends on the electron states of atom and ions and allows us to determine the exchange ion-atom interaction potential.

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EXPLODING WIRE SPIRALS ROLLED UP IN TOROIDAL FORM

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The experimental results concerning of electric exploding metal wires wound up as a spiral on toroidal skeleton are presented. In a number of experiments about 50% of each coil of the spiral was shunted by conductor of double section. Exploding wire of such configuration has variable section, and primary allocation of energy provides in the field with minimal section, which has been structurally formed up that it have been turned same way in relation with the spiral. It led to starting up plasma vortex from exploding wire material, and to possible forming induction discharge inside the vortex because of toroidal magnetic field was reduced with large speed (this field is created by a wire spiral current before the explosion of the spiral). The maximum of the magnetic field induction in experiments reached a value of 3 T, and sometimes the strong magnetic pressure led to premature breaking of conductors and that is why in a number of experiments the energy was supplied by two-level scheme: in the beginning process the conductor got warm under rather small impulse of a current

(up to temperature close to a melting point), and then the basic current impulse led to wire material phase explosion. In kind of wire materials copper and aluminum were used. In experimental electrical explosion processes video shooting had been made, oscillograms of the current impulses passed through the exploding wires were received, and also optical radiation intensities of received plasmas were measured.

**ABOUT THE STATIONARY AND PULSING MODES
OF THE IONIZING GAS FLOW IN THE CHANNEL
OF THE QUASI-STEADY PLASMA ACCELERATOR
(QSPA)**

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The problems of the QSPA [1, 2] and their modern modifications with an additional longitudinal magnetic field [3] suppose the researches a lot of the principle questions of plasma dynamics. The given work continues a cycle of researches of the ionization process in the channel of the traditional coaxial plasma accelerator with an azimuthal magnetic field. At the ionization front there is a nonequilibrium transition from a gaseous condition to plasma. This transition for enough dense medium is considered on the basis of model [4] including the uniform system of MHD-equations and the ionization and recombination kinetics equation within the framework of the modified diffusion approximation [5].

The account of the radiant heat exchange is carried out by means of models of a various level of complexity including the solution of the radiation transport equation with the various mechanisms of the spectral line broadening [6]. The preliminary research of the radiation transport has shown that the most part of the radiation energy of the hydrogen plasma is concentrated in the Lyman alpha line. In this case we can use approximation of the radiative conductivity realized in present model.

The results of the numerical experiments were confirmed with the available data [1, 2] of existence of stationary and pulsing modes of the ionizing gas flow depending on parameters. On basis of the offered model the limit of transition from stationary to pulsing modes is certain and the criterion of existence of the stationary streams of the ionizing gas is formalized.

Work was supported by RFBR (grant 06-02-16707).

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THERMAL FLOW CONTROL

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Our work presents theoretical study of the thermal actuator affecting air flow about the wing section NACA-0015 and a wedge. The thermal effect can result from either a gas discharge or a heater on the contour surface (Joule heat). The wing section NACA-0015 has been examined under a subsonic flow, there being a heater at the wing varying in time to effect the incident air flow. The set of four principle equations: the continuity equation, Navier-Stokes, energy conservation, and equation of state for ideal gas have been solved numerically.

The vector field of velocities pronounces its vortex structure as it was noticed recently [1-4]. Such a vortex structure may be explained by the equation for vorticity (curl) resulting from the Navier-Stokes equation after the curl vector operation:

$$\frac{\partial \vec{\Omega}}{\partial t} + (\vec{V} \cdot \nabla) \vec{\Omega} + (\vec{\Omega} \cdot \nabla) \vec{V} = \frac{1}{\rho^2} \nabla \rho \times \nabla p + \nabla \times \left(\frac{1}{\rho} \nabla \cdot \vec{\sigma} \right).$$

Here the vector product, $\nabla \rho \times \nabla p$ or $\nabla \rho \times \nabla T$ as it follows from the equation of state, appears to be an origin of vorticity. There is an analogy with the dielectric barrier discharge as an actuator, where vorticity is generated by the vector product $\nabla \rho^* \times \nabla \varphi$, ρ^* is the electric density, φ is the electric potential [3, 5].

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DUST-PLASMA LIQUID IN STATISTICAL THEORY OF LIQUID STATE: EXPERIMENTS AN SIMULATIONS

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The measurements in dusty plasma were carried out to find the region of validity of approximate relation in statistical theory of liquid states. The integral equations with the Percus-Yewick and the hyppernetted-chain closures as well as the superposition approximation were chosen as the objects for investigation. We found that the use of experimental methods of analysis of spatial correlation of dust particles in plasma enables one to answer the question about the range of validity of approximate integral equations used in the statistical theory of liquid, in particular, the question about the range of validity of Percus-Yewick and hyppernetted-chain approximations and superposition approximation.

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DUSTY PLASMA STRUCTURES IN SUPERSONIC ION FLOW: EXPERIMENTS WITH DC GLOW DISCHARGE

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Under conditions of typical experiments with dusty plasma structures in dc glow discharges, the use of the mixture of light and heavy gases can make it possible to suppress the ion heating in the electric field and form supersonic flow characterized by large Mach numbers. The drift of krypton ions in helium is considered as an example. Experiments with dc glow discharge at 1–10% of Kr show that the transition to the discharge in mixture leads to increase of dust interaction anisotropy with strong coupling of dust particles in the direction of ion drift. In addition, under certain discharge conditions the phenomenon of abnormal “heating” of dust particles was observed when the particles can obtain high kinetic energy which is several orders of magnitude higher than typical.

DUST PARTICLE CHARGING IN THE UPPER ATMOSPHERE

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The noctilucent clouds (NLC) and polar mesosphere summer echoes (PMSE) are associated with the presence of a charged dust in the upper atmosphere. Simulation of the charging of grains is one of the most interesting problems in dusty plasmas with different electron, ion and atom temperatures. The results of ab initio simulations of dusty plasmas are reported. We use molecular dynamics (MD) and particle in cell (PIC) simulation methods to calculate the charge and mean kinetic energy (temperature) of a dust grain in two temperature plasma.

ABOUT OPPORTUNITIES OF POSITRON DIAGNOSTICS FOR RESEARCH OF DUST SPACE PLASMA

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The analysis the scale-spectra [1], received by an observatory INTEGRAL, has allowed authors to draw a conclusion, that the observable-line with energy 0.511 MeV is caused of positron annihilation from pair-positronium state. In this connection in [1, 2] it has been shown, that positronium formation in dust space plasma with the big concentration of the charged particles of a dust can occur as processes of interaction of positrons to atoms H and free electrons [1], and processes of interaction of a positron with negatively charged particles [3, 4] of dust space plasma with formation of positronium atom [2]. In such space plasma the positronium output about what speak experimental data of space laboratory Integral [1] is possible practically 100%. In the lead reasonings it was supposed, that depth of implantation of positrons in particles of a dust does not exceed length of diffusion of thermalized positrons in the environment, otherwise a part of positrons annihilated in a free condition, or participating in *pick-off-annihilation*, that will lead to increase in a share of the 2γ -annihilation channel. Depth of implantation l depends on energy of positrons E and from properties (density) of environment [5]. Knowing diffusion coefficient (terrestrial experiments) and time of a life of positrons in the environment, it is possible to estimate the size of particles of a dust and initial energy of positrons. So, for example, diffusion lengths of positrons in Si and Al are accordingly equal 0.5 and 0.15 μm [5], and for the majority of the condensed environments have the same order. The share of positrons (positronium), reaching a surface from the general number of positrons in the environment, depends on energy of positrons, i.e. from a parity of length of diffusion and length of absorption. So, lengths of absorption of positrons with energy 1.5 MeV in Si and Al accordingly will be ~ 600 and 500 μm , and for positrons with energy 2 keV the same sizes will be already on three orders less. Broadening of annihilation lines 511 keV in experiments the INTEGRAL makes size 2.37 ± 0.25 keV [1]. To it broadening there corresponds energy of annihilation electron-positron pairs in some 1–2 eV, i.e. energy of quasithermalized positronium.

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ULTRAHIGH CHARGING OF PARTICLES AND COULOMB EXPLOSION IN DUSTY PLASMA INDUCED BY ELECTRON BEAM

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The studying of the dusty plasma properties under electron beam action are of great interest because it gives the unique opportunities for experimental investigation of strongly coupled systems as well as for developing the new dusty plasma technologies of creating the new composite materials. Highly charged dust particle generates electrostatic field that can accelerate positive ions to high power. It gives the unique possibilities of using these macroparticles (for deeply ions implantation, as catalysts for increasing rate of reactions with the high energy barrier, in the new ionic engines etc.).

Presented work deals with the experimental investigation of dust particles charging under direct influence of electron beam. The experiments were carried out with particles of different materials, forms and sizes (10–200 microns) in the atmosphere of different gases (air, helium) at pressures $\sim 10^{-4}$, 0.2, 0.6 Torr and above. The current of electron beam was varied from 1 to 10 mA; energy of electrons was about 25 keV and electron beam diameter was about 3 mm. Under action of electron beam dust particles became charged. Due to Coulomb interaction these macro particles gained the velocity and spread in the different directions.

