

ЛАЗЕРНОЕ ВОЗДЕЙСТВИЕ LASER IRRADIATION

РАСЧЁТНОЕ МОДЕЛИРОВАНИЕ УПРАВЛЕНИЯ ШИРОКОАПЕРТУРНЫМ АДАПТИВНЫМ ЗЕРКАЛОМ ЛАЗЕРНОЙ УСТАНОВКИ «ЛУЧ», ОСНОВАННОГО НА СТОХАСТИЧЕСКОМ ПАРАЛЛЕЛЬНОМ ГРАДИЕНТНОМ АЛГОРИТМЕ

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Численно исследованы методы управления поверхностью широкоапертурного 61-элементного адаптивного зеркала, применяемого в оптической схеме лазерной установки «Луч», основанные на использовании для расчёта управляющих напряжений стохастического параллельного градиентного (СПГ) алгоритма и метода наименьших квадратов (МНК). Найдены предельные возможности адаптивного зеркала по компенсации aberrаций лазерного пучка. Применяя СПГ алгоритм, можно получить более эффективную коррекцию aberrаций по сравнению с реализованной в эксперименте при стандартном управлении адаптивным зеркалом на основе измерения фазы датчиком волнового фронта. Предложен комбинированный метод управления адаптивным зеркалом на основе СПГ алгоритма и МНК, который дает возможность получения доли лазерной энергии в дифракционном угле $\sim 40\%$ и числа Штреля на уровне 0.4.

THE NUMERICAL SIMULATION OF THE WIDE-APERTURE ADAPTIVE MIRROR CONTROL ON THE LUCH LASER FACILITY BASED ON THE STOCHASTIC PARALLEL GRADIENT ALGORITHM

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The methods of the control of a wide-aperture 61-elements adaptive mirror implemented on the Luch facility are numerically investigated. These methods are based on the stochastic parallel gradient algorithm and the least-squares approach for control voltage calculation. The capability of the adaptive mirror is determined as regards to correction of phase aberrations. By means of stochastic parallel gradient algorithm it is possible to obtain more efficient correction of the laser beam aberrations in comparison with that realized in the experiments under conventional adaptive mirror operation mode based on the phase measurement by a wavefront sensor. A combined method (based on the stochastic parallel gradient algorithm and least-squares approach) of adaptive mirror control is proposed. By means of this method it is possible to obtain the laser energy in diffraction angle on a level of 40% and the Strehl number at a rate of 0.4.

NOVEL APPROCHES IN LASER ASSISTED MASS SPECTROMETRY OF ORGANIC COMPOUNDS**S. ALIMPIEV**

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Three novel approaches in laser assisted mass spectrometry of organic compounds will be discussed. The first one SALDI (Surface assisted desorption ionization) is based on laser desorption of protonated organic molecules from nanoscale disordered semiconductor surfaces. The second one is a modification of SALDI technique named as Electron Transfer SALDI is based on laser desorption of molecular ions from semiconductor surface. The third one APLPI (Atmospheric pressure laser plasma ionization) is based on the proton transfer to organic molecule from water molecules ionized by short wavelength laser plasma radiation. This technique is very promising for MS analysis of samples at atmospheric pressure without any probe preparation and in real time scale.

SELF-OSCILLATING PROCESSES DURING THE LASER ABLATION OF CONSTRUCTION MATERIAL**O.G. TSARKOVA, A.A. RUKHADZE, S.V. GARNOV**

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In article features of dependences of the thermodynamic parameters received in experiments at influence of continuous laser radiation 1.3 μm with a pulse energy of 3.5÷90 kJ on the carbon silicon carbide composite material (CSCM) samples [1-2] are analyzed. Intensive ($q=1\div5$ of kW/cm^2) laser heating to temperatures of 1500-3600 K leads to ablation of the material to form the plasma, a plurality of chemical reactions, phase transitions and structural physical and chemical transformations in a sample. Associated with the size of the irradiation spot a specific feature is found. The temperature distribution over the sample volume and effectiveness of the ablation are dependent on the spot size both explicitly and implicitly. These effects are manifested even at identical values of power density of radiation. A set of processes at the interaction of intensive continuous laser radiation with UKKM causes oscillations with nonlinear feedback (self-oscillations) in the bulk and on a surface of the studied samples. It leads to a periodic change in the thermal physic characteristics of the heated area and as a consequence, to fluctuations in the values of the efficiency of the ablation material. Pronounced oscillations with 4÷5 peaks, lying in the limits of upper and lower envelopes, are traced in a variety of experimental graphics: stationary temperature, established on the sample surface, depending on the radiation power density; specific expenses of the laser energy on the ablation depending on the temperature; the ablation rate depending on the temperature; efficiency of the ablation depending on the radiation power density, etc. Besides, with the increase in time of influence of the radiation arises independent discharge on the back of the intact sample supporting burning even after the laser pulse and attenuation of the

plume on the front surface. This leads to the necessity of taking into account the bulk displacement of charge through the 3.5-mm layer of material and its emission from the opposite side.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ АДАПТИВНОЙ ОПТИЧЕСКОЙ СИСТЕМЫ МОЩНОЙ ЛАЗЕРНОЙ УСТАНОВКИ «УФЛ-2М» В РАЗЛИЧНЫХ КОНФИГУРАЦИЯХ

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Проведено численное моделирование распространения лазерного излучения в 4-х проходной оптической схеме усилительного канала мощной лазерной установки УФЛ-2М при наличии аберраций оптического тракта. С помощью различных вариантов использования адаптивной оптики исследована коррекция оптических аберраций, приобретаемых пучком по мере прохождения тракта усилительного канала. Для управления адаптивным зеркалом применен стохастический параллельный градиентный алгоритм. В расчетно-теоретических исследованиях на основе анализа пространственной структуры пучка в диафрагмах пространственных фильтров силового канала определены оптимальные варианты применения адаптивной системы на установке УФЛ-2М с одним и двумя адаптивными зеркалами и даны рекомендации по её конфигурации.

THE NUMERICAL MODELING OF ADAPTIVE OPTICAL SYSTEM OF THE UFL- 2M POWERFUL LASER FACILITY AT VARIOUS CONFIGURATIONS

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The numerical simulation of the laser beam propagation in 4-pass optical scheme of the amplifier section of the UFL-2M powerful laser facility is carried out at aberrations presence in the optical tract. Considering the different configurations of adaptive optical system, we investigate the correction of the optical aberrations that are attained by the beam during its propagation through the amplifier section. The stochastic parallel gradient algorithm is

implemented for control by the adaptive mirror. In the calculations the optimal variants of UFL-2M facility adaptive system with one and two adaptive mirrors are determined basing on the beam spatial structure analysis in the pinholes of the spatial filters of the amplifier section. The recommendations to adaptive system configuration are also given.

**ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ АВТОЮСТИРОВКИ УСИЛИТЕЛЬНОГО
КАНАЛА МОЩНОЙ ЛАЗЕРНОЙ УСТАНОВКИ «УФЛ-2М» С
ИСПОЛЬЗОВАНИЕМ СТОХАСТИЧЕСКОГО ГРАДИЕНТНОГО АЛГОРИТМА**

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Проведено численное моделирование процедуры автоматической юстировки 4-х проходного усилительного канала установки УФЛ-2М при наличии aberrаций в оптическом тракте. В основе процедуры юстировки лежит маркерный метод. Построена расчетная модель распространения излучения юстировочного пучка и световых маркеров ближней и дальней зоны в канале установки. Выделены три логических этапа автоюстировки и определен один из вариантов ее регламента. Для управления контрольными элементами применен стохастический параллельный градиентный (СПГ) алгоритм, который обладает рядом преимуществ по сравнению с обычным детерминированным подходом. Проведена модернизация СПГ алгоритма и определен один из вариантов целевой функции управления. В результате расчетов достигнута точность позиционирования пучка на выходе канала 1% от размера диафрагмы в дальней зоне и 0.1% от размера апертуры пучка в ближней зоне, что с запасом удовлетворяет предъявляемым требованиям к точности юстировки. Однако найдено, что при наличии оптических неоднородностей в усилительном канале точность центрирования юстировочного пучка во внутренних диафрагмах может быть худшей, чем на выходе канала. Вероятно, эта проблема будет иметь место и при стандартном детерминированном управлении контрольными элементами.

**THE NUMERICAL SIMULATION OF THE AUTOMATIC ALIGNMENT
PROCEDURE OF AMPLIFIER SECTION OF THE UFL-2M POWERFUL LASER
FACILITY USING THE STOCHASTIC GRADIENT ALGORITHM**

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The numerical simulation of the automatic alignment procedure of 4-pass amplifier section of the UFL-2M facility is carried out at aberrations presence in the optical tract. The reference method lies in the base of the alignment procedure. The numerical model of the alignment beam propagation, near and far-field light markers propagation in a channel of the facility has been developed. Three logical stages of automatic alignment are defined and an alignment technical schedule is chosen. The stochastic parallel gradient (SPG) algorithm is implemented for management of the control elements. It possesses by a number of advantages as compared with a conventional deterministic approach. The SPG algorithm modernization is

performed and one of the variant of criterion functional is determined. As the result of calculations, the obtained accuracy of the beam positioning at the channel output is 1% of the far-field pinhole size and 0.1% of the beam aperture size in near field that satisfies the technical requirements to alignment accuracy. However, it is found that at the presence of optical aberrations in amplifier channel the centering accuracy of alignment beam in internal diaphragms can be less precise than that at the output of the channel. Probably, this problem will exist under conventional deterministic management of control elements as well.

TEMPERATURE MEASUREMENT OF HIGH ENERGY STATES OF METAL AND GRAPHITE INDUCED BY LASER PULSE

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We suggest to use an original system of calibration for optical scheme of brightness-temperature pyrometer that enables to make temperature measurements of high-heated surface up to $T \sim 105K$. Test measurement of melting points of high-melting metals such as W, Ta, Mo demonstrated coincidence of experimental results with table data, and relative error didn't exceed $\sim 5\%$. During research process we measured the dynamics of temperature, reflectivity and pressure change generated by the pulse of laser irradiation. For Al, the results received at ultra-thin samples agree with earlier data for massive samples. That makes the base for further development of perspective experimental method of "Thermally thin sample".

The result of experimental research enables to plot phase diagrams of laser heating process for Hg, Al and C-carbon in P-T coordinates.

