

## Summaries of All Articles

*I.I. Korel, V.I. Denisov, B.N. Nyushkov, V.S. Pivtsov*

### Precise laser systems with optical fibers

The development and investigation of the main blocks of the all-fiber femtosecond optical clocks on the base by Nd:YAG/I<sub>2</sub> optical standard are considered. The experimental results of the femtosecond comb broadening up to the octave (1÷2 micron) range and numerical modeling of the supercontinuum generation in highly nonlinear optical fibers with complex dispersion profiles are presented.

**Key words:** femtosecond optical clocks, supercontinuum generation, highly nonlinear optical fiber, computing experiments.

*A. Yu. Lizunov, N. I. Zaitseva, V. V. Zosimov*

### Account of intraligand interactions by the knowledge based potential improving the docking accuracy in flexible ligands

We propose a universal algorithm for accounting interatomic ligand-ligand interactions in docking studies. The proposed algorithm can be implemented with any scoring function of interatomic interactions. We implement the algorithm in the program Algocomb on the basis of the Tarasov-Muryshv scoring function. We demonstrate a significant improvement in selfdocking Rognan test for flexible ligands, taking into account the internal interactions of the ligand by the proposed algorithm.

**Key words:** docking, intraligand interactions, scoring function, knowledge based scoring function, statistical scoring function, noncovalent interactions, flexible ligands.

*O.I. Markov, Yu.V. Hripunov*

### Influence of atomic hydrogen on the restructuring of the cleaved surface of a bismuth single crystal

The results of the research morphology of the cleaved surface of a bismuth single crystal after the treatment in an environment of atomic hydrogen are presented in the paper. It is shown that the application of atomic hydrogen is restructuring surface to form nanoscale structures.

**Key words:** bismuth single crystal, chip, surface, atomic force microscopy.

*I.V. Matyushkin, S.V. Korobov, R.R. Vildanov*

### Features of hexagonal cellular automata on a flat surface in nanotechnology

The results of computational experiments via our SoftCAM program with cellular automata of totalistic type on a hexagonal grid are presented. Some semantic interpretations in the context of nanotechnology are proposed.

**Key words:** cellular automata, surface, nanotechnology, hexagonal grid, boundary, Fredkin's rule.

*E.A. Menkovich, S.A. Tarasov, I.A. Lamkin, S. Suihkonen, O. Svensk, H. Lipsanen*

### Study of the physical processes occurring at low temperatures and currents in the light-emitting nanoheterostructures based on semiconductor nitrides

In this paper, light-emitting nanoheterostructures with multiple quantum wells on the basis of (Al, Ga, In)N solid solutions are studied. The properties of the two types of structures were investigated: containing superlattice (type A) or with greater number of quantum wells (Type B) are also studied. Experiments are conducted at cryogenic temperatures (10 – 300 K) and low currents (10 nA – 2 mA). The parameters of various types of nanoheterostructures are compared. It is found that the structure of type A has a higher stability and better work performance. The superlattice influence on the elastic stresses, the lattice deformation at heterointerfaces and in the built-in electric field is considered. An increase in the intensity and reduced self-heating effects in the structure of A is shown. This may be due to the decrease in defects in such nanostructures.

**Key words:** nanoheterostructures, luminescence, superlattice, cryogenic temperatures, elastic stresses, piezoelectric.

*A.V. Trifonov, N.V. Averev, I.A. Charaev, V.A. Seleznev, A.A. Korneev, A.V. Semenov, G.N. Golt'sman, G.M. Chulkova*

### Study of the nature of dark counts in a superconducting single photon detector

We compare with the experiment a model of thermally activated single vortexes, which describes dark counts of superconducting single photon detectors. We find that the model provides a rather good description of the dependence of the dark count rate on a bias current if the latter is close enough to the critical current ( $I_b \geq 0.9I_c$ ).

**Key words:** superconductivity, superconductive single photon detector, thermally activated single vortexes, dark counts.