Simple technique of particle charge estimation was developed. The changing of particle temperature and time of it charging under experimental conditions were estimated. Role of secondary electronic emission and thermal emission of electrons in processes of macroparticle charging was considered.

The estimations of the 200 microns alumina particle charge was performed. It was about 10^8 elementary charges at pressure $\sim 10^{-4}$ Torr.

This work was partially supported by the U.S. Civilian Research & Development Foundation (Project RUP2-2891-MO-07) and the NWO project 047.017.039.

EXPERIMENTAL STUDY OF ELECTRON BEAM PASSING THROUGH THE LAYER OF AEROSOL WHICH CONTAINS SOLID PARTICLES

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In this work we experimentally studied the electron beam passing through the layer of aerosol that contains solid particles. Namely, effects of influence of a beam on individual particles of an aerosol and on aerosol volume as a whole were studied. Besides, measurements of integral power of the beam which has passed through dispersion medium, and distributions of flux density of electrons were made at various parameters of a beam, the gas environment and a material of firm particles.

Beam-plasma formations containing the dispersive medium have been created by preliminary preparation of plasma-forming environment: an aerosol layer where the electron beam was injected was created by means of mechanical dispersive device. In this work we studied the behavior of aerosol depending on the pressure of residual gas and speed the passage of particles through the impact zone of the beam. For working gas air it was established that at pressure above 1 Torr, activation of an electron beam did not lead to any visually observed changes of character of particles motion. When the pressure was reduced to 7.5 Torr the particles started to deviate from the initial falling direction: the continuous layer of an aerosol influenced by the electron beam was divided into two streams. It occurred because the particles were charged and had electrostatic repulsion. From the geometry of the experiment we estimated the charge of the particles, which it receives being subject to electron beam. For particles of the micron size (30 microns) its value forms 10^4 elementary charges. At the subsequent pressure decline (~ 3.5 Torr) we observed stronger projection of particles. Thus there is a preferred direction of the aerosol projection along the electron beam opposite to movement of electrons. With the greatest possible pumping (~ 0.1 Torr) aerosol projection becomes very intensive, and the preferred direction of projection of particles now is the direction of the movement of the electron beam.

The given researches are interesting from the point of view of calculation of working processes of plasma-chemical reactors with reactionary volume in the form of electron-beam plasma of aerosol, as well as optimization of their design.

EXPERIMENTS WITH DUSTY PLASMA GENERATED BY A PROTON BEAM

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Investigations of processes in dusty plasma are usually performed in inert gases when initially a gas discharge of some kind is initiated and then dust grains are being inserted into the ionized medium. At the same time the ionized medium can be created by fast charged particles incoming with the initial energy 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.

Results of experimental study of self-organization of dusty structures formed under an action of a proton beam in inert gases are presented. The experiments were performed at the electrostatic accelerator producing a proton beam with the energy of 2.5 MeV and the current from 0.5 up to 5.0 μA . The experimental cell was separated from the evacuated ion duct by the grounded titanium foil. The beam moved in an inert gas from the titanium foil to the electrode to which the negative potential was applied. The illumination of the internal volume of the experimental cell was made through optical windows by the laser knife. Dusty formations were registered with the help of a videocamera. The experiments

were performed for different gases (He, Ne, Ar, Xe, Kr) with monodisperse and polydisperse particles with diameters of 1–10 microns. The plasma component density was $n_e \cong n_i \cong 10^{11} \text{ cm}^{-3}$, the dust grains density was $10^4\text{--}10^7 \text{ cm}^{-3}$. The values of dust charges were in the range of 130–200 units of electron charge. The electrode voltage was varied from 0 up to 500 V. The gas pressure was varied in the wide range from 1 up to 800 Torr. Two orientations of the proton beam were used for the experiments. In one case we used the proton beam with a horizontal direction of the beam. A great amount of data on self-organization of the dust component at different gas pressures and the applied electric field was obtained. It should be noted that the horizontal direction of the beam is optimal from the point of view of compensation of the gravity force. In the experiments with the vertical proton beam we used melamine-formaldehyde monodisperse particles of $d = 3$ microns. When the electric potential is applied to the electrode dust structures are formed in the near electrode region. The shape of a structure depends on the gas pressure, the electrode potential value and density of dust grains injected into the experimental cell. The study performed has the interest both for the basic research and for developing foundations of the technological application of the dusty plasma formations in different power installations.

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DUST CLUSTER RESPONSE TO THE HIGH VOLTAGE NANOSECOND PULSES

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Influence of high-voltage nanosecond pulses on the dust particles levitating in a plasma of a rf discharge is studied. The experiments are performed in a modified GEC cell. Additional ring-shaped electrode, to which we applied the high-voltage pulses (20 ns duration, 1–11 kV amplitude, up to 200 Hz repetition rate), was introduced into the chamber 30 mm above the rf electrode. A confinement ring was installed on the rf electrode coaxially with the high-voltage electrode to provide the radial confinement of the dust grains. Melamineformaldehyde spheres of 7.17 micron levitated between the rf electrode and the high-voltage ring and were highlighted

with a laser sheet in order to be observed with a high-speed videocamera either from top or from side. The influence of these impulses on the plasma was monitored by measuring the voltage on the bottom electrode. It was found that after the action the voltage on the bottom electrode becomes more negative. The relaxation lasts several hundreds microseconds. Therefore pulse produces significant influence on the plasma. Since the plasma is affected by the high-voltage pulses, dust particles also are. They start to oscillate as the repetitive pulses are applied. They exhibited resonance curves, known from low voltage excitation. Dust particles formed clusters in the horizontal plane. These clusters exhibited parametric instabilities when the repetition frequency of the pulses equaled doubled the frequency of one of the cluster modes and was close to the resonance of the vertical oscillations. A simple model of the plasma response to the high-voltage pulse shows that the dynamics of the dust particles must be significantly affected by the nanosecond high-voltage pulses. The model allows us to explain the observed resonance amplitudes of the oscillation of the dust particles.

ELECTROSTATIC INTERACTION OF SPHERICAL CONDUCTING MACROPARTICLES IN A PLASMA

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Electrostatic interaction of finite size spherical macroparticles in an plasma is studied. Primarily, the interaction of a point-like charge in the equilibrium plasma with a conducting sphere is considered. Subsequently, the interaction of two conducting spheres in a plasma neglecting shielding effects is fulfilled. This problem was previously studied in papers [1, 2, 3] for constant charges on the conducting spheres. In this paper we study the cases of constant, independent on interparticle distance, macroparticle charges and constant macroparticle potentials. The last case is more suitable to description of the electrostatic interaction of macroparticles in a plasma where the macroparticle potential is controlled by the floating plasma potential. It is shown that the interaction is different in this two cases and is weaker in the case of constant potentials. It is shown that electrostatic energy cannot be used as interaction potential energy in the case of constant potentials. This is consequence of that the external source holds the constant macroparticle potential and exchanges energy with macroparticles. Consideration on the basis of the Maxwell stress ten-

sion allows us to establish the form of interaction potential energy also in the constant potential case.

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DYNAMICS FEATURES OF DUST PLASMA STRUCTURES IN MAGNETIC FIELDS IN A DC DISCHARGE

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An explanation of the rotation inversion of the dust plasma structures in the vertical magnetic field in dc discharge observed in a number of experiments is presented. The ions azimuthally drift in the crossed axial magnetic field and radial electric field, and the dust plasma structure rotation is due to the ion drag force. It is shown that the rotation inversion occurs because of the inversion of the radial ion flux. At low magnetic fields, the radial ion diffusion flux from the axis (where the dust structure is placed) to walls prevails over the flux absorbed by the dust particles structure. As the magnetic field increases, the plasma is magnetized and the radial flux toward the wall decreases. At a certain magnetic field value, the total flux on the dust particles becomes larger than the flux generated in the volume of the dust structure. Therefore, the inversion of the radial ion flux occurs in the central discharge region and leads to the change in the rotation direction of dust particles. With the further increase in magnetic field, the inversion region of the diffusion flux is expanded, the potential trap disappears, and the dusty structure decays.

THE DYNAMICAL AND STRUCTURAL FEATURES OF DUSTY PLASMA STRUCTURES IN RF DISCHARGE

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In this paper we report about experimental research of dynamical and structural features of gas rf discharge dusty plasma with spherical melamine-formaldehyde particles 12 micron in diameter. We studied a formation of dust plasma structures in near-electrode layer of rf discharge, including an investigation of influence of discharge parameters and sort of gas on quantity of levitated particles in structure. The diagnostics of dusty plasma structures with measuring of basic parameters of dusty component (quantity of particles in a layer, mean interparticle length, particle temperature subject to discharge parameters such as pressure of buffer gas and power consumption) was carried out. Varying a quantity of particles, a conditions of formation a new layer, mechanisms of such a formation, dynamics and structural features of such processes were studied. Using synchronized sistem of video surveillance on horizontal and vertical plane, we measured kinetic temperatures of dust particles on horizontal and vertical sections of dusty plasma structures and made comparative analysis of measurement.