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PLD GROWN THIN FILMS STOICHIOMETRY AND STRUCTURE STUDYV. M. Brendel¹, T. F. Yagafarov¹, S. V. Garnov¹, V. A. Terechin², U. A. Trutnev²¹ *Prokhorov General Physics Institute, Russian Academy of Sciences, 119991, Moscow, Vavilov Str., 38*² *FSUE RFNC - VNIIEF, 607188, Sarov, Nizhny Novgorod region, Mira Ave, 37
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Dielectric and semiconducting films on metal substrate are good candidates for photocathodes, which can withstand exposure to air [1]. Initially we used PLD technique to produce CsI, CsBr thin films on copper substrate and measured quantum yield of such photocathodes [2]. In this work we decide to carefully investigate stoichiometry and structure of PLD films. GaAs is chosen as promising material for durable photocathodes [3].

We have made thin films of CsI, CsBr and GaAs on dielectric substrates (glass). The films were made by pulse laser deposition with Nd:YAG electro-optically Q-switched laser. The laser parameters: wavelength 1064 nm, pulse duration - 20ns, the maximum pulse energy - 1000mJ, the maximum frequency - 20 Hz. Coating was carried out in a vacuum chamber with oil-free evacuation to 10^{-5} mbar. Coatings were deposited for 2 hours (20Hz) at various temperatures of substrate: room temperature, 50⁰ C, 100⁰ C. The laser pulse energy was minimal, but one in which the target ablation occurred. During the deposition process was performed manually adjust the focus of the laser spot on the target.

After production samples were transferred to stoichiometry and film structure study by X-ray diffraction analysis and scanning electron microscopy. We found that the stoichiometry of CsI and CsBr is ideally coincides with the initial state of target. GaAs films have increased Ga content in all our samples, including specially produced samples on Cu substrate. All films are polycrystalline with spherical clusters (fig. 1, fig. 2). Increase of substrate temperature leads to increase coating density in all cases.

We attribute stoichiometry breach with low laser energy density used. Laser density was kept small enough to produce plasma plume but no to produce a lot of smithers of target material on to deposited film. Melting point of both CsI and CsBr is about twice smaller than GaAs. So GaAs was not ablated properly, instead it was melted and a lot of Ga transferred to substrate because of much hire vapor pressure than As. To ensure our proposed explanation is correct additional experiments need to be done.

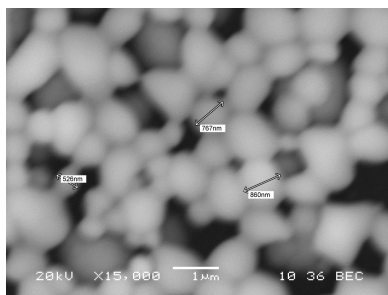


Fig. 1. CsBr film on glass (room temp).

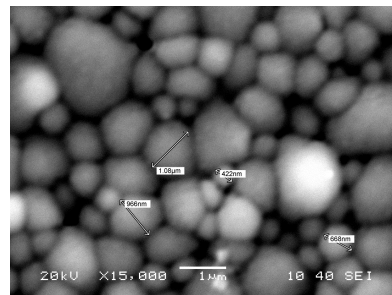


Fig. 2. CsI film on glass (room temp).

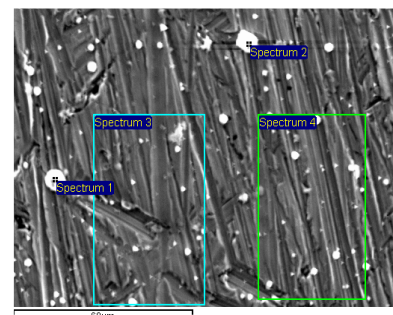


Fig. 3. GaAs film on Cu (room temp).

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**EXPERIMENTAL AND NUMERICAL STUDY OF FS LASER PULSE
PROPAGATION THROUGH C-SI BULK**

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Recently, a method of local structure modification inside various transparent materials has been demonstrated. The structure modification was caused by nonlinear absorption of fs laser pulses in the focal region (e.g. [1]). This method can be hypothetically applied to crystalline silicon as it has ability to change its structure to amorphous [2]. However, pulses of energies up to 100 μJ ($\lambda=1.2 \mu\text{m}$, $\tau=250 \text{fs}$, focused by 8mm aspherical lens) was found to be unable to induce any transformation in c-Si. Experimental and mathematical study of this phenomenon was performed.

Femtosecond interferometry experiments [3] revealed two specific features of fs pulse propagation through c-Si bulk. The first is high energy losses before focus, the second is formation of light filament up to several millimeters long. Simple calculations showed that two-photon absorption (TPA) is responsible for the energy losses. To study the nature of the filamentation, numerical solution of electromagnetic wave equation coupled with continuity equation for the free-carrier density was done. We used wave equation written for slowly varying envelope in paraxial approximation. Inclusion of nonlinear terms responsible to optical Kerr effect, TPA and plasma defocusing in the wave equation led to solution that was in qualitative agreement with experimental data (fig 1).

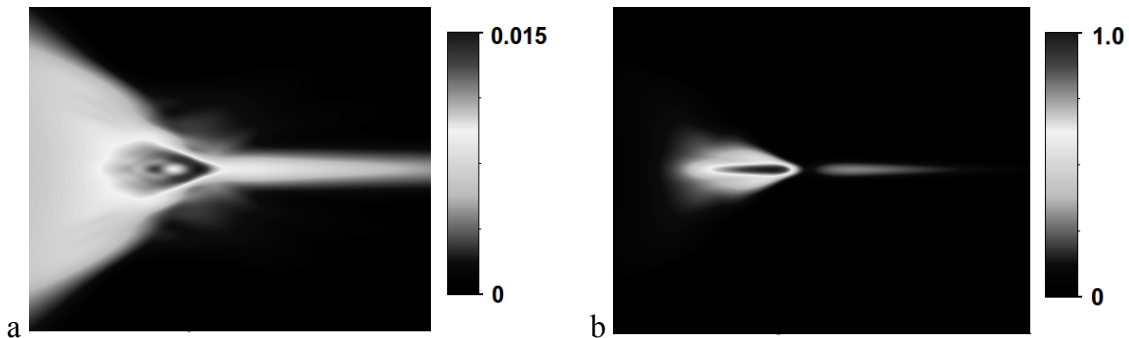


Fig.1 Simulation of 2 μJ laser pulse propagation through silicon: a) fluence map (J/cm^2); b) photo-induced free-carrier density map ($10^{19}/\text{cm}^3$). Map size is $2.5 \times 0.08 \text{mm}$.

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ELECTRO-OPTIC SYSTEM FOR TIME DEPENDENT DETECTION OF ELECTRICAL FIELD OF HIGH-POWER MICROWAVE NANOSECOND PULSES

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Electro optics (EO) is widely used nowadays for electric field measurement due to its intrinsic advantages such as absence of field disturbance, adequate sensitivity, high damage threshold and galvanic isolation of the instruments. There are several papers regarding electro-optic field sensing devices [1,2]. The papers demonstrate convenience of such technique, especially its flat frequency response, which could not be achieved with frequency-resonant antenna techniques. Investigation of radiation of broadband HPM sources poses a problem that the field magnitude and frequency differs at every point of the generator's aperture in each pulse [3]. Therefore for determination of actual field mode it is crucial to measure the field at different points of the aperture simultaneously. Such requirements could be met in a system of multiple EO crystals positioned all the way across the HPM generator horn aperture. We hereby present the results of creating one element of that system and measured signals from a conventional magnetron and experimental broadband plasma relativistic HPM source [4].

The experimental setup (shown in Fig. 1) consists of a 3 mW 1064 nm DPSS laser, Y-cut 5x5x5 mm lithium tantalate EO crystal, a quarter wave plate with polarizer for management of the working point and a fiber collimator to get the optical signal into a fiber cable. The fiber transported the signal to a 12 GHz NewFocus amplified photoreceiver model 1554-B mounted on a 16 GHz DPO71604C Tektronix oscilloscope.

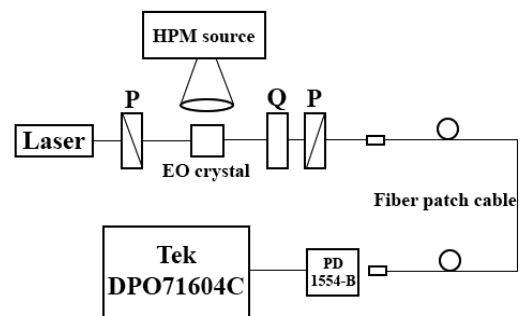


Fig. 1. Scheme of the EO system.
P – polarizers, Q – quarter wave plate

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ELECTRON DENSITY DYNAMICS OF FEMTOSECOND FILAMENT PLASMA CHANNEL IN GASES

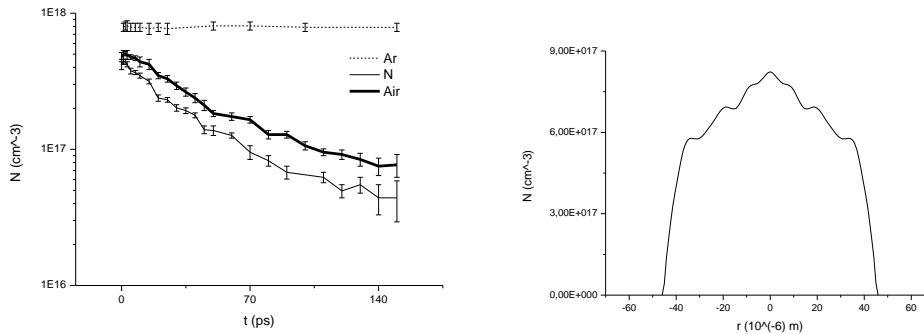
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We report results on decay of femtosecond filament plasma channel. The results for air, nitrogen and argon under atmospheric pressure conditions are obtained due to interferometry method[1,2]. Our investigation covers time scale from the formation of the filament plasma channel to 150 picoseconds after it for air, N₂ and 600 picoseconds for Ar. Patterns of phase shift due to plasma and corresponding electron density patterns are obtained.

Our results show that electron density decreases faster in N₂ than in air. Also they show that plasma channel in Ar exists much longer and its decay is negligible on 150 ps time scale.

We also studied formation stage of the femtosecond filament plasma channel. We report observation of phase shift due to Kerr effect which is necessary for the channel to appear.



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TUNABLE TWO-FREQUENCY σ -POLARIZED ND:YVO₄ -YVO₄ LASER

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The two-frequency nanosecond and picoseconds laser pulses can be efficiently converted in terahertz emitters and nonlinear optical crystals [1-3]. The general aim of our research is to obtain two-frequency emission with ps-pulse duration on vanadate crystal under longitudinal diode pump. The scheme of laser setup to demonstrate the capabilities of laser double-wavelength tuning is shown in Fig.1. As active laser elements, we used the a-cut composite Nd: YVO₄ - YVO₄. As a selecting element, we used an intracavity Fabry-Perot cavity standard [4] made of a YAG crystal in the form of a plane-parallel plates about 80, 97, 130, 270 μm thick. In this work, we proposed and realized a promising method of wavelength tuning for the a-cut (σ -polarization) YVO₄: Nd: YVO₄ crystal. Realized restructuring difference wavelengths in the range of 1.2 to 4.4 nm. Fig. 2. shows the output spectrum of the laser radiation at entry to the cavity FP standards in continuous generation. A stable two-frequency lasing at the ${}^4F_{3/2}$ - ${}^4I_{11/2}$ transition of the neodymium ion in YVO₄:Nd:YVO₄ crystals is obtained in the cw regime, acousto-optic Q-switched regime, active acousto-optic mode-locked regime.