*E.L. Shangina*

### Energy relaxation in heterodyne detectors based on two – dimensional electron systems

We discuss the application of the theoretical results of the energy relaxation of two-dimensional electrons via the emission of acoustic phonons in the semiconductor  $A^{III}B^V$ ,  $A^{II}B^{VI}$  and group IV structures with a cubic lattice for the analysis of the intermediate frequency band of a heterodyne detector. The process of hot-electron energy loss through the emission of phonons dominates in the long ( $L > 1$  mkm) AlGaAs/GaAs bars; on the contrary, the hot electrons cool in contacts of the shorter channels. We predict the jump of the rate of the energy losses in the metallic Si samples experienced the metal – dielectric phase transition. We predict a jump in the energy loss rate in the metallic Si samples at the metal – dielectric phase transition. We also discuss the importance of this effect for satellite- and earth- based terahertz monitoring.

**Key words:** energy relaxation, two-dimensional electron gas, semiconductor structures, acoustic phonons, hot electron bolometer (mixer), quantum phase transition, scaling, terahertz region of frequencies, heterodyne, intermediate frequency band.

*M.V. Yakunin, S.M. Podgornykh, V.N. Neverov, A.P. Savelyev, Anne de Visser, Gianni Galistu*

### **Interference of spin and tunneling gaps in quantum magnetotransport of the n-InGaAs/GaAs double quantum well**

Complicated transformations of the magnetoresistivity oscillations in the  $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}$  double quantum well are found with a tilt of samples relative to the magnetic field, which reflects the behavior of the gaps in the calculated magnetic level picture. In a tilted field, the tunneling gaps oscillate with the field for large Landau level numbers, which is manifested in sharp transformations of certain magnetoresistivity features within narrow ranges of fields and angles. The minimum for the small filling factor  $\nu = 3$  changes gradually but nonmonotonously with a tilt as the corresponding gap transforms from spin to tunneling gap.

**Key words:** double quantum well, quantum magnetotransport, tilted magnetic fields, spin gap, tunneling gap.

*Zh. A. Devizorova, V. A. Volkov*

### **Nonlinear and anisotropic spin splitting of Landau levels in GaAs-based nanostructures**

An original boundary condition for the effective wave function (envelope wave function of an electron in a crystal) is obtained from general requirements. This condition describes an atomically sharp boundary in  $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$  heterojunction and depends on a single phenomenological constant. It is shown that the atomically sharp boundary and spin splitting of the conductance band due to lack of inversion symmetry lead to anisotropic and nonlinear in the magnetic field spin splitting of Landau levels in a two-dimensional electron system. The corrections to the electron  $g$ -factor linear in the magnetic field are obtained. It is shown that these corrections depend on the bulk constant of cubic spin-splitting of the conductance band (Dresselhaus constant), the parameter  $R$ , characterizing the boundary and the order number of the corresponding Landau level. The results correlate with the recent experimental data.

**Key words:** heterostructure, two-dimensional electron system, spintronics, Lande factor, Landau level.

*P. A. Eroshkin, E. P. Sheshin*

### **Electron gun for an X-ray tube with a field emission cathode**

A design of an electron gun with a field emission cathode based on a beam of polyacrylonitrile carbon fibers for an X-ray tube is proposed. The simulation of the electronic system is made. The optimal design parameters are determined.

**Key words:** X-ray tube, field emission, carbon materials.

*V. V. Vyshinsky, A. G. Nalivaiko*

### **Computational research of the effectiveness of the inhaler of the turbo-jet marine engines**

Inertial separator for air rectification from the sea water droplets, salt and sand at the entrance of turbo-jet mariner engine is the object of the investigation. Computational researches of the different construction schemes inertial separators were made. Their effectiveness and wall friction were analyzed. The optimal construction scheme of inertial separator with minimum wall friction and simple structure at proper effectiveness of separation was proposed.