EXPERIMENTAL STUDY OF DUSTY PLASMA WITH ROD-LIKE MACROPARTICLES

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In the majority of the experimental and theoretical works deal with researching of properties of strong non-ideal dust plasma, spherical particles were used. Only during the latest time works in which dust particles have the strongly asymmetric form appeared. Using of such particles should lead to occurrence of new states of dusty plasma structures (liquid crystal and crystal phases with various degree orientation and position ordering), those demonstrate a great number of unstuded properties and new phenomena. These phenomena may be studed at the kinetic level. Thus,

experimental studying of the dusty plasma structures formed by particles of the asymmetrical form represents significant interest.

The present work deals with the experimental investigation of structural and dynamic properties of dusty plasma with rod-like macroparticles in the high-frequency gas discharge. These plastic particles were 300 micron in length and 15 micron in diameter. A series of experiments were carried out at various pressure in a range of 0.11-0.28 Torr. Movements of particles was recorded by two videocameras. On the basis of experimental data three-dimensional coordinates were obtained. Also dependence of speed of the centre of mass of the particles on time and dependence of speed of their rotation on time were calculated. It should be noted that at low pressure (0.11–0.15 Torr) all particles were orientated in a horizontal plane and changed their orientation with pressure increasing (0.15–0.28 Torr).

THE IMPACT OF DUSTY CLOUD ON THE DC DISCHARGE POSITIVE COLUMN STRUCTURE

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An influence of the dusty cloud on plasma parameters of dc discharge plasma is investigated by numerical simulations using non-local 2-D kinetic model of the dc discharge positive column in neon. The effect of dusty particles on ion drift and the recombination of electrons and ions on dusty particles are taken into account. Dusty particles charges are calculated in response to plasma parameters. Calculations are performed for various dusty cloud dimensions, densities and dusty particles sizes.

COULOMB CLUSTERS OF CHARGED DIAMAGNETIC MACROPARTICLES IN INHOMOGENEOUS MAGNETIC FIELDS

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We have theoretically and experimentally confirmed the possibility of the stable levitation of Coulomb clusters of charged diamagnetic macroparticles in inhomogeneous magnetic fields. We present an experimental setup

for keeping in a stable state the Coulomb clusters with small number of charged graphite grains of 100–300 μm in size. The grains levitate in the upper part of the space between the electromagnet pole pieces where the magnetic field $B \sim 1$ T with $|\nabla B| \sim 10$ T/cm. The pole pieces of special form have been designed for the creation of the magnetic field configuration trapping a diamagnetic grain cluster. An analysis of the cluster structure and dynamics is performed. We have developed a simple theoretical model for calculations of the equilibrium levitation place of the diamagnetic grains and the frequencies of their oscillation. The calculation results are in agreement with the experimental data. We conclude that, using stronger magnetic fields $B > 10$ T in terrestrial conditions, one can form stable 3D dust crystals and liquids containing several thousands of grains. For investigations of such structures formed under microgravity conditions onboard a space station, much smaller magnetic fields are necessary, $B \sim 0.1$ T, $|\nabla B| \sim 0.1$ T/cm.

CHARGING AND SCREENING OF SMALL DUST PARTICLES IN PLASMAS OVER A WIDE RANGE OF COLLISIONALITY

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We present results of numerical calculations of the dust grain charging in weakly ionized plasmas. The relations between the grain size and ion and electron mean free paths are assumed arbitrary. If the grain size is small in comparison with the mean free paths, we take into account the collisionless layer of thickness on the order of the mean free path around the grain. Inside the layer, the ion and electron motion is governed by the moment and energy conservation laws. Outside the layer, it is described by the continuity and Poisson's equations. The system of these equations is solved numerically. We allow for the volume ionization and recombination as well as the recombination on the grain surface. We can also take into account the influence of electron emission from the grain surface. As a result we have obtained the time dependence of the grain charge and the ion and electron density distributions around the grain. Our results are compared with those of the analytical models and numerical calculations available in literature.

EFFECT OF TRANSPORT OF GROWING NANOPARTICLES ON CCRF DISCHARGE DYNAMIC

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The influence of movable dust on the discharge properties and even the dust distribution on the initial stage of the nanoparticle growth are still open questions. We have developed kinetic model of the ccrf discharge with mobile nanoparticles of different radii taking into account the particle charging. New aspects in our study of ccrf discharge plasma with nanoparticles are as follows: a) we consider dust particle charging by using the electron and ion energy distribution functions taken from the kinetic PIC-MCC simulation, b) the motion of dust is calculated self-consistently with the discharge parameters, and c) we analyze the role of movable dust on the transition process between the different discharge regimes.

It is found that at initial stage of growth the nanoparticles are accumulated near the sheath-plasma boundaries, where the ionization by electron impact have maxima. The growing nanoparticles suppress the ionization absorbing fast electrons and stimulate a quick change of plasma parameters followed by the transition between different modes of discharge operation. At the moment of the transition the ratio of the ion drag to the electrostatic force changes because of a drop of the ion density, and the dust peaked distribution transforms to a flat one. The results of our PIC-MCC calculations showed that the quick change of plasma parameters observed in Refs. [1, 2] in the beginning of dust formation is explained by the influence of nanoparticles in the discharge volume. In the ccrf discharge before dust formation the ionization rate has a maximum near the sheath-plasma boundary. At the initial stage of particle growth (up to 20 nm) more dust is accumulated near the sheath-plasma boundary which suppresses the ionization rate, absorbing observed in the experiments.

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MODE TRANSITION IN CAPACITIVELY COUPLED
RADIO-FREQUENCY DISCHARGE IN
ARGON/ACETYLENE MIXTURE

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The gas discharge in hydrocarbon mixtures is widely used for carbon film growth. These thin films are of great interest for a wide range of industrial applications due to their extraordinary material properties.

The advantage of a capacitively coupled radio frequency (CCRF) discharge is that it can be used for producing non conducting films. Noble gases like argon and neon are often used as main background gases for hydrocarbon mixtures as their presence changes morphology of diamond like carbon films and leads to fewer crystalline defects.

The existence of different regimes of radiofrequency glow discharges corresponding to specific mechanisms of electron energy gain and deposition have been demonstrated experimentally and studied theoretically for different atomic and molecular gases. The transition from volume dominated regime to electrode-sheath regime is characterized by a sudden increase in the plasma density and decrease in the electron temperature of the bulk plasma. Such a transition affects film deposition rate and for example a higher rate of α -Si:H film deposition was measured for the volume-dominated discharge mode.

In previous work devoted to study of plasmachemical processes in Ar/C₂H₂(5.8%) we observed changes in argon discharge properties associated with addition of small acetylene portion. These changes are characterized by decrease in plasma density and decrease in the electron temperature of the bulk plasma. In spite of decrease in plasma density this changes are similar to regime transition described above.

In this work we study the plasma dynamics in a capacitive 13.56 MHz discharge in a Ar/C₂H₂ mixture for the conditions of Bochum experiments. The interelectrode distance is 7 cm, the gas pressure is 75 mTorr, and the amplitude of applied voltage is 92 V. The portion of acetylene was varied.

Changes in plasma dynamics associated with acetylene addition were analyzed. It was shown that secondary electron emission and electron attachment processes are not responsible for this transition.

BEHAVIOR OF CHARGED DUSTY PARTICLE SYSTEMS OF SPHERICAL AND CYLINDRICAL SYMMETRY UNDER PULSE LOADING

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Dusty or complex plasma has been the subject of intensive investigation for more than 10 years. Now it is well known that microparticles of matter in plasma of different origin can acquire high electric charges and exhibit properties of gas, liquid or a solid. The aim of the present report is to study the internal structure of a Coulomb Balls (CB) of different symmetry by means of MD simulation. The interparticle interaction is described by the Yukawa isotropic pair potential. The theoretical estimation of the dust particle charge as the particle size function was carried out within an analytical approach, which is a generalization of the known charge theory in the orbit motion limited (OML) approximation in case if ion scattering on neutral atoms is taken into account.

Peculiarities of dust particle systems behavior at external confinement field under different types of impulse loading are investigated. Loadings performed by adding center oriented velocity to particles on the outer shell.

Simulations showed that outer shell oscillations have beat form. The main reason of such response is close values of frequencies of outer shells. Beat amplitude almost decays after few dozen periods. That occurs since synchronization of outer shell oscillations. Oscillation amplitude increases with loading intensity, while oscillation frequency remains the same. It should be pointed out, that shell oscillation frequency depends substantially on CB size. This dependence can be written as $T \approx 0.006 + 0.009e^{-\frac{N}{1200}}$. It is shown that two regimes of structural response of dust particle systems on impulse loading exist.

A binary mixture of dust particles in plasma which is in the field consisting of gravitational, thermophoretic, and electrostatic force is simulated. The structural properties of the binary mixture of particles depending on composition are investigated. The segregation features of a system of particles of two species under the conditions of recent experiments on Coulomb ball formation are studied.