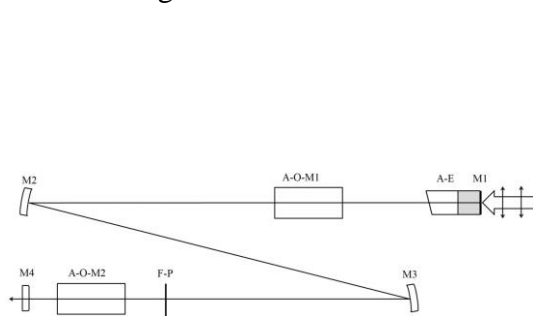


Fig.1. Scheme of the laser. M1- mirror deposited on the A-E, A-E – active element, A-O-M1,2 – acousto-optic modulators, M2,3 – spherical mirrors=340mm, F-P - Fabry-Perot cavity standard, M4 – output mirror.

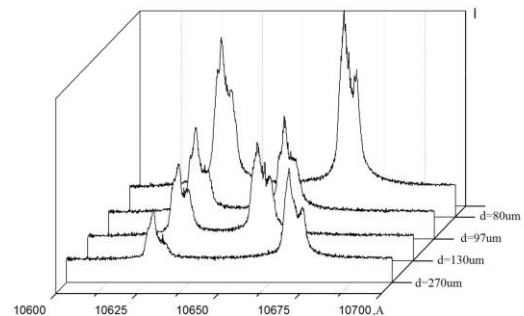


Fig.2. Dual-frequency spectrum of the radiation Nd: YVO₄-YVO₄-laser FP thickness 80, 97, 130 and 290 μm , respectively.

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PUMP-PROBE INTERFEROMETRY OF FEMTOSECOND LASER PLASMA

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The pump-probe technique of femtosecond laser plasma diagnostics is described. This technique is based on recording interference patterns of a laser plasma using a time-delayed probe laser pulse. We report results on studying of laser microplasma formation and femtosecond filamentation by pump-probe interferometry. The experimental results on plasma formation and decay are shown. Temporal profiles of the peak electron density and density distribution are presented.

Acknowledgements: The reported study was partially supported by RFBR, research project No. 12-02-31572.

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ВЗАИМОДЕЙСТВИЕ ЛАЗЕРНОГО ИЗЛУЧЕНИЯ С ГРАФЕНОМ И НАНОСТРУКТУРАМИ НА ЕГО ОСНОВЕ

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В последние годы графен стал одной из самых горячих тем в физике. Необычные электронные и оптические свойства, которые демонстрирует этот 2D материал, позволяют предложить широкий спектр будущих приложений для графена. Среди них: оптоэлектронные приборы, лазерные модуляторы, солнечные батареи и сверхбыстрые фотодетекторы. Однако, несмотря на интенсивные исследования свойств графена в последние годы, многие свойства остаются недостаточно исследованными.

Данная работа посвящена экспериментальному исследованию свойств графена и материалов на его основе при взаимодействии с интенсивным лазерным излучением. Результаты, полученные в данной работе, показали возможность использования новых материалов на основе графена в лазерах для генерации сверхкоротких импульсов (вплоть до фемтосекунд). Такой тип ультракоротких импульсных лазеров может быть использован в оптической обработке, связи, медицине. Другим перспективным результатом работы является демонстрация возможности использования графена в качестве эффективного источника электромагнитного излучения в терагерцовом диапазоне.

В докладе будет приведен обзор экспериментальных результатов исследования нелинейно-оптических свойств графена, полученных авторами.

**МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ
MATHEMATICAL MODELING**

**ATOMISTIC AND CONTINUUM APPROACHES TO MODELING THE
KINETICS AND DYNAMICS OF FAST PHASE TRANSITIONS INDUCED BY
ULTRASHORT LASER PULSES**

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We consider the results of modeling of the kinetics and dynamics of fast phase transitions in aluminum film induced by ultrashort laser pulses. We study the mechanisms of homogeneous and heterogeneous melting and crystallization, and spall phenomena in Al films. To describe the processes used atomistic and continuum approaches. On the continuum level used hydrodynamic nonequilibrium 2T model with a kinetic condition at the interface. Atomistic description is carried out within the framework of molecular dynamics with EAM potential. Figs. 1-2 shows the spatial condition of target and the spatial distribution of temperature and the hydrodynamic velocity at $t = 50$ ps.

The work was partially supported by RFBR grants №№ 12-07-00436a, 13-07-00597a.

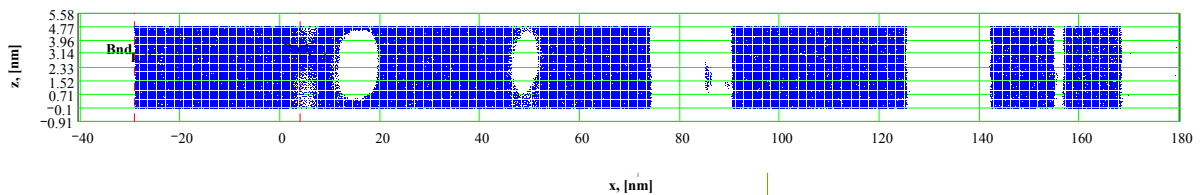


Fig. 1. The target condition at $t = 50$ ps.

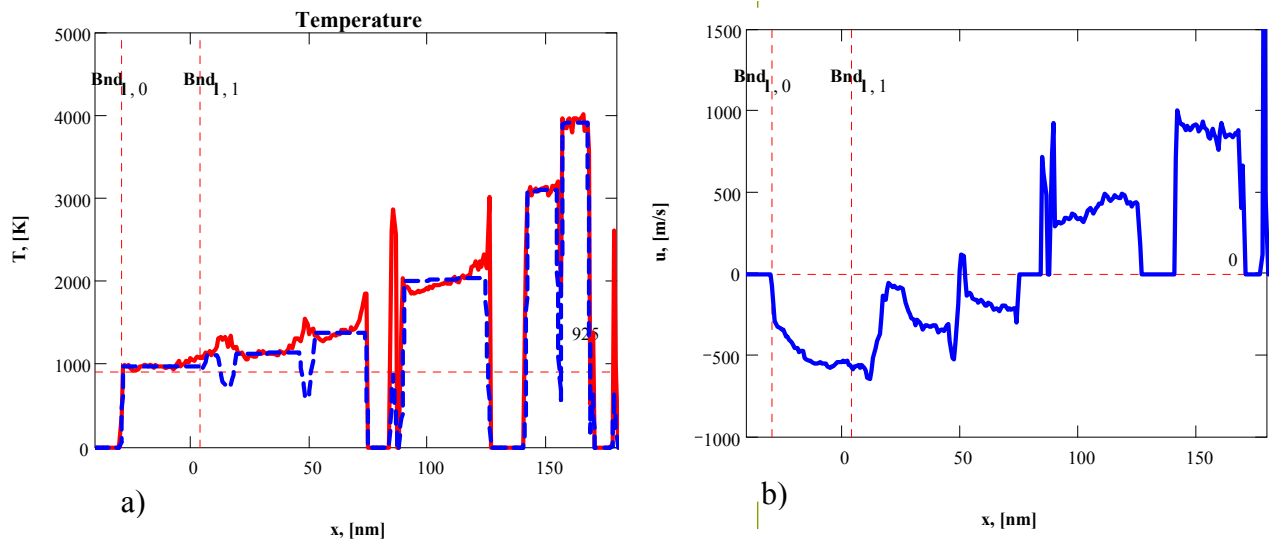


Fig. 2. The spatial distribution of temperature (a) and the hydrodynamic velocity (b) at $t = 50$ ps.

**МОЛЕКУЛЯРНО-ДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ
НЕРАВНОВЕСНОГО ФАЗОВОГО ПЕРЕХОДА ЖИДКОСТЬ-ПАР ПРИ
СУБНАНОСЕКУНДНОМ ОДНОРОДНОМ НАГРЕВЕ ТОНКОЙ ПЛЕНКИ**

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**MOLECULAR DYNAMIC CALCULATION OF NON-EQUILIBRIUM LIQUID-
VAPOR PHASE TRANSITION DURING SUB-NANOSECOND
HOMOGENEOUS THIN FILM HEATING**

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In the framework of molecular dynamics the behavior of thin liquid film during its rapid homogeneous heating with rate 2-100 K/ps is studied. The initial film thickness through the Z axis is 48 nm. The overall number of particles is 96 000 and the length of calculation area is 268 nm in that direction. In the film plane periodic boundary conditions were used with the main dimension 8x8 nm. The calculation results are presented in a form of distributions of temperature, density and particle velocity in the calculation area averaged over the film plane and also in the form of two-dimension particle density distributions in the zx plane in the range of heating time from 0 to 800 ps. In some calculations the heating was switched off with subsequent monitoring of the film behavior. The obtained results suggest the existence of four different regimes of film behavior depending on the heating rate: quasi-stationary regime with surface evaporation, explosive (volume) boiling, spinodal decomposition and overcritical expansion.

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MATHEMATICAL SIMULATION OF RADIATION ACCELERATED OUTFLOWS

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The RMHD model for formation of astrophysical jet outflow from the vicinity of a compact object surrounded by a thin accretion disk and immersed into the nebula of a galactic plasma is considered.

The numerical methods for solving the systems of magnetic hydrodynamics (MHD) equations and radiation transport equation in two-dimensional axis - symmetrical statement on triangular unstructured grid were developed. The numerical algorithms are based on division by physical processes and include a difference scheme for the MHD system and discrete directions method for radiation transfer equation.

The numerical methods were implemented as a software system designed for high performance systems with shared memory, including systems with graphical accelerators.

Parallel implementation of RKDG method for solution of two-dimensional equations of ideal magnetic hydrodynamics on triangular unstructured grids was considered. The software complex was built with the MPI and OpenMP technologies. The algorithms for monotization and divergence – free reconstruction of magnetic field are presented. They allow getting physically adequate results with high order accuracy. The results of test calculations and obtained from parallel technologies values of computation accelerations are discussed.

The modeling results show the formation of the accelerating channel and acceleration of jet plasma up to $1/5$ luminal speed and comply with the available observation data. Computations are performed on a KIAM K-100 cluster.