**Key words:** air rectifier, inertial separator, wall friction, multistage air rectification, mathematical simulation, Reynolds averaged Navier-Stokes equations.

*Zay Yar Myo Myint, A. Yu. Khlopkov, Kyaw Zin*

### Monte-Carlo method for solving high-altitude aerodynamics

The experimental determination of aerodynamic data for high altitudes is difficult not only from the technical but from economic viewpoint. Therefore, the main tools for the study of aerodynamic characteristics of a spacecraft are numerical methods of rarefied gas dynamics. The development of numerical methods in rarefied gas dynamics is primarily due to the use of direct simulation (Monte Carlo method). In this paper, we present an algorithm of the Monte Carlo method and various gas-surface interaction models. The results of the aerodynamic characteristics of spacecrafts obtained by the Monte Carlo method using various gas-surface interaction models are described.

**Key words:** Monte-Carlo method, rarefied gas dynamics, gas-surface interaction models, Maxwell model, Cercignani-Lampis-Lord model, space vehicle, high-altitude aerodynamics.

*A.M. Gaifullin, G.G. Soudakov, A.V. Voevodin, V.G. Soudakov, Yu. N. Sviridenko, A.S. Petrov*

### Effect of fuselage length on civil aircraft aerodynamics at high angles of attack

The experimental investigation of a civil aircraft model in cruise configuration is carried out in the T-103 wind tunnel of TsAGI for different fuselage length (three versions). The objective of the study is to explore the longitudinal and side characteristics of the model at high angles of attack in the presence of yawing. The main goal is to get information on the behavior of the model in these regimes and investigate the effect of fuselage length on aerodynamic characteristics. A comparison of the experimental data and numerical results in the framework of RANS is given. Regions of the abnormal behavior of the side force at high angles of attack are revealed. It is shown that at angles of attack  $a > 15^\circ$ , a sharp decrease of the force acting on the vertical tail can occur, while the vertical tail at  $a > 20^\circ$  is in the aerodynamic shadow of the wing vortex system. In this case, loss of control of the side characteristics can occur.

**Key words:** aircraft, fuselage, aircraft vortex system, side stability, large incidences, large sideslip, vertical tail efficiency.

*M.I. Lipatov, D.X. Do*

### Structure of compressible vortex Couette–Taylor flow

The Couette–Taylor flow of compressible gas at high Reynolds numbers is studied. On the basis of asymptotic analysis at high Reynolds numbers, the mathematical models of the flow and the similarity parameters are defined. The diagram of typical flow regimes at different wavelengths of disturbing flow is built.

**Key words:** Couette–Taylor flow, compressibility influence, flow structure.

*Ya. N. Soe*

### **The flow of delta wing with small sweep angle of the leading edge on the regime of strong interaction**

This paper presents the investigation of the flow on spatial boundary layer on a semi-infinite flat delta wing at small angles to the leading edge sweep on regime of strong viscous-inviscid interaction. In the vicinity of the leading edges of the expansion of functions performed in the course of the power series are formulated and solved the boundary value problems for the functions of flow and on the edge of their own numbers. In the vicinity of the plane of symmetry of the wing held the expansion of functions of flow in power series in the transverse coordinate and the small parameter associated with the sweep angle. The corresponding boundary value problems for calculating the coefficients of members coordinate — parametric expansions and calculated the coefficients of the first six terms of the expansion. Held merging of the obtained expansions to determine the dependence of the induced pressure from the transverse coordinates for different values of a small parameter

**Key words:** spatial boundary layer, delta wing, the strong interaction, series expansion, splice.

*Amirov R. Kh., Vorona N. A., Gavrikov A. V., Zhabin S. N., Lizyakin G. D., Polistchook V. P., Samoylov I. S., Smirnov V. P., Usmanov R. A., Yartsev I. M.*

### **Experimental research of processes of vacuum arc evaporation and substance (gadolinium) ionization, modeling of uranium for plasma technology development of spent nuclear fuel reprocessing**