Structure with cylindrical symmetry is obtained to investigate wave propagation process. This structure is formed under non-isotropic confinement field (confinement field of cylindrical symmetry). Perturbation is generated in the dusty plasma during loading.

DYNAMICS OF CHARGED CLUSTERS IN LIQUIDS IN THE PSEUDO-STEADY REGIME

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Discussed in the paper are details of the Ohmic conduction of the solution of a binary 1-1 electrolyte. The study is motivated by the desire to have a consistent equation of motion for a charged particle in normal (non-superfluid) liquid with finite viscosity η . Usually, employed for this purpose is the so-called Langevin equation where the particle mass M is assumed to be constant and the characteristic relaxation time is expressed through viscosity η . However, this scenario is not self-consistent: If the friction force has the Stokes origin, the effective ion mass consisting of its bare mass and associated hydrodynamic mass due to arising flow of adjacent liquid should not be constant (for example, in case of oscillatory motion it exhibits a strong frequency dispersion: $M^{ass}(\omega \rightarrow 0) \simeq \omega^{-1/2}$). Although the scenario with $M = \text{const}$ is also in principle possible (we refer to it as the Drude scenario below), in that case the friction force which is linear in the ion velocity should have a different (non-Stokes) origin. The performed analysis of frequency dispersion of electrolyte conductivity for the two scenarios reveals qualitative differences which can be detected experimentally in their behaviour allowing to distinguish between the Drude and Stokes models. An important problem for ion dynamics in liquids is the structure of charged clusters (arising around the ions) whose radius R_s is usually considered to be an adjustable parameter. We discuss the physical mechanisms governing formation of R_s .

KINETIC TEMPERATURE OF CHARGED DUST PARTICLES IN NONIDEAL DUST PLASMA

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The “heating” phenomenon (increase in the kinetic temperature) charged dust particles in plasma to the temperatures considerably exceeding own temperature of a particle and kinetic temperature of electrons and ions is investigated. The mechanism of energy transfer from an external source to dusty particles in plasma is investigated and its influence on a

spectrum of particles oscillations is discussed.

Frequency intervals of various types of fluctuations in dusty plasma are analyzed: a range of eigenfrequencies of particle vertical oscillations in near-electrode plasma; a range of eigenfrequencies of horizontal particle oscillations in a field-trap; a range of eigenfrequencies of oscillations in a chain of dust particles; a range of eigenfrequencies of dust particle oscillation in numerical simulation of two-dimensional dust-plasma crystal, in which dust particles interact via Yukawa potential; a range of frequencies of charge fluctuation of a dust particle; a range of characteristic frequencies of external field of rf discharge; a range of electronic, ionic and dust plasma frequencies. Due to overlapping of different frequency ranges mentioned above with an interval of eigenfrequencies, it is possible to propose a parametrical resonance model that explains an anomalous high kinetic temperature of dust particles.

The estimations of the kinetic temperature values of dust particles in plasma for the considered mechanisms of “heating” are carried out. The comparison of results obtained with the data of Quinn and Goree 2000, Vaulina et al 2006, Samarian et al 2001 is carried out. The correspondence between the potential of interparticle interaction of dust particles and the dust plasma properties is discussed as well as the specificity of nonideal dust plasma in comparison with the condensed matter systems.

CRITERIA OF FORMATION OF NEW LAYERS IN DUSTY PLASMA WITH ISOTROPIC PAIR INTERACTION POTENTIALS

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In this work, the conditions of formation of quasi-two-dimensional dusty structures are considered, which are held in the gravity field by the external electric fields. At present, it is common to use the Debye potential $U = (eZ_p)^2 \exp(-l/\lambda)/l$ (where l is the distance, λ is the screening length, eZ_p stands for the grain charge) as the main approximation of the pair interaction potential of charged grains in plasma. Note that this approach fits the experimental and numerical simulation data only if the distance between the grains in plasma is small: $l < 4\lambda_D$, where λ_D is the Debye screening length [1]. With increasing of distance l the screening weakens, and the interaction potential U for $l \gg \lambda_D$ can transform into power-law function: $U \propto l^{-2}$ [2] or $U \propto l^{-3}$ [3].

In present work, the following power-law pair interaction potentials were investigated: $U = a_m (eZ_p)^2 l_p^{m-1} / l^m$ (where $m = 2, 3$), and also the screened Coulomb potential. For each of the potentials under study, the relations between the radial and the vertical gradients of electric field and the number of grains in the layer were found, that define the criterion of formation of new dusty layer. The process of formation of quasi-two-dimensional system of dusty grains was studied also numerically. The simulations were carried out for two cases: 1) for the system, restricted radially by the electrical field $E_r = \alpha r \neq 0$, and 2) for the uniform dusty layer in periodical boundary conditions in the horizontal directions \mathbf{x} and \mathbf{y} ($E_r = 0$). In both cases, the results of numerical simulation agreed well with the analytical criteria of formation of a new layer. The presented results can be easily adapted to any pair potential, given analytically, and can be used for the passive diagnostics of the interparticle interaction parameters in quasi-two dimensional structures, forming in the near-electrode area of rf-discharge.

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NEW TECHNIQUE FOR RESTORATION THE PAIR POTENTIAL OF INTERACTING PARTICLES IN NON-IDEAL SYSTEMS

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The purpose of the given work was to develop a technique for restoration parameters of dusty-plasma systems in laboratory plasma, such as pair potential of interacting dust particles in plasma, their factors of friction and parameters of external holding back potential. The technique based on finding a solution of the inverse problem describing movement of dust particles by system of the Langevin's equations.

Unlike the techniques proposed by the statistical theory of liquids, in the offered technique we does not use any additional assumptions of rela-

tionship between pair correlation function $g(\rho)$, direct correlation function $c(\rho)$ and potential of pair interaction $U(\rho)$ and therefore can be applied to strongly correlated systems of interacting particles.

The peculiarity of the solved problem consists in “irreversibility” of the Langevin’s equations in the sense that they include actions of casual forces.

That’s why the restoration can’t be provided in a correct way when the number of the equations and unknown parameters of a problem are equal.

In certain cases when considering inverse problem it’s possible to solve a system that contains more equations, than number of unknown parameters. In this way we get a chance to define unknown parameters by reducing random errors.

In our case we achieve good results restoring unknown parameters of system of the Langevin’s equations by finding the best match between the solution of a direct problem on movement of particles and the information on coordinates and displacement of these particles that can be easily found both in numerical, and in real experiments.

A method was tested on the results of numerical experiments with dusty-plasma structures of the various sizes.

RADIATION CHARACTERISTICS OF HIGH CURRENT PULSED DISCHARGE IN HIGH DENSITY HYDROGEN IN VISIBLE AND SOFT X-RAY SPECTRAL RANGES

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Results are presented from experimental studies of self-constricted discharge (Z-pinch) in dense hydrogen at initial pressure of hydrogen up to 35 MPa and current amplitude up to 1600 kA. Current half-period was varied from 100 to 150 μ s. The discharge burns in metal vapor of initiating wire and eroded electrode material, surrounded with hydrogen.

The brightness temperature of the discharge channel at the wavelengths 695 and 550 nm was measured by two identical monochromatic pyrometers. Brightness temperature of an external hydrogen shell of the discharge channel is 1–9 eV. Data of spectroscopic measurements of the transient layer of hydrogen around the discharge channel in visible spectra are presented. The SXR intensity was measured with SPD-8UVHS photodiodes.

Temperature of the central metal zone, from which x-ray radiation is registered, achieves several hundreds eV. On based of the experimental data the estimations of discharge parameters were produced. The equalization of the magnetic and gaskinetic pressures in the course of the contraction and subsequent expansion of the channel is accompanied by oscillations of the channel diameter. These oscillations, which are clearly seen in optical streak images, correlate with spikes in the voltage waveform and oscillations in the intensity of x-ray emission.

The constricted discharge channel surrounded by hydrogen shell can be used for producing pure photoionized hydrogen plasma, for modelling various astrophysical processes (radiative energy transfer in the outer shells of stars, oscillations of stellar brightness due to the arrival of shock waves at the stellar surface, etc.).

ON THE NATURE OF CATHODE EROSION IN TRICHEL PULSE NEGATIVE CORONA

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Cathode erosion has been investigated in Trichel pulse regime of negative corona discharge in atmospheric pressure air in point-to-plane electrode configuration on copper, aluminum, carbon and tungsten cathodes. It is found that negative corona causes the erosion of cathode surface in form of nanometer-size craters.

In Trichel pulse negative corona discharge current is performed as a consequence of nanosecond-scale pulses and the current between pulses is low. One can assume that erosion process in Trichel pulse regime of negative corona is also performed as a consequence of elementary erosion acts. Each elementary erosion event is associated with a single Trichel pulse and discharge current flows on the cathode through the surface the area of which equals to cross section of elementary erosion fragment or crater.