The processes of creation and development of magneto-rotational instability of near – star plasma disc were investigated. The results show that instability leads to withdraw of the angular momentum on the periphery of the disk and the accretion on a star.

Acknowledgements. The investigation is partially supported by RFBR (projects 12-01-00109, 12-01-31193, 12-02-12096, 12-02-00687), grant of President of Russian Federation for state support of leading scientific schools of RF (project NSH-1434.2012.2).

MODELLING OF NONUNIFORM HEATING OF LASER-PRODUCED PLASMAS BY DSMC-BASED METHOD

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Numerical simulation of plasma dynamics on the kinetic level is a difficult problem. It is natural to consider separately (a) continuous motion of electrons and ions in external and self-consistent electro-magnetic fields (Vlasov-Maxwell kinetic equations) and (b) Coulomb collisions (Landau-Fokker-Planck (LFP) equations). The particle methods for solving the first stage (a) of "collisionless" plasma are very well developed and discussed in literature. To model collisions of charged particles Monte Carlo methods are usually used for operating linear problems. This is because such an approach faces severe difficulties for the interaction potentials of the infinite radius of action.

We propose a general approach to stochastic methods (DSMC) for Coulomb collisions. Its key idea is an approximation of the nonlinear LFP equations by the Boltzmann equations of a quasi-Maxwellian kind. This means that the total collision frequency for the corresponding Boltzmann equation does not depend on velocities. This allows one to make the simulation process very simple since the collision pairs can be chosen arbitrarily, without restriction. The suggested new numerical scheme is simple, effective and easily can be combined with the particle methods. We derive it for the general case of multi component plasmas.

DSMC numerical simulation is tested for the classical problems of plasma physics. The developed method can be also applied not only to Coulomb potential but for other long-range potentials such as dipole-dipole interactions, van der Waals attractions between atoms, etc. Some results related to nonequilibrium plasma dynamic and to the nonlocal transport and nonuniform heating of laser-produced plasmas are discussed.

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ELECTRON PRESSURE IN THE PROBLEM OF FEMTOSECOND LASER HEATING OF METALS**V.I. MAZHUKIN, M.M. DEMIN, A.V. SHAPRANOV, V.E. PEREZHIGIN**

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The statement of the problem of the femtosecond laser action on metals is considered. It takes into account the effects of non-equilibrium part of the pressure of the collectivized electrons subsystem.

Modeling of action of 180-fs laser pulse on an aluminum target is performed with and without account of electron pressure.

Account of electron pressure results in a change in the ablation behavior:

- during the initial stage of the process, spallation of a thin subnanometer subsurface region of the target occurs;
- during the later stage, disintegration of the target has a tendency for spallation of thinner films.

The work was partially supported by RFBR grants №№ 12-07-00436a, 13-07-00597a.

DSMC MODELING OF ELECTRON HEATING FOR THE NONLINEAR COLLISION KINETIC EQUATION WITH QUASILINEAR DIFFUSION**I.F. POTAPENKO**Keldysh Institute of Applied Mathematics, RAS, 125047 Miusskaya Pl., Moscow, RF
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We propose a general approach to stochastic methods (DSMC) for Coulomb collisions. Its key idea is an approximation of the nonlinear LFP equations by the Boltzmann equations of a quasi-Maxwellian kind. This means that the total collision frequency for the corresponding Boltzmann equation does not depend on velocities. This allows one to make the simulation process very simple since the collision pairs can be chosen arbitrarily, without restriction. The suggested new numerical scheme is simple, effective and easily can be combined with the particle methods. We derive it for the general case of multi component plasmas.

Solution of the time dependent spatially uniform nonlinear collision kinetic equation in the course of heating is studied numerically. Coulomb collisions are treated with the Landau-Fokker-Planck collision integral. The considered heating source is a quasilinear diffusion operator with variable coefficient acting in a full velocity space. DSMC method is used to investigate the process. The time-dependent solutions are examined.

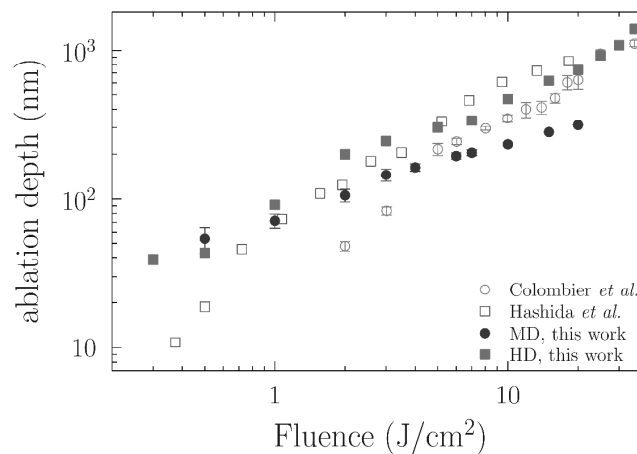
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**COMPARISON OF CONTINUUM AND MOLECULAR DYNAMICS APPROACHES
 FOR SIMULATION OF LASER ABLATION OF METALS**

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We perform comparison of two approaches for simulation of laser ablation of metals. In molecular dynamics model (MD) the atomic subsystem is described by a group of atoms with material-dependent interatomic potential. This approach is supplemented by the electron system which allows description of interaction of laser pulses with matter, similar to paper [1]. The electron subsystem helps to describe the effects of laser energy absorption by free electrons, an electron-ion coupling, and fast electronic heat conductivity. The atomic subsystem, in turn, reproduces melting, nucleation, spallation and spinodal decomposition processes. Hydrodynamic approach is based on Lagrangian model [2] and includes a multi-phase equation of state which reproduces stable and metastable solid, liquid and gas phases. The HD method contains also a model of homogeneous nucleation of liquid state. By means of both methods the dependence of crater depth on laser fluence is investigated for aluminum and comparison with experimental data [3, 4] is done.



Acknowledgements: The research was sponsored by the Russian Foundation for Basic Research (Project Nos. 13-08-01179 and 13-02-91057-CNRS).

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NON-EQUILIBRIUM MELTING AND EVAPORATION OF SILICON UNDER THE INFLUENCE OF ULTRA-SHORT LASER PULSE

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Interaction of powerful laser radiation , having the form of short pulses (picosecond or femtosecond range) with semiconductor materials leads to a cascade of energy conversion processes, including the excitation and relaxation of the electronic subsystems of the electron-phonon relaxation phonon- phonon relaxation and thermal processes (heating, melting and evaporation) . Parameters of the electron-hole plasma produced in the semiconductor in this reaction may be strong enough to change (the carrier density $10^{12} < N < 10^{22} \text{ cm}^{-3}$, temperature $10^4 < T < 10^5 \text{ K}$). To describe the non-equilibrium heating of the semiconductor and dynamics of fast phase transitions in metal silicon was used two-temperature hydrodynamic model. Computational problems associated with the presence of mobile phase boundaries, were resolved by the method of dynamic adaptation.

In this paper, we consider the dynamics of non-equilibrium melting and vaporization of a silicon wafer by laser radiation power of $2.5 \times 10^{11} \text{ W/cm}^2$, with the wavelength $\lambda = 0.53 \mu\text{m}$, pulse duration $\tau = 20 \text{ ps}$. Time profiles of the temperature on the target surface and the velocity of the melting front are shown in Fig . 1-2.

Acknowledgements: The work was partially supported by RFBR grants №№ 13-07-00597, 12-07-00436.

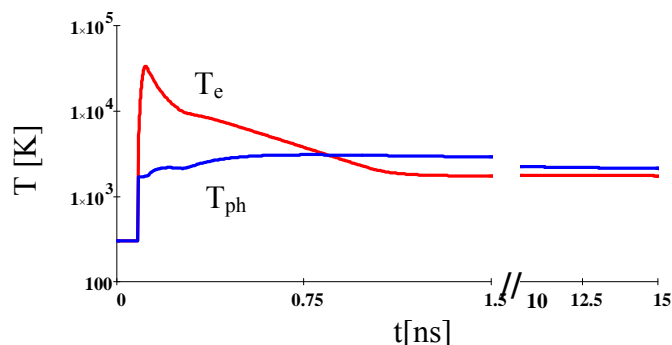


Fig.1. The time dependence of the temperature on the target surface.

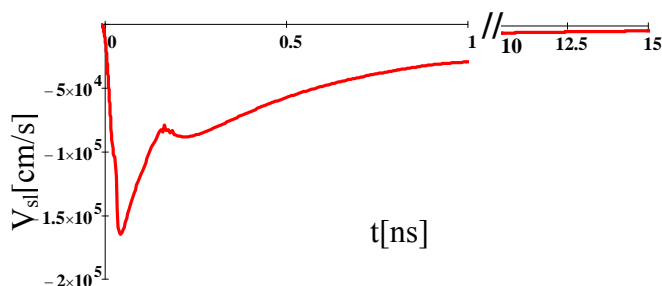


Fig. 2. Velocity of the melting front.

MOLECULAR DYNAMICS MODELING OF THE HETEROGENEOUS MELTING/CRYSTALLIZATION OF ALUMINIUM

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According to the results of molecular dynamics modeling constructed the dependence speed of the interface solid-liquid from value of overheating/hypothermia in aluminum. Dependency is defined in a broad temperature range in which the deviation from the equilibrium temperature is $(-600 \div 200)^\circ\text{K}$. Results of modeling is showed a weak dependence on the pressure in the range $(0 \div 80 \text{ kbar})$. Determined the fitting coefficients, allowing to use the dependence of the velocity of the front of solid-liquid from the value of overheating/hypothermia received from the kinetic performances. Fig. 1 shows the deviation from the equilibrium melting temperature.

The work was partially supported by RFBR grants №№ 12-07-00436a, 13-07-00597a.