One of the main problems of the plasma technology development of spent nuclear fuel (SNF) reprocessing is to design a plasma source using a solid SNF as a raw material. This paper is devoted to the experimental study of processes of evaporation and ionization of a substance (gadolinium), modeling of SNF. A vacuum arc on a heated gadolinium cathode is created for this purpose, and parameters of different arc regimes are studied. During the experiment the cathode temperature, voltage, discharge current and vacuum arc plasma spectrum are measured. Also, the probe diagnostics is carried out. It is found that with increasing cathode heating, the arc voltage considerably decreases (down to 3 ?? ). This allows one to reduce the electron energy and obtain singly ionized plasma with high degree of ionization and thus satisfy one of the requirements for plasma technology of SNF reprocessing. This conclusion is confirmed by spectral analysis and the results of probe diagnostics.

**Key words:** plasma technology of SNF reprocessing, vacuum arc, plasma source, gadolinium.

*R. T. Islamov, A. A. Dereviankin, I. V. Zhukov, M. A. Berberova, S. S. Dyadyura, Ju. A. Mardashova, R. Sh. Kalmetiev*

### **Risk Assessment for NPPs with RBMK and WWER reactors**

We make a comparative risk assessment for NPPs with RBMK and WWER reactors and give the results of risk index calculations required for Kursk NPP and Rostov NPP safety passports, which are compulsory for each hazardous industrial facility in accordance with the legislation of the Russia Federation. The output of this research is the assessment of risk index systems in physical and economic terms, social risk (F-N curves) and material damage (F-G curves) charts for Kursk and Rostov NPPs. Key words: risk assessment, safety, NPP, reactor, RBMK, WWER, safety passport.

**Key words:** risk assessment, safety, NPP, reactor, RBMK, WWER, safety passport.

*V.I. Golubev*

### **Technique of visualization and interpretation of full-wave seismic modeling results**

The problem of the visualization and interpretation of the results of computer simulation of dynamic processes in heterogeneous geological media in the process of seismic survey of oil and gas fields is investigated. The author proposes a technique for drawing synthetic seismograms based on the results of 2D and 3D numerical full-wave modeling. The research software «Seismograph» for drawing images in the semi-automatic regime and saving them as graphic files is developed. Examples of important practical geophysical results obtained by «Seismograph» are given. The effective format of data presentation not only at the save time but also at postprocessing stage is proposed. Algorithms for saving data using a single-process and multi-process approach are described.

**Key words:** Mathematical modeling, numerical grid-characteristic method, seismic survey, experimental data interpretation.

*Yu. V. Dorn*

### **Detecting inefficient arcs in transportation networks**

The problem of detecting inefficient arcs in transportation network is considered. An efficient algorithm is presented.

**Key words:** Braess Paradox, Selfish Routing, Network Design, Congestion Games.

*A.V. Kulikov, N.O. Malykh, A.A. Stezhkin*

### **Bang-bang control of swing option price by a binomial asset pricing model**

We use a lattice method for price swing option. We show that the payoff function at each node of the lattice is concave and piecewise affine. The conclusion of this result is that there exists bang-bang control such that if the loan at the moment is an integer, then  $[0, 1]$ -valued optimal purchased quantity at this moment is equal to 0 or 1. If the loan at the moment is not an integer, the fair price is a convex combination of the nearest payoff values with integer loans.

**Key words:** swing option, lattice approach, bang-bang control.

*E.A. Umnov, A.E. Umnov*

### **Method for investigation of the dependence of the solution of a linear programming problem on parameters**

This article is devoted to a scheme of using the smooth penalty functions method for investigating the dependence of the solutions of linear programming on the parameters. A comparative analysis of different types of penalty functions and the assessment of the effectiveness of methods for solving various classes of optimization problems are given.

**Key words:** linear primal and dual programming problems, penalty functions method, parametrical programming problem, dependence of the optimal solution on parameters.