Current density on the cathode surface equals to relation of Trichel pulse amplitude to area of a single crater and was estimated as 10^8 A/cm². To the same value leads proposition that current density equals to relation of Trichel pulse amplitude to cross-section of elementary erosion fragment, size of elementary fragment was calculated as relation of total cathode erosion during experiment to number of Trichel pulses.

The value of integral of specific current action of Trichel pulse which depends on the cathode current density and pulse duration and serves as a criterion of electro-explosion has been calculated as $10^9 \text{ A}^2\text{s}/\text{cm}^4$. This value argues that cathode erosion in Trichel pulse negative corona discharge is caused by local electro-explosions due to pulsed discharge current.

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THE PHASE STATE OF A TUNGSTEN CATHODE SURFACE IN HIGH CURRENT ATMOSPHERIC PRESSURE ELECTRIC ARCS

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The present day understanding of the phase state changes at the surface of refractory cathodes operating in high current (several hundred amperes) electric arcs is still in its infancy. The relevant empirical data are mostly fragmentary and often conflicting. The existing theory starts from the assumption that the energy flux onto the cathode surface and surface electric current density are solely the functions of the near-cathode voltage drop and the surface temperature and exhibit no dependence on the total arc current [1]. On this basis, the bifurcation analysis and numerical simulation of the arc stability are performed [1]. Such an approach is not, however, universal and meets with failure in the case when the arc generates the resonance photon fluxes onto the cathode surface being comparable with other incident energy fluxes [2]. No account is also taken in [1] of the existence of a liquid phase at high enough surface temperatures. Both the features mentioned are typical of high current atmospheric pressure nitrogen arcs.

A greater insight into the physics of high current atmospheric pressure arcs, whatever the plasma-forming gas, can only be gained on a self-consistent consideration of the system “plasma–electrode surface”. As the first step towards this target, the present paper reports on investigating the phase changes resulting in a liquid phase formation on the surface of a tungsten cathode in powerful nitrogen arcs. Also drawn are some qualitative inferences of relevance to the phenomena observed.

The formation of a liquid film of the molten cathode metal is regularly observed at arc currents less 200 A, while at currents of 300 A and above the molten state disappeared completely or partly. The molten region is removed by 0.2–0.4 mm from the arc attachment and resembles a 0.1–0.2 mm wide roll slipped over a conic cathode. The former is contradictory to the results of [3] wherein the surface melt is stated to occur just along the boundary of the arc attachment. In whole, the effects we observe in the melt region are as follows:

1. Ejection of small-sized (~ 0.01 mm) fragments from the melt at speeds of ~ 100 m/s.
2. Swirling and formation of ball-shaped surface fragments (bubbles) followed by their full or partial carryover into the arc plasma or solidification at the cathode tip.
3. Blowing of the liquid film by plasma-forming gas to expose a solid cathode structure.

All the phenomena mentioned are observed in nitrogen arcs and none of them does in argon arcs except for a few details concerning the bubble formation as described in [4]. This being kept in mind, the problem of a comparative analysis of the energy exchange mechanisms in argon and nitrogen arcs takes on great importance. Some relevant aspects are to be touched up in this paper.

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STUDY OF GAS FORMATION IN THE TRANSFORMER OIL IN THE PULSE ARC DISCHARGE

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The processes of gas formation in the high-voltage oil-filled equipment with the appearance of internal short circuit determine the value of pressure in the expanding steam-gas bubble and, as a result, the scales of emergency. These processes also determine the requirements for the operation of the safety devices. The intensity of gas formation with the electrical discharges in the transformer oil is determined by resistance to gas formation (Bg) and is characterized by the volume of the formed gases per the energy unit of the discharge. In the electric arc the results of measuring the specific gas formation, obtained in the known works, differ to two orders in the value: from 80 to 7000 l/MJ.

Authors fulfilled the volume measurements of the isolated gases with a change in the energy of arc in the range from 10 to 100 kJ. The energy source was a capacitive storage. Arc has burnt in the special reactor by the volume about 18 litres. The volume, occupied with oil, was about 8 litres, the remained volume was filled up with nitrogen. Discharge appeared after the electrical explosion of copper wire with the diameter of 0.1 mm. The distance between the parallel cylindrical electrodes was about 20 mm, the length of electrodes was 180 mm. The duration of arcing reached 5 ms, the maximum current was about 50 kA. Characteristic arc voltage was about 1 kV and the maximum voltage was about 3 kV. Under the action of own magnetic field the arc was drawn out and it was moved. The velocity of arc motion, according to the estimations, reached 30 m/s.

The volume of the isolated gases was calculated from an increase of the pressure in the vessel. Experiments showed that the coefficient of gas formation in the transformer oil practically does not depend on energy of arc in the investigated range and is about 110 l/MJ.

ENGINEERING FOUNDATION OF PULSED GENERATOR ON INDUCTIVE STORAGE AND COMBINATION OF VACUUM INTERRUPTER AND PLASMA OPENING SWITCH

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Development of nanosecond pulsed technique of terawatt power is connected with such problem as primary storing of energy. At present generators of such kind are based on capacitor storages (CS) which have low density and high cost [1, 2].

At approach to terawatt power nanosecond pulses generation based on inductive storage is offered to consideration in paper [3, 4, 5]. Combination of vacuum interrupter (VI) and plasma opening switch (POS), which allow to equalize maximum voltage VI and POS in self insulation condition, and their modification offered in [6] are the base of the generator. The second characteristic of the construction is current zero battery transformation into Marx bank. It provide for forced current zero break in 2–3 μs and allows to decrease significantly volume of current zero battery and to use it power for current multiplication in transformer storage (TS) circuit. The third construction peculiarity of the generator connected with circuit of current multiplication in TS. Effect of primary wining screening is used under current output from secondary winding for time of output from storage. Coupling coefficient here is inversely prepositional to coefficient of current multiplication [6].

The offered complex of the engineering solution allows to use effectively IS for generation of nanosecond power pulses. Constructive characteristics of current zero banks and possible ways of their usage with IS as well as with TS are emphasized in the article.

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THE INDUCTIVE LIMITER OF A SHORT-CIRCUIT CURRENT

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Fundamental possibility of creating of high-speed inductive limiters of short-circuits current in power lines of 110 kV and above is discussed. The inductive limiter is capable of detecting and limiting of a short-circuit current at the first rise, i.e. in less than 3 ms. The inductive limiter of a short-circuit current comprises a transformer and a high-speed explosive opened switch. The results of numerical simulation of the inductive current limiter are presented. The paper presents results of nominal load and short-circuits load testing of the inductive current limiter in power lines with a voltage of 10 kV on the 'SRC HVA' bench. The proposed inductive limiter can be used for protection of electrical equipments rated to 220 kV, improving of the quality of electricity and increasing of safety level.

ON FRACTIONAL SEPARATION OF SUBMICRON SIZE POWDERS WITH THE HELP OF PLASMA DISCHARGE

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Modern high technologies widely use powders, including the submicron size, received in the various ways. One of the basic ways of reception of this type powders is detonation synthesis. There are also technologies with application of electronic beams, supersonic gas streams, microwave heating in water, etc. In all these technologies output powder suspension, in which the necessary fraction (for example, 30–50 nanometers) contains only partially, turns out. In this connection the problem of powder suspension division on fractions becomes urgent. The purpose of work is the estimation of an opportunity of submicron size powders division on fractions with use of the plasma discharge in a magnetic field.

Limited orbital motion approximation known in physics of dust plasma is accepted as the basic model of charging particles. Use of cold nonequilibrium plasma received at pressure about 0.1 Torr and electrons temperature about 1 eV is supposed. In work the estimation of key parameters of the division unit, without which the process of submicron powders separation is impossible is carried out. The estimation of resolution of the received device is made for division unit with the sizes of about 0.5 μm .

Result of work became the draft design of unit intended for division particles on fractions. The basic opportunity of realization of process of particles division with comprehensible resolution in a range about 50 nanometers is shown. The basic technical difficulties of realization of the given process are revealed. Work is development of researches submitted on the previous conference in the report "the Analysis of an opportunity of application the plasma discharge for clearing powders of the micron size".

LOW TEMPERATURE ECR PLASMA TECHNOLOGY TOWARDS NANOSCALE DEVICES CREATION

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Low temperature ECR plasma has apparent advantages for nanotechnology applications. Among them are high plasma density (up to 10^{13} cm^{-3}) and low energy of plasma particles (20–30 eV with absence of external bias) and low working pressure (10^{-3} Torr). Low level of energy flow going down to a sample opens the way to use sensitive materials as a substrate. However, further improvements and optimizations for both etching and deposition processes are required for a nanoscale objects treatment. The suitable parameters to be tuned are bias voltage applying to a substrate surface and power of magnetron and configuration of shields and reflectors are placed in reactor etc. The main tasks are solved consist of removing plasma glow region from wafer and increasing of plasma uniformity for reproductivity of processes to be grown.

By optimization of plasma parameters for nanometer resolution targets so-called "gecko-style" dry nanoadhesives were already obtained [1]. The nanoadhesives are constituted from pillars with length 700 nm and width 400 nm etched in a bulk of polyimide. The mask was constructed by optic lithography onto 6 cm^2 square surface. Also, sensing elements of tunnel accelerometers were minimized down to 500 nm [2].