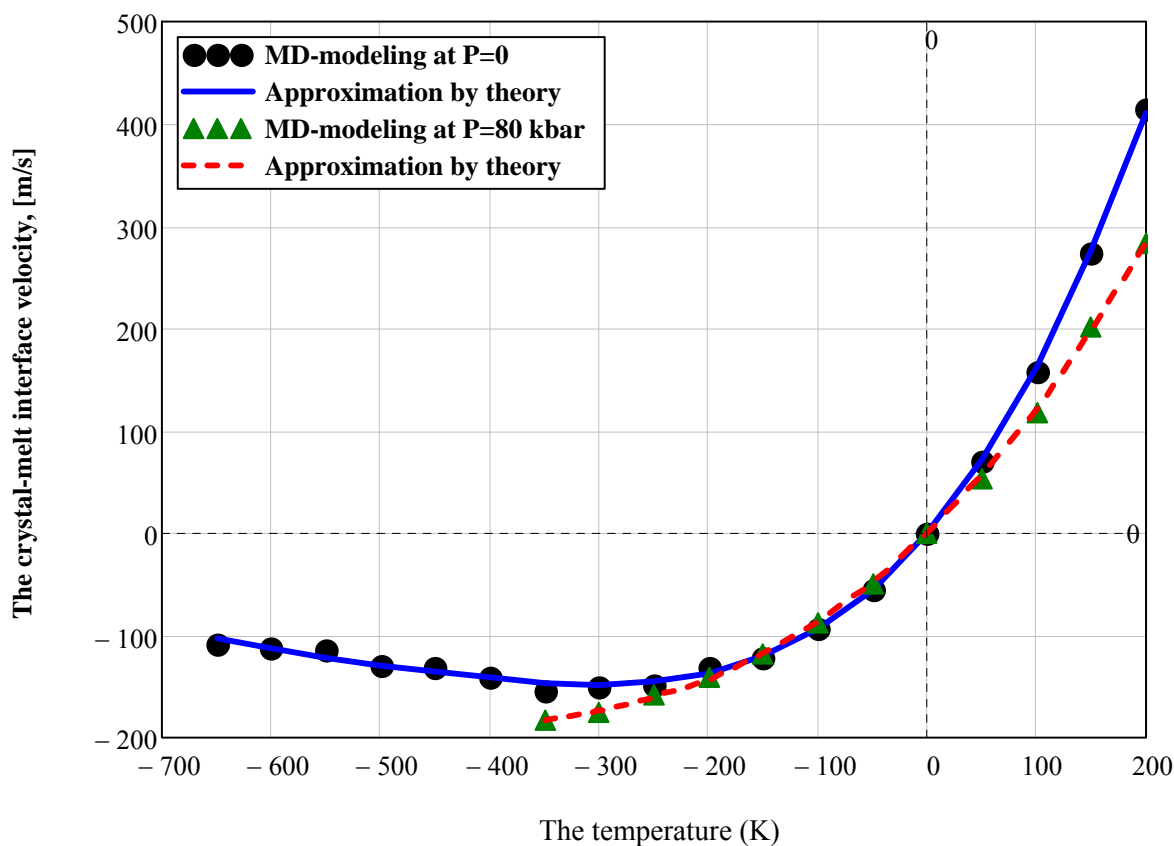


Fig. 1. The deviation from the equilibrium melting temperature.

COMPARATIVE STUDY OF INTERATOMIC POTENTIALS FOR CRYSTALLINE SILICON

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On the basis of molecular dynamics modeling using semi-empirical potentials of Stillinger-Weber (F. Stillinger, T. Weber) and its modifications (SWM), Tersoff (J. Tersoff), EDIP, Ehrhart-Albe (P. Erhart, K. Albe) and KIHS (T. Kumagai, S. Izumi, S. Hara, and S. Sakai) were investigated thermo-physical and mechanical properties of single crystal silicon.

The following characteristics of these potentials are compared: temperature dependence of thermal expansion coefficient and heat capacity, pressure dependencies of isothermal compressibility, melting temperature and melting heat. Numerous calculations show that none of these potentials can reproduce well all the examined macroscopic characteristics in a wide range of temperatures and pressures. Nevertheless in this regard KIHS, SW and Erhart-Albe are found to give the best overall performance. It is proposed also to use a linear combination of two potentials SWM and KIHS giving the resultant potential with the properties, more acceptable for simulating the crystalline silicon in a wide range of pressures and temperatures.

Acknowledgment. This study was partly supported by RFBR grants nos 13-07-00597-a, 12-07-00436-a.

МОДЕЛИРОВАНИЕ ОГНЯ И ДЫМА В ВИДЕО ТРЕНАЖЕРНЫХ КОМПЛЕКСАХ

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Во многих тренажерных комплексах (например, в видео тренажерах ликвидации чрезвычайных ситуаций) возникает проблема моделирования и визуализации огня и дыма. В этих комплексах ставятся задачи и отрабатываются действия по обнаружению, локализации и ликвидации возгораний и источников задымления.

Для моделирования огня и дыма можно использовать математическую модель несжимаемой невязкой однородной жидкости в трехмерном пространстве. Она описывается уравнениями Эйлера (для концентрации красителя и скорости распространения) и уравнением непрерывности. В качестве области моделирования выбирается параллелепипед, разбитый на квадратные ячейки одинакового размера. Выбранная система уравнений представляется в разностном виде и дополняется начальными и граничными условиями. Считается, что жидкость в начальный момент времени имеет во всей области нулевую скорость и нулевое давление. Кроме того, жидкость не выходит за границы параллелепипеда моделирования, а на нижней границе имеется постоянно действующий источник огня (дыма). Для решения системы на каждом шаге моделирования используется метод суммарной аппроксимации и теорема Гельмгольца-Ходжа о декомпозиции.

Для визуализации результатов каждого шага моделирования вычисленные значения скорости и концентрации записываются в трехмерные текстуры. Использование пиксельных шейдеров позволяет в реальном масштабе времени проводить синтез изображений прозрачного параллелепипеда моделирования с наложенными на него вычисленными трехмерными текстурами.

Моделирование тушения огня или устранения источника дыма заключается в уменьшении интенсивности источника на нижней границе области моделирования.

Работа выполнена при поддержке Программы фундаментальных исследований ОНИТ РАН, проект № 2.9.

**AN APPROACH TO MODELING IN A CONTINUUM MODEL OF A
 HOMOGENEOUS MELT AL FILM INDUCED BY AN ULTRASHORT LASER
 PULSE**

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Modeling of a homogeneous melting is based on the continuum hydrodynamic non-equilibrium model. Homogeneous melting mechanism characterized by the birth of a new phase (liquid) in a volume of superheated crystal. For each material there is a maximum superheating temperature of the solid phase, after which begins the volume (homogeneous) melting. Liquid phase of subnanometer thickness is introduced into the solid phase at the point of reaching a maximum temperature of overheating. The initial temperature in this liquid region is recalculated taking into account the heat of fusion and the law of conservation of energy. Fig. 1 shows the spatial profiles of temperature.

The work was partially supported by RFBR grants №№ 12-07-00436a, 13-07-00597a.

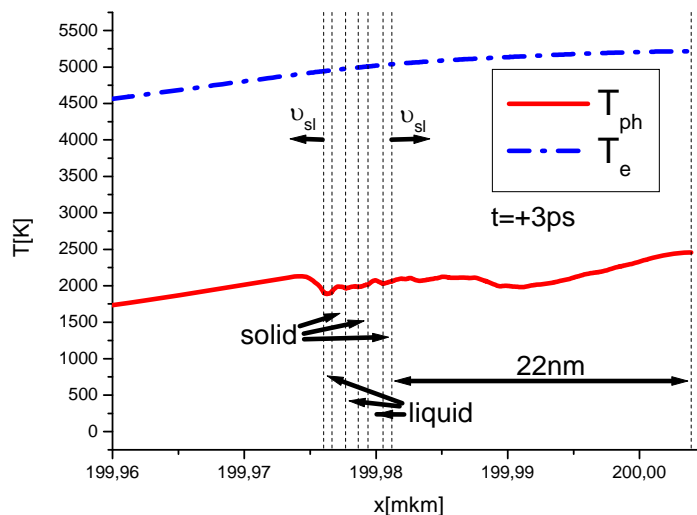


Fig. 1. The spatial profiles of temperature

**MODELS OF THERMODYNAMIC PROPERTIES AND PHASE TRANSITIONS
OF MATERIALS UNDER INTENSE LASER INFLUENCES**

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An equation of state (EOS) of matter in a broad region of the phase diagram is necessary for numerical simulations of laser–plasma processes. Accuracy of calculated results is determined mainly by adequacy of description of thermodynamic properties of materials in question. In this work, different approaches to EOS calculations are considered.

For modeling of adiabatic processes, it is sufficient to know a relationship of pressure P , density ρ and internal energy E , so-called caloric EOS, $P = P(\rho, E)$ or $E = E(\rho, P)$. A simple caloric EOS model is proposed for various metals, inorganic and organic compounds over a wide range of pressures and densities. This model is used for simulation of shock and spall experiments with ns and ps laser pulses [1].

A thermodynamically full model of free energy potential as a function of density and temperature $F = F(\rho, T)$ with taking into account polymorphic transitions, melting and evaporation is also presented. On the basis of this model, multiphase EOS calculations are carried out for some metals, alkali halides, oxides and polymers over a wide range of pressures and temperatures.

Obtained results are in a good agreement with data from experiments at high energy densities, such as measurements at static compression to high pressures as well as in shock and release waves. The presented EOS models can be used efficiently in numerical simulation of physical phenomena in materials and plasmas under intense laser influences [2, 3].

Acknowledgements: The work is supported by the Russian Foundation for Basic Research (grants 11-08-01225, 13-08-12248 and 13-02-91057).

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Modeling of plasma short wavelength source for nanolithography

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Sources of short (extreme) ultraviolet radiation are necessary for future lithography to produce highly packaging integrated circuit elements with details less than ~ 10 nm [1]. Such sources are based on tin plasma produced by CO₂ laser and have very high efficiency in the wavelength range around 13.5 nm. The tin plasma at density of 10^{19} 1/cm³ and at temperature of ~ 50 -100 eV up to tenfold ionization is optically thick, and the level kinetics coupled with the radiation transport in many ways determine the dynamics of such a plasma.

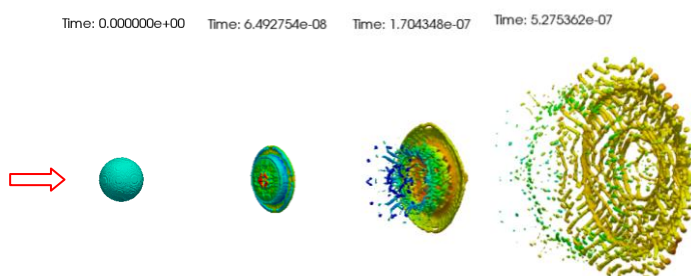


Fig.1. Dynamics of defragmentation of liquid tin droplet after laser pre-pulse

After the laser pre-pulse with duration of ~ 30 ns relatively low intensity (with energy ~ 20 mJ and pressure $P \sim 2$ kbar), a droplet of liquid tin diameter of 30μ disintegrates into fragments of $\sim 1 \mu$ in time ~ 1 ms. To simulate this process there was used open package OpenFoam [2] (see Fig.1).

To describe the plasma dynamics after the main laser pulse onto the target, broken into fragments, there was used 2D code RZLINE [3], which includes refraction, reflection and absorption of the laser radiation, time-dependent ionization, electron and ion conductivity, spectral transport of nonequilibrium radiation and so on. To account for radiative processes there was used THERMOS-BELINE package, which enables self-consistent calculation of radiative transfer in overlapped spectral lines together with level kinetics of multiply-ionized non-stationary plasma in different geometries [4]. Some results of calculations are presented on Fig.2. The optimization of conversion efficiency over laser pulse parameters and target forms were fulfilled.

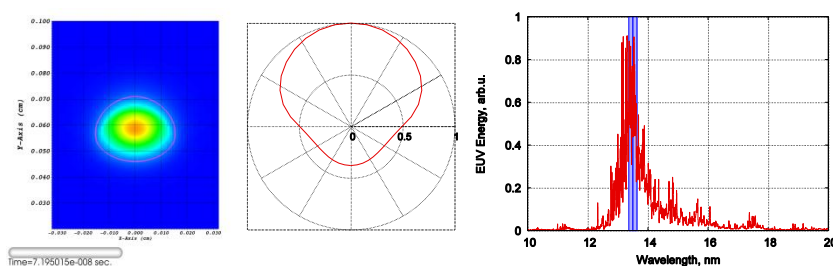


Fig.2. Snapshot, anisotropy and spectrum of tin source

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LOCAL TWO-DIMENSIONAL PERTURBATIONS EVOLUTION IN SMALL-CONDUCTIVITY GAS FLOW IN MAGNETIC FIELD

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In the beginning of 1970, during the numerical solution of some class of magnetic hydrodynamics problems the T-layer effect was discovered. The T-layer is a high-temperature self-sustaining area in plasma moving in a magnetic field. The T-layer derivation is caused by nonlinear connections between electromagnetic and gasdynamic plasma parameters. Conditions of derivation, evolution and stability of this phenomenon for one-dimensional task are rather fully studied. This work is dedicated to further research of T-layer derivation and evolution conditions for two-dimensional problem. The impact of temperature perturbation of initial parameters and the flow characteristics is investigated.

Let's consider the two-dimensional flat channel on (x, y) coordinate plane with constant width D (along y axis) filled with homogeneous compressible gas moving along channel axis (x axis). The gas conductivity that depends on its temperature is not enough for making gas interact with the magnetic field. At the initial moment of time the magnetic field is homogeneous and has only one non-zero component directed along z -direction. Nonperturbed initial temperature is equal to T_0 . At the initial time moment $t=0$ a local temperature perturbation up to value $T_1 > T_0$ is introduced into the gas flow. Due to this gas conductivity also increases and becomes enough significant to provide gas and magnetic field interaction. We are interested in this perturbation further development in time and space.

In the perturbing gas motion intensive Joule heating liberation arises. That leads to internal energy and pressure increase. Because of pressure rise the perturbation enlarges and compresses adjoining gas layers. That causes additional temperature elevation. This enlargement proceeds principally along channel axis. Therefore the flow gradually transforms to one-dimensional structure that is homogeneous along this direction.

The numerical results confirm the proposition about the possibility of T-layer nascence and evolution because of the corresponding process that initiates temperature rise caused by Joule heating liberation. A number of parameters that significantly affect the T-layer nascence ability and evolution speed are detected.

The main result of work is the verification and confirmation of T-layer nascence criterion in two-dimensional case. The T-layer arises if the magnetohydrodynamic interaction parameter $R_M = \sigma u l H^2 / (2c^2 p)$ exceeds certain critical value depended on problem geometric parameters.

The numerical solution algorithm is based on original method that was designed in Moscow State University and is called quasiacoustic scheme.

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МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ЗАДАЧ ФЛУКТУАЦИОННОЙ ГИДРОДИНАМИКИ С ИСПОЛЬЗОВАНИЕМ АЛГОРИТМОВ СЛЕДУЮЩЕГО ПОКОЛЕНИЯ

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При использовании метода молекулярной динамики (MD) для моделирования кинетики свертываемости длинных белковых молекул в водной среде необходимы вычислительные ресурсы, на много порядков превышающие ожидаемый в ближайшие десять лет экзафлопс. Однако, используя подходы, развиваемые в последние годы для расчетов сильно разномасштабных физических процессов (multi-scale) можно попытаться приблизить это время.

Основная идея уменьшения вычислительных затрат на расчеты процессов свертывания длинных белковых молекул в водной среде заключается в замене молекулярной среды в «боксах», примыкающих к «охвосту» белковой молекулы, на сплошную среду с учетом тепловых флуктуаций. Это, по идее, должно привести к кардинальному увеличению величины шага интегрирования по времени. При удалении от зоны «охвоста», размеры «боксов» могут постепенно возрастать до мезомасштабного уровня. Соответственно будет увеличиваться и величина шага интегрирования. Таким образом, мы приходим к асинхронным многомасштабным и мультифизическим (multi-physics) алгоритмам.

При описанном подходе возникает множество трудноразрешимых проблем. Первая и наиболее принципиальная из них заключается в постановке граничных условий между соседними ячейками («боксами») с разными физическими приближениями – молекулярно-динамическим и флуктуационно – гидродинамическим.

Вторая по значимости проблема заключается в выборе численного метода для решения уравнений Ландау-Лифшица. Исходной точкой было предположение, что определяющую роль при вычислении гидродинамических флуктуаций играют внутренние диссипативные характеристики базовой газодинамической схемы. Поскольку амплитуды стохастических возмущений в уравнениях Ландау-Лифшица определяются на основании флуктуационно – диссипативной теоремы, то при определенном из теории уровне флуктуаций важно соблюдать баланс диссипативных свойств, складывающихся из физического эффекта молекулярной вязкости и вычислительного эффекта аппроксимационной вязкости. В соответствии с указанной концепцией за основу были выбраны бездиссипативные разностные схемы второго порядка аппроксимации «крест» (Leap-Frog) и CABARET (Upwind Leap-Frog). Вычислительная эффективность предложенных методов была подтверждена на ряде модельных и тестовых расчетов, отвечающих существующим мировым стандартам.

Работа выполнена при поддержке РФФИ, грант № 11-07-93938-ДЖИ8_a.

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ЭЛЕКТРОМАГНИТНОГО ПОЛЯ В ЗАДАЧАХ С ВЫДЕЛЕННЫМ ФРОНТОМ ИОНИЗАЦИИБерезин А.В.¹, Крюков А.А.², Марков М.Б.³¹к.ф.-м.н., с.н.с. ИПМ им. М.В.Келдыша РАН, Москва, Россия²к.ф.-м.н., м.н.с. ИПМ им. М.В.Келдыша РАН, Москва, Россия³д.ф.-м.н., зав. сектором ИПМ им. М.В.Келдыша РАН, Москва, Россия*anton.krv@gmail.com*

Представлен численный алгоритм решения задачи Гурса для уравнений Максвелла [1]. Алгоритм предназначен для моделирования генерации электромагнитного поля импульсами фотонов в трехмерной постановке. Рассмотрены уравнения Максвелла в системе отчета, связанной с фронтом излучения фотонов. Построена полностью консервативная разностная схема [2]. Предложена методика решения сеточных уравнений, основанная на итерационном методе Крыловского типа. Алгоритм решения сеточных уравнений адаптирован для распределённых вычислений методом декомпозиции расчетной области. Методика реализована для кластерных систем с гибридной архитектурой. Рассмотрен метод дискретизации расчетной области нерегулярными декартовыми сетками. Представлены результаты расчета параметров электромагнитного поля, генерируемого при рассеянии в атмосфере импульса тормозного гамма-излучения.

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3D MOLECULAR DYNAMIC SIMULATION OF GAS MIXTURE PROPERTIES

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In this work we consider the molecular dynamic simulation of gas mixture atom systems in the micro-channel. The molecular dynamic method (MMD) allows to get information about processes on molecular scale, and at times of a few nanoseconds. We deal with supersonic binary gas flow and metallic micro-channel. The gas mixture involves such gases as hydrogen and nitrogen, the micro-channel walls consist of nickel atoms. The Verlet scheme was used as a numerical algorithm for solving of motion atoms equations. The system of molecular dynamic equations is used as a grid algorithm. Within the MMD algorithm the interactions of gas particles are described by the Lennard-Jones potential, which is determined by the properties of the mixture components and their thermal conditions. Calculating the characteristics of metal used as bases an embedded atom model (EAM) analytical form. The interactions between the gas flow and the metallic wall were described by the Morse and Lennard-Jones potential functions.

For calculations a hybrid computing system was used. The system has a central processing units (CPU) and graphic processing units (GPU). Decomposition of the computational domain on the nodes of the computing system was realized. This decomposition is a grid that is similar to used computational mesh. As a result, each node of a computer system processes some subset of cells. The gas dynamic parameters are produced by molecular dynamic method on GPU.

Two 3D mathematical tasks were considered and analyzed numerically with the help of elaborated approach. The first task describes the interaction of molecules of gas mixture far from the walls. The second task describes the interaction of molecules of gas mixture near the walls. In the last case the interaction of gas molecules with the walls atoms was taken into account. Some properties of these interactions were studied in numerical experiments.

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МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ГЕНЕРАЦИИ ТОРМОЗНОГО ИЗЛУЧЕНИЯ ЭЛЕКТРОННЫМ ПУЧКОМ УСКОРИТЕЛЯ

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Рассматривается процесс генерации тормозного гамма-излучения при взаимодействии пучка электронов с мишенью. Для описания переноса излучения используется модель индивидуальных соударений, в основе которой лежит обработка данных по сечениям процессов взаимодействия электронов и квантов с веществом [1]. Модель не использует распространенные приближения (непрерывное замедление, теория многократных столкновений, теория энергетических потерь Ландау), что позволяет проводить анализ распределений частиц с детальным учетом всех столкновений. Кроме того, такая модель является удобной и эффективной при распараллеливании расчетов на гибридной вычислительной технике.

Созданы статистические алгоритмы для моделирования переноса квантов и электронов в веществе на гибридной вычислительной технике. Алгоритмы основаны на весовых модификациях метода Монте-Карло, учитывающих особенности распараллеливания вычислений с помощью технологии NVIDIA© CUDA [2, 3]. Построены экономичные методы описания рассеивающей среды. Алгоритмы и методы реализованы в виде программ, предназначенных для проведения расчетов на гибридной вычислительной технике с использованием графических ускорителей в качестве арифметических сопроцессоров.

Проведено моделирование процесса генерации тормозного излучения при взаимодействии сфокусированного пучка электронов с танталовой мишенью. Получены спектральные и пространственные распределения квантов тормозного излучения. Расчеты взаимодействия излучения с веществом и переноса электронов и гамма-квантов выполнены на гибридном вычислительном кластере K-100 (<http://www.kiam.ru/MVS/resources/k100.html>). Достигнуто удовлетворительное согласие с экспериментальными данными.