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**UTILIZATION OF HIGH ENERGY ELECTRIC
DISCHARGE TECHNIQUES FOR PRODUCTION
OF CARBON NANOMATERIALS**

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New technologies were developed for manufacturing of novel carbon nanomaterials (CNM)—amorphous carbon, fullerene-like clusters of the C₆₀–C₇₀ types and higher, nanotubes, nanodiamonds, etc.—with use of the methods of electrical wire explosion and electric breakdown of organic liquids.

The suggested methods are characterized by an impact of high temperatures and pressures (which amount to 10000 K and 300–500 MPa, respectively), electrical and magnetic field on the material. It causes an evaporation of carbon in the form of clusters, plasmochemical reactions of synthesis with following ultraspeed quenching of the reaction products, what results in appearing new allotropic forms of carbon. It has been ascertain the effective possibility to control the spectral composition of the produced CNM through variation of the time-energy parameters of the synthesis process, type of material (graphite, iron, nickel, copper and others) and surrounding mediums (toluene, kerosene, ethanol, hexane and others), and catalyst use.

DEVELOPMENT AND EXPERIMENTAL INVESTIGATION OF THE CARBON NANOTUBES SYNTHESIS PROCESS USING A PLASMA TORCH

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The work consists in the experimental investigation of the influence of pressure, type of gas (helium and argon), carbon vaporization speed, and bimetallic catalyst (Ni and Co) concentration on the synthesis of carbon nanotubes in the plasma jet reactor [1, 2]. The main goal is development of highly productive process of carbon nanotubes synthesis from the carbon powder in the thermal plasma jet. In this study the synthesis occurs in the plasma volume during the simultaneous vaporization of fine-dispersed carbon and catalyst. The final goal of this investigation is the optimization of the synthesis process in the plasma jet reactor using a specific dc plasma torch with expanding anode channel.

Plasma torch with 10–20 kW power input with argon and helium as working gas was used in experiments. Current value varied in the range 150–300 A. Soot, nickel and cobalt were used as material input. Mass rate of soot was in the range 0.15–1 g/min, weight concentration of bimetallic catalysts being 6 and 15%. Parameters of experiment with the argon are as follows: gas flow rate 1–3.6 g/s under 300–500 Torr during 45–60 min. Corresponding parameters with the helium: gas flow rate 0.4 g/s under 300 Torr during 15 min. The analysis of carbon-bearing products on the metallic target using Raman spectroscopy shows that in the spectrum there are thin lines representatives for single-layer carbon nanotubes.

The intensity of carbon vaporization into soot reached up to now at the existing installation makes 1 g/min and if synthesis efficiency would reach 20–70% the rate of production of nanotubes would surpass the corresponding figures for the installations using arc discharge, and the hope for the 20–25 times greater nanotubes production rate appears. Taken into consideration the possibility of steady state work, limited only by the resource of replaceable cathode, the selected approach shows certain feasibility.

Results obtained demonstrate the possibility of carbon nanotubes synthesis in a wide range of parameters, and the determination of the optimal conditions for the synthesis would be possible.

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EXPERIMENTAL AND THEORETICAL INVESTIGATION OF THE PLASMA TORCH WITH EXPANDING CHANNEL FOR THE COATING PURPOSES

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For the sake of investigation the special designed plasma torch was developed with the electric arc of self-establishing length in the expanding channel. In experiments a number of plasma torch parameters were measured for different regimes of the plasma spraying. The influence of regime technological parameters and of the composition of plasma forming gases on the plasma torch operation and the spraying process was investigated. Practically important fact was established: three-fold increase of the voltage and arc power occurs due to the addition of the nitrogen. This is in well concord with other spraying experiments [1].

Corundum particles velocities after the plasma torch nozzle were measured using the visualization method, that was realized by the infra-red and high-speed cameras. They were focused on the location 10 cm downward from plasma torch nozzle [2]. Particles were illuminated by laser beam. Track processing program was providing the velocity and the particle temperature. Using tracks got by high-speed camera, there was a possibility of manual determination of particle velocity. Measured data were compared with results of numerical modeling.

Based upon [3] the system of differential equations use derived for the velocity and the temperature of the carrying gas and of corundum particles. Average values were considered as particle temperature (the temperature drop between the center and the surface of the particle being assessed as negligible). For the particles with diameter 40–60 μm a comparison was performed of the results of numerical modeling with measured data. The coincidence may be considered as well satisfactory.

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DEVICE FOR FREQUENCY PUMPING OF Ar-Xe-LASER BY A NON-SELF-SUSTAINED DISCHARGE

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Main problems during creation of Ar-Xe-lasers with a high average lasing power are concerned with both formation of powerful rep-rated pumping pulses and heating of gas mixture. A device which provides solution of the both problems is presented here. The device is a special removable block attached to a multi-functional laboratory complex. The complex is described in [1].

The removable block is a vacuum diode with a longitudinal explosive emission cathode and gas chamber for a formation of non-self-sustained volume discharge initiated by electron beam. An electron beam and discharge pulse have the following parameters: energy of beam electrons up to 170 keV, beam current up to 25 A, beam pulse duration 5–10 ns, beam cross-section 20 cm per 3 cm, voltage on the discharge gap up to 20 kV, discharge current up to 1 kA, discharge pulse duration up to 200 ns, pulse repetition rate up to 50 Hz.

In experiments [2] maximum pulse repetition rate of lasing (25 Hz) was limited by parameters of electron accelerator and supply circuit of non-self-sustained discharge. Moreover, high electric field strength resulted in increase in possibility of contraction of the volume discharge. Our device allows to use more optimum pumping pulse duration and lower values of electric field strength. Average pumping power may be increased by growth of pulse repetition rate.

It is shown [3] that limitation of lasing power during frequency pumping of Ar-Xe-laser by pulsed electron beam is explained by heating of working gas mixture. Our device provides an effective cooling of the gas mixture in close cycle by pumping the mixture through a liquid-nitrogen-cooling chamber.

All these features of the device will allow to obtain frequency Ar-Xe-lasing with a high average power.

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PLASMA NEEDLE WITH FIBER SYSTEM FOR INPUT-OUTPUT AN OPTICAL RADIATION

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Last years rf electric discharge atmospheric pressure such as plasma needles it was investigated by various authors [1, 2] in connection with possible medical applications. We develop the shaper of a plasma needle supplied with fiber system for input-output of the optical radiation. For this purpose the quartz optical fiber in diameter of 500 microns was used. The axis of a plasma needle and an optical axis of a fiber were colinearity. Thus we had an opportunity to brighten a torch plasma needle and an area of interaction of plasma with object various using laser sources. For this purpose the first and second harmonics of YAG-Nd laser, the nitrogen laser or the dye laser have been used. Using of laser radiation allows to excite various radicals and molecules contained both in a torch of a plasma needle, and on a surface of object selectively. At a conclusion of radiation with the help of a fiber we investigate radiating spectra interactions of plasma needle corresponding to three modes an operation with biological object. The first mode is a mode of on object top of free torch of a plasma needle practically. Next modes are a transitive mode with the increased current of influence and mode rf of an arch. Study of spectra has shown that they adequately reflect a corresponding mode of process of interaction of plasma with object. Last circumstance enables to organize in further effective opto-electronic system of a feedback intended for management of operating modes of a plasma needle.

In the report the measured parameters of a plasma needle are represented geometrical factors, thermal power, rotary and oscillatory temperatures the molecules of nitrogen determined on spectra, also parameters of laser radiation to pass through the torch of a plasma needle.

This work is a part of final work a degree on the engineer executed on department of laser engineering and biomedical optics of TU IFMO.