Работа выполнена при поддержке гранта РФФИ №11-01-00342.

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ВЫЧИСЛИТЕЛЬНАЯ МАТЕМАТИКА COMPUTATIONAL MATHEMATICS

ДИНАМИЧЕСКИ АДАПТИРУЮЩИЕСЯ СЕТКИ В ГАЗОДИНАМИЧЕСКИХ ЗАДАЧАХ С ИСКУССТВЕННОЙ ВЯЗКОСТЬЮ

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Рассматривается использование динамически адаптирующихся сеток для решения газодинамических задач с искусственной вязкостью. Численные результаты сравниваются с решениями, полученными другими методами без выделения разрывов (WENO3, WENO5 и MUSCL). Функция адаптации определяется исходя из двух условий: условия квазиравномерности расчетной сетки и автоматического сгущения узлов в областях изменения искомого решения. Полученная функция используется для решения методом динамической адаптации двух тестовых задач: задачи о распаде произвольного разрыва и задачи о двух встречных ударных волнах.

Работа выполнена при поддержке РФФИ, грант №№ 12-07-00436а, 13-07-00597а.

DYNAMICALLY ADAPTING GRIDS FOR GAS-DYNAMIC PROBLEMS WITH ARTIFICIAL VISCOSITY

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Dynamically adapting grids are used to solve gas-dynamic problems with artificial viscosity. Numerical results are compared with solutions obtained by other shock-capturing techniques (WENO3, WENO5 and MUSCL methods). The adaptation function is determined by two alternative conditions: computational grid is quasi-uniform and grid points are concentrated in the steep-gradient regions. The dynamic adaptation method with the adaptation function thus determined is used to solve SOD problem and two blast wave's problem.

The work was partially supported by RFBR grants №№ 12-07-00436а, 13-07-00597а.

**РЕШЕНИЕ БОЛЬШИХ ЗАДАЧ МАТЕМАТИЧЕСКОЙ ФИЗИКИ
НА СУПЕРКОМПЬЮТЕРАХ:
ИСПОЛЬЗОВАНИЕ РАСЧЕТНЫХ СЕТОК СЛОЖНОЙ СТРУКТУРЫ**

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На протяжении ряда лет коллективом, который представляют авторы, проводилось решение различных задач в областях сложной геометрической формы с использованием неструктурированных сеток, а также разработка программных средств для решения таких задач. Появление большого числа новых аппроксимаций и методик, наличие разных подходов к дискретизации расчетной области (сетки регулярной структуры, конформные неструктурированные сетки, восьмеричные деревья и т. д.), необходимость декомпозиции сетки для использования высокопроизводительных параллельных вычислительных систем – все это приводит к необходимости создания специального набора программных средств для хранения и обработки сеток сложной структуры, независимых от предметной области решаемой задачи.

Подобный набор средств был разработан в рамках проекта MARPLE 3D, предполагавшего создание кода для моделирования широкого круга физических процессов в высокотемпературной излучающей плазме в трехмерной постановке с использованием неструктурированных сеток. Сеточная инфраструктура кода MARPLE содержит классы C++ для хранения и обработки неструктурированных сеток и атрибутов, связанных с теми или иными элементами сетки (такими как расчетные величины в узлах или ячейках).

Принципиальным моментом было введение понятия нумерованного множества элементов и соответствующего ему C++ класса. Это позволило обеспечить связь между множеством пронумерованных элементов (таких, например, как узлы сетки) и всеми массивами атрибутов, определенных на этих элементах. Любое изменение множества (например, в результате динамической адаптации сеток) автоматически приводит к соответствующим изменениям во всех массивах атрибутов. Также в виде классов C++ реализованы бинарные отношения между множествами, такие как отношения инцидентности и смежности между элементами сетки. Неструктурированная сетка представляется набором узлов, ребер, граней и ячеек с определенными на них отношениями инцидентности (топологическими связями). Наконец, для распределенных приложений предусмотрены средства для установления соответствия между элементами сетки при межпроцессорных обменах.

Планы по дальнейшему развитию сеточной инфраструктуры предполагают обеспечение большей общности при работе с сетками. Предполагается поддержка сеток с последовательным дроблением ячеек (как, например, в восьмеричных деревьях). Кроме того, поддержка сеток более простых типов в качестве частного случая более общего и более сложного типа сетки (например, сетка регулярной структуры может быть формально описана как неструктурированная) требует существенно больших затрат памяти и времени, чем непосредственная поддержка более простых типов сеток. Поэтому сетка должна чистой абстракцией напоминать итератора в концепции STL библиотеки.

НОВЫЙ БЕСПАРАМЕТРИЧЕСКИЙ ВЫЧИСЛИТЕЛЬНЫЙ МЕТОД ПРЯМОГО МОДЕЛИРОВАНИЯ ТЕРМОКОНВЕКТИВНЫХ ТЕЧЕНИЙ В ЗАМКНУТОЙ ОБЛАСТИ В ФОРМЕ ПАРАЛЛЕЛЕПИПЕДА

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В докладе изложен новый вычислительный алгоритм для прямого моделирования нестационарных турбулентных термоконтвективных течений в замкнутой области в форме параллелепипеда при высоких числах Рэлея. Этот вычислительный алгоритм, получивший название «метод КАБАРЕ», не содержит никаких настроечных параметров и имеет в своей основе только нестационарную систему уравнений Навье-Стокса, записанную с приближением Буссинеска, уравнение теплопроводности и ряд базовых принципов вычислительной математики (таких как принцип максимума и принцип наименьшего возрастания парциальной локальной вариации [1]). Метод «КАБАРЕ», являясь консервативным, 2-го порядка аппроксимации, позволяет использовать достаточно грубые сетки, точно передавая при этом все особенности термоконтвективного турбулентного течения, в том числе, образование и взаимодействие вихрей, перенос тепла, пульсации температуры и т.д.

Несмотря на накопление богатого багажа публикаций, посвященных естественной конвекции, в мире до сих пор мало надежных экспериментальных данных высокого качества, которые можно было бы использовать как надежный и качественный тест (бенчмарк) для отработки новейших вычислительных методов моделирования термоконтвективных течений при высоких числах Рэлея. В докладе описано несколько экспериментов, признанных вычислителями во всем мире и взятых за основу для тестирования схемы «КАБАРЕ». Например, один из таких бенчмарков — эксперимент по термоконтвекции в вытянутой по вертикали замкнутой области [2].

В описанных экспериментах и в проведенных численных расчетах методом «КАБАРЕ» получены нестационарные временные зависимости температуры (пульсации) с высоким разрешением по времени в различных точках области, спектральные характеристики температурных флуктуаций. Проведено сравнение осредненных тепловых характеристик на активных стенках, средних профилей температур и скоростей в различных сечениях области, а также профилей среднеквадратичных отклонений температур и скоростей. Показано, что результаты численных расчетов имеют очень хорошую согласованность с данными представленных экспериментов. Продемонстрированы преимущества схемы «КАБАРЕ» в сравнении с другими численными подходами.

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МЕТОД АДАПТИВНОЙ ИСКУССТВЕННОЙ ВЯЗКОСТИ РЕШЕНИЯ УРАВНЕНИЙ ГАЗОВОЙ ДИНАМИКИ НА НЕСТРУКТУРИРОВАННЫХ ТРЕУГОЛЬНЫХ И ТЕТРАЭДРАЛЬНЫХ СЕТКАХ

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В работе предложен метод адаптивной искусственной вязкости (АИВ) для решения уравнений газовой динамики. В предлагаемой работе этот метод переносится на случай треугольных сеток для двумерных уравнений в переменных x, y и r, z а на тетраэдральных сетках для уравнений в декартовых переменных x, y, z . Приводятся результаты расчетов тестовых задач.

COMPOSITION HYPERRINGS

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In this paper we introduce the notion of composition hyperring. We show that the composition structure of a composition hyperring is determined by a class of its strong multiendomorphisms. Finally, the three isomorphism theorems of ring theory are derivated in the context of composition hyperrings.

HARMONIC FUNCTIONS AND THE HYPERBOLIC METRIC

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We give a proof that positive harmonic functions in the upper half-plane do not increase the hyperbolic metric. Motivation for our work are some recent results of Kalaj and Vuorinen.

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**АСИМПТОТИКА СОБСТВЕННЫХ ЗНАЧЕНИЙ ОПЕРАТОРА ТИПА ШТУРМА-
 ЛИУВИЛЛЯ С ПЕРЕМЕННЫМ ЗАПАЗДЫВАНИЕМ**

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В данной работе обсуждается асимптотика ноль характеристической функции оператора $D^{(2)}$, который генерируется дифференциальным уравнением

$$-y''(x) + q(x)y(\alpha(x)) = \lambda y(x)$$

где $0 < \alpha(x) < x$, $x \in (0, \pi]$ и $\alpha(0) = 0$, и начальными условиями $y'(0) - hy(0) = 0$ и $y'(\pi) + H(\pi) = 0$. Отыскивается асимптотика ноль, для ранее полученной автором характеристической функции F оператора $D^{(2)}$, имеющей форму:

$$\begin{aligned} F(z) = & \left(-z + \frac{hH}{z}\right) \sin \pi z + (h + H) \cos \pi z + \int_0^\pi q(t_1) \cos z(\pi - t_1) \cos z\alpha(t_1) dt_1 + \\ & + \frac{H}{z} \int_0^\pi q(t_1) \sin z(\pi - t_1) \cos z\alpha(t_1) dt_1 + \frac{h}{z} \int_0^\pi q(t_1) \cos z(\pi - t_1) \sin z\alpha(t_1) dt_1 + \\ & + \frac{hH}{z^2} \int_0^\pi q(t_1) \sin z(\pi - t_1) \sin z\alpha(t_1) dt_1 + \\ & + H \sum_{l=2}^{\infty} \left\{ \frac{1}{z^l} \int_{D_l} Q(T_l) \sin z(\pi - t_1) P(T_l, z) \cos z\alpha(t_1) dT_{l1} + \right. \\ & \left. + \frac{h}{z^{l+1}} \int_{D_l} Q(T_l) \sin z(\pi - t_1) P(T_l, z) \sin z\alpha(t_1) dT_{l1} \right\} + \\ & + \sum_{l=2}^{\infty} \left\{ \frac{1}{z^{l-1}} \int_{D_l} Q(T_l) \cos z(\pi - t_1) P(T_l, z) \cos z\alpha(t_1) dT_{l1} + \right. \\ & \left. + \frac{h}{z^l} \int_{D_l} Q(T_l) \cos z(\pi - t_1) P(T_l, z) \sin z\alpha(t_1) dT_{l1} \right\}, \end{aligned} \quad (1)$$

где $D_l = D_l(\pi)$, $D_l(x) = \{(t_1, t_2, \dots, t_l) | 0 \leq t_1 \leq x, 0 \leq t_2 \leq \alpha(t_1), \dots, 0 \leq t_l \leq \alpha(t_{l-1})\}$,

$Q(T_l) = \prod_{i=1}^l q(t_i)$, $P(T_l, z) = \prod_{i=1}^{l-1} \sin z(\alpha(t_i) - t_{i+1})$ и $dT_l = dt_l dt_{l-1} \dots dt_1$, $z^2 = \lambda$.

THE STRINGS METHOD IN A NUMERICAL SIMULATION OF LASER TREATMENT

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Heat treatment of material surface with laser procedure can get working surfaces of tools with high hardness characteristics due to high-speed heating and cooling, as well as the ability to handle hard surfaces of the parts and the absence of deformation of workpieces. Especially effective laser processing amorphous pyrolytic coatings, not only leads to the formation of hard carbides, but also to the formation of chemical bonding (sintering) to a substrate material, significantly increases adhesion of the coating.

The features of laser treatment that should be considered in the simulation are the high temperature gradients, changes in thermal properties of materials, as well as diffusion processes leading to the formation of local stable chemical compounds. Standard methods of sampling and solutions of difference equations in these cases often lead to an oscillating approximate solutions that do not meet the actual behavior of the system. The problem is two-dimensional surface treatment as modeling to determine the depth and width of the heat action zone (HAZ). To solve this problem have been used a new method of mathematical modeling, based on the integral describing the process of heat transfer. The developed method was named by strings, because its distinctive feature is the representation of the solution of the problem as a set of strings, similar to a tennis racket, each of which are written the law of conservation of energy and Fourier's law, which connects the heat flux with temperature. The resulting system of integral equations can be applied rapidly converging iterative procedure, making it possible to calculate the temperature field in two-dimensional and three-dimensional cases [1-3].

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USING „WOLFRAM MATHEMATICA 9.0“ TO SIMULATE PROBABILITY PROBLEMS

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The topic and objective of this paper is to illustrate how Wolfram Mathematica 9, through her symbolic programming environment, can be used to simulate probability problems. Apart from the general discussion of its uses, several examples of Mathematica's application will be shown. The examples will clarify Markov Chains and Queues whose symbolic representation in this software makes visualisation the process, simulation process path and computation the stationary distribution much easier.

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МАТЕМАТИЧЕСКИЕ МОДЕЛИ И МОДЕЛИРОВАНИЕ В ПЕРЕДОВЫХ НАУЧНЫХ ТЕХНОЛОГИЯХ

MATHEMATICAL MODELS AND MODELING IN ADVANCED SCIENCE TECHNOLOGIES

ОДНО МАТЕМАТИЧЕСКОЕ РАССМОТРЕНИЕ ПОКУПКИ И ПРОДАЖИ

ЖАРКО ПАВИЧЕВИЧ

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Возможно ли, что снижение цены уменьшает возможность покупки продукта-компании, а увеличение эту возможность увеличивает?
Психологический фактор не учитывается.

МАТЕМАТИЧЕСКИЕ ПОНЯТИЯ В СКАЗКАХ, ЛЕГЕНДАХ И БАСНЯХ

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Предмет исследования - некоторые знакомые рассказы. Попытаемся разъяснить некоторые его скрытые смыслы с помощью математических понятий.

ACADEMIC HISTORY AND RAS REFORMATION

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Russian academic history is considered briefly from its beginning to present days. Current reformation of Russian Academy of Sciences is discussed in more details taking into account various reasons (internal and external) of this turmoil.

THE IMPACT OF INFLATION ON THE EFFECTIVENESS OF THE PROJECT

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Changing inflation is one of the major external factors affecting the cash flow of projects. Accounting for the effects of inflation, provides a real project performance indicators. In this paper we investigate the real effectiveness of long-term and short-term projects in different rates of inflation. Inflation is taken into account by observations over a long period of time, the Federal State Statistics Service. [1] Project performance is evaluated on such parameters as the real rate of return, taking into account the temporal structure of projects, loss of profits, the real present value, the probability of favorable market conditions.

To calculate the actual performance indicators used by the annual inflation rate $J(t)$ in the years 1999-2012 (Figure 1). Fig. 2 shows the real return projects, calculated for two variants of inflation: 2004-2012 and 1999-2008.

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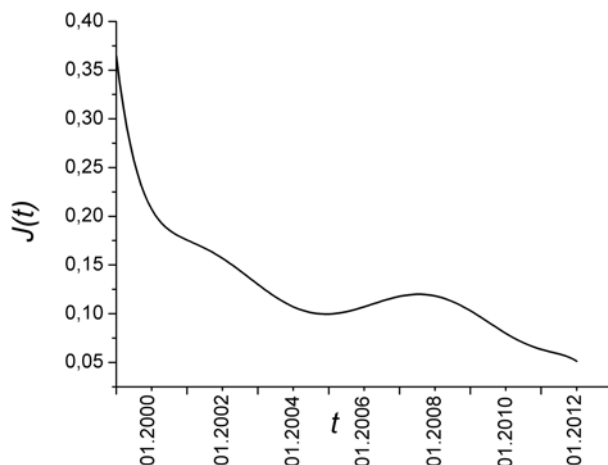


Fig. 1 Rate of inflation

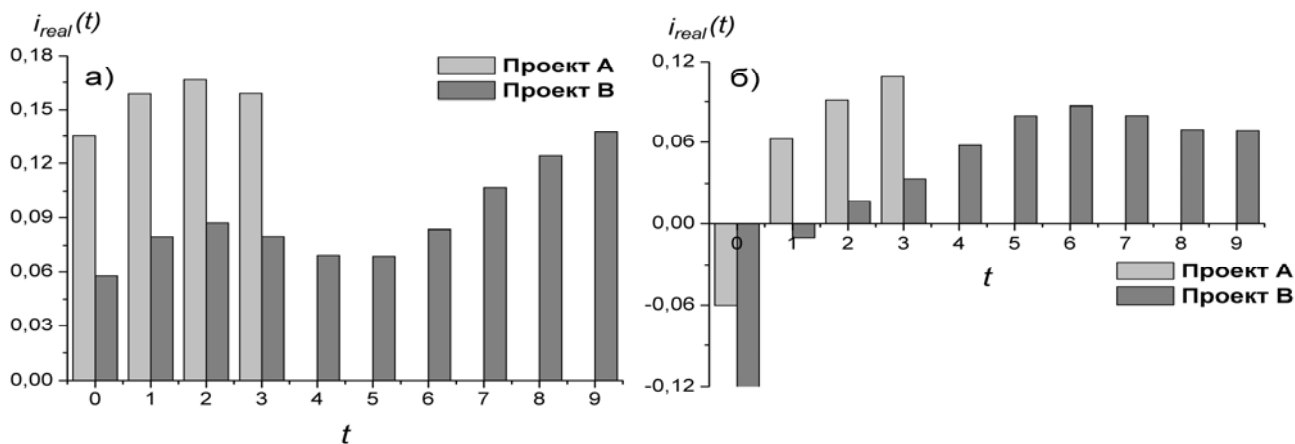


Fig. 2. Real rates during the project: a) – the rate of inflation 2004-2012; б) – the rate of inflation 1999-2008 years.

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EFFECT OF REINVESTMENT OF INCOME FOR THE PROJECT RATE OF RETURN

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A qualitative evaluation of the effectiveness of investment, taking into account the features of the economic situation and the alternatives is essential to making an investment decision for or against the project. Of particular interest are projects with the reinvestment of income.

The problem of determining the rate of return on the project for re-use of income from the investment in the same project. To study the return the investment project, allowing for feedback in the scheme of investment flows, are used indicators such as the marginal rate of return of the project, the net present value, the increment of income on a set of opportunity costs.

Fig. 1 shows the change in the set of opportunity costs net present value of the project with the reinvestment of income and no reinvestment.

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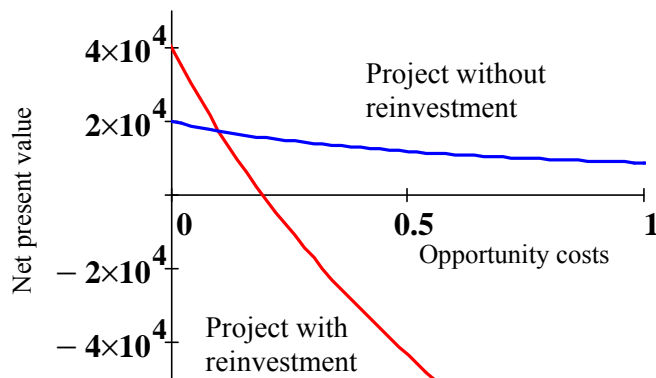


Fig. 1. Net present value of the project with and without reinvestment

**ANALYSIS AND MODELING OF MORPHOLOGICAL AND PRODUCTIVE
CHARACTERISTICS OF SPECIES OF THE GENUS *AMARANTHUS L.***

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This paper includes research of ten genotypes of introduced species of the genus *Amaranthus L.* Raw materials from the genus *Amaranthus L.* contain high quality starch, pectin, lipids, vitamins and other physiologically active substances, and can be used as important nutritional supplements.

The experiment was monitored in a three-year work, at the same location, under different climatic and meteorological conditions. Morphological and productive characteristics, number of leaves per plant, medium leaf length, medium leaf width and leaf mass per amaranth plant, were studied. Coefficients of variation and standard deviation were calculated for the above characteristics.

A mathematical model was developed, by whose application, in a short time and in a simple way, it was possible to predict the leaf mass of all ten genotypes of introduced species of the genus *Amaranthus L.*

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МЕХАНИЗМЫ РАЗВИТИЯ ШОКОВЫХ СОСТОЯНИЙ

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Механизмы развития шоковых состояний чрезвычайно сложны и многообразны. Центральным и общим звеном при различных шоках является падение артериального давления. Это угрожает жизни больного, так как нарушает кровообращение прежде всего в сосудах мозга и сердце. Организм выработал много защитных процессов, направленных на восстановление низкого давления. Многие из этих механизмов известны. Например, возбуждение симпатической нервной системы, централизация кровотока, активация ренин-ангиотензин-альдостероновой и гипотааламо-гипофизарно-надпочечниковой систем. Однако обратная сторона этих реакций может стать причиной срыва компенсации. Непрогрессирующий шок, при котором достигнута стабилизация состояния больного, в том числе по величине артериального давления, может внезапно перейти в прогрессирующий и терминальную стадию. Есть убедительные представления, что этот переход связан с развитием феномена реологических расстройств. Познакомить с этим феноменом математиков является нашей задачей. Возможно, их методы позволят клиницистам предсказать условия развития этого прогнос тически неблагоприятного феномена.