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AUTHOR INDEX

- Abdrashitov A.V., 211
Abdulagatov I.M., 170
Adams J., 179
Adushkin V.V., 90
Adzhiev A.H., 137
Agranat M.B., 21–24, 31
Aksenov A.G., 57
Akunets A.A., 51
Aleksandrov A.L., 209, 210
Amirov R.H., 173, 216, 224
Anan'ev S.S., 50, 51
Andreev N.E., 25–27, 38, 143
Andreev V.G., 167
Andrievskaya V.U., 137
Anisimov S.I., 21, 22, 24
Antipov S.N., 198, 205
Apfelbaum E.M., 54, 144, 188
Ariskin D.A., 209, 210
Ashitkov S.I., 21–24
Asinovsky E.I., 165
Avdonin V.V., 80
Azizi N., 39
Babushkin A.N., 157, 158
Baev V.P., 167
Bagdasarov G.A., 53
Bakhmutova A.A., 36
Baklanov D.I., 120, 128, 129
Bakshaev Yu.L., 50, 51
Bakulin V.N., 61
Balagansky I.A., 112
Barabanenkov M.Yu., 192
Bardin A.A., 222
Barenbaum A.A., 108
Bartov A.V., 50
Basharin A.Y., 162–165
Baturin V.A., 146, 147
Bayandina D.V., 201
Bayandin Yu.V., 88, 89
Bazhenova T.V., 122
Bekuliva I.Z., 28
Belevtsev A.A., 217
Belyakov A.A., 78
Belyatinskaya I.V., 78
Benuzzi-Mounaix A., 35
Berry R.S., 145
Bessmertnyh A.V., 133
Bezruchko G.S., 76, 77
Bisti V.E., 66
Blinov P.I., 50, 51
Bogachev S.S., 202
Bogomaz A.A., 215
Boguslavskii L.Z., 223
Boldarev A.S., 34
Bolton P., 34
Bonitz M., 178
Borodina T.I., 75, 78
Borzov D.N., 148
Bragin M.V., 123
Brambrink E., 35
Bronin S.Y., 127
Budin A.V., 215
Bugay I.V., 62
Bukharkina T.V., 168
Bulanov S.V., 34
Bulgakova N.M., 42
Bulgakov A.V., 42
Burov Yu.M., 117
Chernenko A.S., 50, 51
Chikina J.V., 212
Chinnov V.F., 217
Cros B., 27
D'yachkov L.G., 205, 207, 208
Daido H., 34
Daito I., 34
Dan'ko S.A., 50, 51
Darian L.A., 54, 219

Davydov I.A., 106
 Degtyareva O., 142
 Degtyareva V.F., 142
 Demchenko N.N., 32
 Dementiev Yu.A., 54
 Demidova E.V., 82
 Demidov V.S., 82
 Demin D.A., 106
 Deputatova L.V., 202
 Dikinov H.J., 137
 Dinariev O.Yu., 176
 Director L.B., 132, 133
 Dobrinskiy E.K., 167, 168
 Dolov M.Kh., 169
 Doskoch I.Ya., 32
 Dozhdikov V.S., 163
 Drakon A.V., 125
 Dubovskoy A.N., 90
 Dudin S.V., 55, 56, 82
 Dyachenko S.V., 53
 Efimchenko V.S., 155
 Efremov K.V., 136
 Efremov V.P., 54, 118
 Egorov O.G., 220
 Emelianov A.V., 124, 127
 Eremin A.V., 70, 124–127
 Evseev N.V., 176
 Faenov A.Ya., 34, 35
 Falyakhov T.M., 128
 Fedorov V.Yu., 30
 Fedulov M.V., 183
 Fel'dman V.I., 78
 Filatov I.E., 226
 Filinov V.S., 178
 Filippov A.V., 204
 Fortova S.V., 57, 103
 Fortov V.E., 25, 27, 54–56, 74, 75,
 82, 101, 102, 118, 124,
 178, 181, 197, 198, 207,
 221
 Frenkel M.M., 170
 Fridman V.B., 59
 Frolova N.Yu., 84
 Fruchart D., 223
 Fukuda Y., 34
 Galburt V.A., 113
 Ganiev A.S., 192
 Gasilov S.V., 34
 Gasilov V.A., 34, 53
 Gatskevich E.I., 46
 Gavrikov A.V., 200, 206
 Gericke D.O., 32
 Ghoranneviss M., 39
 Ghorbanalilu M., 40
 Glazkov V.S., 83
 Glazkov V.V., 225
 Golovastov S.V., 121, 128, 129
 Golubev A.A., 36, 82
 Golub V.V., 119–122, 128, 129
 Golyshev A.A., 81
 Goncharov A.V., 189
 Gordon E.B., 154
 Gorelski V.A., 99
 Gorshkov A.B., 147
 Goryachev S.V., 217
 Grafutin V.I., 199
 Gregory C., 35
 Griбанov V.M., 63
 Grinenko A.Yu., 32
 Grushin A.S., 140
 Gryaznov V.K., 181
 Gurentsov E.V., 70
 Gus'kov S.Yu., 32, 33
 Habibi M., 40
 He X.T., 39
 Hihluha D.R., 190
 Hokamoto K., 112
 Homma T., 34
 Hora H., 39
 Ignatova O.N., 83

Inogamov N.A., 21–24
 Iorish V.S., 54
 Iosilevskiy I.L., 178
 Isakaev E.Kh., 217, 224
 Ivanov A.V., 105
 Ivanov D.S., 20
 Ivanov E.N., 116
 Ivanov K.V., 120, 129
 Ivanov M.F., 54, 113, 114, 116
 Ivaschuk L.I., 223
 Ivlev A.V., 203
 Ivlev G.D., 46
 Izvekov O.Y., 97
 Kalinin Yu.G., 50, 51
 Kameshima T., 34
 Kandidov V.P., 30
 Kando M., 34
 Kanel G.I., 73, 76, 77
 Kantsyrev A.V., 82
 Kanunova L.I., 74
 Karpenko S.V., 159
 Kashkarov A.O., 109
 Kashtanov P.V., 154, 189
 Kato Y., 34
 Kawachi T., 34
 Kawase K., 34
 Kazakov E.D., 27, 50, 51
 Kedin N.A., 69
 Kedrov V.V., 45
 Keshev R.M., 28
 Kheifets O.L., 157, 158
 Kheifetz A.E., 84
 Khishchenko K.V., 25–27, 54, 74,
 76, 77, 81, 102, 107, 142,
 143, 156
 Khizriev K.Sh., 152
 Khokhlov V.A., 22, 24
 Khokonov A.Kh., 169
 Khokonov M.Kh., 28
 Khomkin A.L., 187
 Khomskaya I.V., 84
 Khorev I.E., 99
 Khrapak A.G., 79, 127
 Kimura T., 34
 Kim V.V., 58
 Kingsep A.S., 50
 Kiseev S.V., 175
 Kiselev V.I., 165, 224
 Kislenko S.A., 173
 Kiverin A.D., 54, 113, 114
 Klassen N.V., 45
 Klimovskii I.I., 166–168
 Kochesokov G.N., 169
 Koenig M., 35
 Kolesnikov S.A., 82, 194
 Komarov P.S., 21, 22, 30
 Komissarov V.V., 74
 Konovalov V.S., 195
 Konyukhov A.V., 101, 102
 Koptseva A.A., 153
 Korolev V.D., 50, 51
 Kosarim A.V., 193
 Kosov V.F., 133, 135
 Kosov V.V., 135
 Koss X.G., 213
 Kostanovskaya M.E., 49
 Kostanovskiy A.V., 49, 59
 Kostanovskiy I.A., 208
 Kostenko O.F., 25–27, 38
 Kostin V.A., 43
 Kostyukov I.Yu., 29, 30
 Kotaki H., 34
 Kouhi M., 39
 Kovalchuk A.V., 222
 Kovalev A.E., 74, 81
 Kozlov A.N., 195
 Kozlov A.V., 55, 219, 221
 Kraiko A.N., 130
 Krivko O.A., 45
 Krukovsky A.Yu., 53

Kryzhevich D.S., 92
 Kudinov I.V., 176
 Kudrenko E.A., 45
 Kuehl Th., 27
 Kuksin A.Yu., 92, 93
 Kulikauskas V.S., 59
 Kulikov S.V., 125
 Kulipanov G.N., 75
 Kuper K.E., 110
 Kurilenkov Yu.K., 33
 Kuskova N.I., 223
 Kuznetsova I.V., 215, 227
 Kuznetsov D.L., 226
 Kuznetsov S.V., 27
 Kuzovnikov M.A., 149
 Lankin A.V., 184–186
 Laskin I.N., 122, 129
 Lavrov V.V., 56
 Lenkevich D.A., 129
 Leont'ev A.A., 55, 56
 Levashov P.R., 25–27, 107, 142,
 143, 156, 178
 Likhachev A.P., 101, 102
 Lin Z., 20
 Lisanov M.V., 136
 Lisin E.A., 214
 Loktionov E.Yu., 41
 Lomonosov I.V., 74, 102, 141
 Lorenzen S., 179
 Losev S.Yu., 215
 Loupias B., 35
 Lozitski I.M., 106
 Lukyanchikov L.A., 75, 109
 Lukyashin V.E., 36
 Luzganov S.N., 219, 221
 Lysenko I.Y., 164, 165
 Maikov I.L., 71, 132, 133, 135
 Maiorov S.A., 198
 Makarov D.V., 123
 Makeich A.A., 124, 126
 Malashin S.I., 167, 168
 Malekynia B., 39
 Malevich V.L., 46
 Malyshev A.N., 83
 Malyshev A.V., 221
 Mamchuev M.O., 160
 Manikandan P., 112
 Manohin A.A., 201
 Manoshkin A.B., 194
 Manykin E.A., 190
 Marchenko V.A., 53
 Markov A.V., 133
 Martino G., 36
 Matrosov A.D., 112
 Matveichev A.V., 58
 Maynard G., 27
 Melnikova N.V., 157, 158
 Mendeleev V.Y., 165
 Merkulov V.V., 224, 225
 Merzhievsky L.A., 109
 Mezhevov A.B., 74
 Mikushkin A.Y., 121
 Miley G.H., 39
 Milyavskiy V.V., 75, 76, 78, 111
 Mingaleev A.R., 52
 Mintsev V.B., 55, 56, 82, 181
 Mironchik A.I., 60
 Miyoshi H., 112
 Mizhiritsky V.I., 50
 Mohammadi M.O., 40
 Molkov V.V., 123
 Molodets A.M., 79, 81
 Mora P., 27
 Mordinsky V.B., 225
 Morfill G.E., 203
 Moslehi Moslehabadi A.M., 40
 Murtazaev A.K., 150, 152
 Mutailamov V.A., 150
 Myasnikov M. I., 191
 Nadezhin S.S., 83

Nagorskiy N.M., 35
 Naimark O.B., 87–89
 Nasonov P.A., 84
 Nasretdinov Y.A., 173
 Nazin S.S., 212
 Nerush E.N., 30
 Nikolaenko I.V., 69
 Nishihara K., 22–24
 Norman G.E., 94, 184, 186, 212
 Novikov M.G., 74, 81
 Novikov N.L., 221
 Novikov V.G., 140, 183, 195
 Oborin V.A., 89
 Olkhovskaya O.G., 53
 Oreshkin V.I., 223
 Ostriuk A.V., 61–64, 147
 Ovchinnikov A.V., 21, 30, 31
 Ovechkin A.A., 140
 Palmichenko A.V., 80
 Panin V.V., 194
 Parfenov N.A., 91
 Parshikov A.N., 105
 Pasko E.G., 86
 Peletsky V.E., 174
 Pernik L.M., 90
 Petrenko M.V., 215
 Petrovsky V.P., 31
 Petrov A.A., 216
 Petrov A.M., 106
 Petrov O.F., 197, 198, 200, 205–
 207
 Petrov Yu.V., 21–24
 Petukhov V.A., 113
 Pikalov G.L., 175
 Pikuz Jr. S.A., 35, 36
 Pikuz S.A., 50, 52
 Pikuz T.A., 34, 35
 Pimenov V.G., 51
 Pinchuk M.E., 215
 Pinigina K.S., 158
 Pisarev V.V., 94
 Piskunov V.N., 106
 Podurets A.M., 83
 Pokhil G.P., 59, 60
 Polistchook V.P., 54, 165, 219
 Polushkin E.A., 222
 Polyakov D.N., 203
 Popel S.I., 90
 Postovarov P.I., 201
 Potashevsky S.S., 194
 Povareshekin M.N., 219, 221
 Povarnitsyn M.E., 25–27, 107
 Pozubenkov A.A., 215
 Presnyakov D.V., 49
 Privalov V.E., 47
 Prokopiev E.P., 199
 Protasov Yu.Yu., 41
 Pruel E.R., 75, 109, 110
 Psakhie S.G., 91, 92, 211
 Pustynnik M.Y., 203
 Röpke G., 179, 181, 182
 Rabec le Gloahec M., 35
 Radchenko A.V., 98
 Radchenko P.A., 98
 Raevsky V.A., 83
 Rainish V.A., 221
 Raitza Th., 179
 Raybul S.V., 47
 Razinkova T.L., 199
 Razorenov S.V., 76, 77
 Reinholz H., 179, 181, 182
 Reutov B.F., 170
 Romadinova E.A., 61, 64
 Romanova V.M., 52
 Rosmej O.N., 27
 Rozanov V.B., 32
 Rudenko V.V., 106
 Rud A.D., 223
 Rusin S.P., 65
 Rutberg Ph.G., 215

Rykov V.A., 202
 Saakyan A.G., 174
 Saitov I.M., 186
 Saleh Kotahi M.O., 40
 Samoylov I.S., 165, 173, 216
 Savintseva S.A., 68
 Savintsev Yu.P., 68
 Savinykh A.S., 76, 77
 Savin S.F., 207
 Schardt D., 36
 Schweigert I.V., 209, 210
 Semin N.V., 119, 122, 128
 Sengebusch A., 179
 Sergeev O.V., 172
 Severov D.S., 192
 Shabashova O.A., 157
 Shakaryan Yu.G., 221
 Shakhray D.V., 79, 80
 Shakirov E.F., 157
 Shapoval S.Yu., 192, 222
 Sharkov B.Y., 82
 Shelkovenko T.A., 50, 52
 Shemanin V.G., 47
 Shemyakin O.P., 156
 Shevchenko V.S., 68
 Shevelko V.P., 193
 Shikin V.B., 212
 Shipachev A.N., 100
 Shishakov V.V., 170
 Shorokhov E.V., 84
 Shpatakovskaya G.V., 139
 Shpilrain E.E., 133
 Shumikhin A.S., 187
 Shumova V.V., 118
 Shurupova N.P., 55, 221
 Shurupov A.V., 54–56, 219, 221
 Shurupov M.A., 221
 Shur B.A., 174
 Shustov Ye.N., 225
 Shutov A.V., 82, 104
 Shveikin G.P., 69
 Sidorov N.S., 80
 Silaev A.A., 43, 44
 Simonov I.V., 103
 Sin'ko G.V., 142
 Sinelshchikov V.A., 133, 135
 Sinkevich O.A., 225
 Sitnikov D.S., 21
 Skobelev I.Yu., 34
 Skovorod'ko S.N., 165
 Skripnyak E.G., 86
 Skripnyak V.A., 85, 86
 Skripnyak V.V., 85
 Smekhova A.G., 117
 Smirnova E.A., 51
 Smirnov B.M., 37, 145, 154, 189,
 193
 Smirnov G.N., 82
 Smirnov N.A., 142
 Smirnov V.P., 50
 Sobina O.A., 164, 165
 Sofyin A.S., 136
 Sokhareva N.S., 158
 Sokol G.F., 133
 Solomyannaya A.D., 183
 Sosikov V.A., 96
 Stadnichenko I.A., 112
 Starikov S.V., 171
 Stegailov V.V., 94, 144, 171–173,
 212
 Steinman E.A., 67
 Stepanov R.V., 32
 Sumskoï S.I., 136
 Surkov Yu.S., 226
 Tahir E., 20
 Tahir N.A., 58
 Tajima T., 34
 Tarakanov V.P., 33
 Tarasenko I.N., 128
 Ten K.A., 75, 109, 110

Ter-Oganesyan A.E., 52
 Tereshonok D.V., 196
 Thomas D.A., 20
 Thomas H.M., 203
 Timirkhanov R.A., 206
 Timofeev A.V., 212
 Tishkin V.F., 32
 Titov V.M., 75, 109
 Tkachenko S.I., 50, 52, 53
 Tolochko B.P., 75, 109
 Torchinsky V.M., 71
 Troshkin O.V., 57
 Tsirlina E.A., 27
 Tsyba N.E., 219
 Turchaninov M.A., 163–165
 Turtikov V.I., 82
 Tyulina N.A., 85
 Tyupanova O.A., 83
 Uchvatov A.N., 219, 221
 Urakaev F.Kh., 68
 Ushakov A.A., 84
 Ushnurtsev A.E., 55, 56
 Ustroev G.I., 50, 51
 Ustyuzhanin E.E., 170
 Utkin A.V., 82, 96
 Uvarin V.V., 226
 Uvarov S.V., 88, 89
 Valiano G.E., 75
 Valiyev Kh.F., 130
 Vasilieva E.V., 206
 Vasiliev M.M., 205, 207
 Vasiliev M.N., 200, 201
 Vasilyak L.M., 203
 Vaulina O.S., 197, 213, 214
 Vergunova G.A., 32
 Verzhichinskaya S.V., 168
 Veselov R.A., 106
 Vetchinin S.P., 203
 Veysman M.E., 25, 27, 143
 Vichev I.Yu., 183
 Vikhrev V.V., 51
 Vladimirov V.I., 202
 Vlasov A.N., 194
 Vokhmyanina K.A., 60
 Volkov G.S., 183
 Volkov S.A., 227
 Volodin V.V., 120, 128, 129
 Vorob'ev V.S., 144
 Vorona N.A., 200
 Voronin B.L., 106
 Vvedenskii N.V., 43, 44
 Wierling A., 179, 182
 Winkel M., 182
 Yakhin R.A., 32
 Yanilkin A.V., 93
 Yankovskiy B.D., 111
 Zaitchenko V.M., 71, 133, 135
 Zaitsev V.I., 183
 Zakharenkov A.S., 107
 Zakharov A.F., 199
 Zakharov V.S., 183
 Zaporozhets Yu.B., 181
 Zashakuev Z.T., 137
 Zeldovich V.I., 84
 Zelener B.B., 190
 Zelener B.V., 190
 Zelenin A.A., 50, 51
 Zelepugin S.A., 100
 Zhakhovskii V.V., 22–24
 Zhernokletov M.V., 74, 81
 Zhgiliev I.N., 84
 Zhigilei L.V., 20
 Zhilyaev P.A., 93, 94
 Zhilyakov L.A., 59
 Zhirnov K. V., 37
 Zhogin I.L., 109
 Zhukov A.N., 80
 Zhukov V.P., 42
 Zhulanov V.V., 75
 Ziborov V.S., 118

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Zobnin A.V., 207

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