CONFERENCE ABSTRACTS

International Student Conference

“Science and Progress”

DAAD

Санкт-Петербургский государственный университет

Freie Universität Berlin

German-Russian Interdisciplinary Science Center

St. Petersburg – Peterhof
November, 15-19
2010

Programme International Student Conference

"Science and Progress"

November, 15-19

St. Petersburg – Peterhof

November, 15 (Monday)

- **09.30 – 10.30**
  Registration (hall, 1-st flow, Faculty of Physics)
- **10.30 – 10.40**
  Opening Ceremony, aud. B-04
- **10.40 – 11.20**
  "Photoionization in Variable-Size Matter", Prof. Dr. Eckard Ruehl, Institute of Chemistry and Biochemistry, Physical and Theoretical Chemistry, Freie University Berlin, aud. B-04
- **11.20 – 12.00**
  "Rare-Earth and Actinide Compounds – Physics of Strongly Correlated Electrons", Prof. Dr. Clemens Laubschat, Freie Universität Berlin, Germany, aud. B-04
- **12.00 – 12.40**
  "Bifurcation without parameter", Prof. Dr. Stefan Liebscher, Institute of Mathematics, Freie University Berlin, Germany, aud. B-04
- **12.40 – 13.00**
  Coffee-break
- **13.00 – 14.00**
  Oral Sections
  C – Mathematics and Mechanics, part I, aud. B-04
  G – Theoretical, Mathematical and Computational Physics, part I, aud. B-02
  H – Biophysics,part I, aud. 210
  Steering Committee of G-RISC, Office G-RISC in Institute of Physics
- **14.00 – 15.00**
  Lunch
- **15.00 – 16.30**
  Oral Sections
  C – Mathematics and Mechanics, part II, aud. B-04
  G – Theoretical, Mathematical and Computational Physics, part II, aud. B-02
  Steering Committee of G-RISC, Office G-RISC in Institute of Physics

- **15.00 – 16.00**
  Oral Sections
  H – Biophysics, part II, aud. 210
- **16.00 – 17.00**
  Poster Section, hall, 2-nd flow, Faculty of Physics
  H –Biophysics
- **16.30 – 17.00**
  Coffee-break
- **17.00 – 18.00**
  Oral Section
  C – Mathematics and Mechanics, part III, aud. B-04
  G – Theoretical, Mathematical and Computational Physics, part III, aud. B-02
  Steering Committee of G-RISC, Office G-RISC in Institute of Physics
- **18.00 – 19.00**
  Supper

November, 16 (Tuesday)

- **09.00 – 10.00**
  Breakfeast
- **11.30 – 12.30**
  Annual Metting of G-RISC "First results and perspective", aud. B-04
- **12.30 – 13.00**
  Coffee-break
- **13.00 – 14.00**
  Annual Metting of G-RISC (*continue*)
- **14.00 – 15.00**
  Lunch
- **15.00 – 17.00**
  Poster Section, hall, 2-nd flow, Faculty of Physics
  G – Theoretical, Mathematical and Computational Physics
- **18.00 – 19.00**
  Supper

November, 17 (Wednesday)

- **09.00 – 10.00**
  Breakfeast
- **10.00 – 11.30**
  Oral Section
  A – Chemistry, aud. B-04
  With a lection "Thermodynamic Properties of Pure Ionic Liquids", Prof. Dr. Andreas Heintz, Department of Physical Chemistry, University of Rostock, Germany
  B – Geo- and Astrophysics, part I, aud. B-02

- **11.30 – 12.00**
  Coffee-break
- **12.00 – 14.00**
  Poster Section, hall, 2-nd flow, Faculty of Physics
  A – Chemistry
- **12.00 – 13.30**
  Oral Section
  B – Geo- and Astrophysics, part II, aud. B-02
- **13.30 – 14.30**
  Poster Section, hall, 2-nd flow, Faculty of Physics
  B – Geo- and Astrophysics
- **14.00 – 15.00**
  Lunch
- **15.00 – 18.00**
  Excursion to Pushkin (Tsarskoye Selo - Catherine Palace, Amber room)
- **18.00 – 19.00**
  Supper

November, 18 (Thursday)

- **09.00 – 10.00**
  Breakfeast
- **10.00 – 11.30**
  Oral Section
  D – Solid State Physics, part I, aud. B-04
  E – Applied Physics, aud. B-02
  F – Optics and Spectroscopy, aud. 210
- **11.30 – 12.00**
  Coffee-break
- **12.00 – 14.00**
  Poster Section, hall, 2-nd flow, Faculty of Physics
  E – Applied Physics
  F – Optics and Spectroscopy
  Oral Section
  D – Solid State Physics, part II, aud. B-04
- **14.00 – 15.00**
  Lunch
- **15.00 – 17.00**
  Poster Section, hall, 2-nd flow, Faculty of Physics
  D – Solid State Physics
- **18.00 – 19.00**
  Supper
- **19.00 – 24.00**
  Excursion “Night Petersburg” (start from the Faculty of Physics)

November, 19 (Friday)

- **10.00 – 11.00**
  Breakfeast
- **11.00 – 11.45**
  "Thermodynamics in an icy world: The atmosphere and internal structure of Saturn's moon Titan", Prof. Dr. Andreas Heintz, Department of Physical Chemistry, University of Rostock, Germany, aud. B-04
- **11.45 – 12.30**
  "Inverse ill-posed Problem, Regularization and Application in Aerosol Physics", Prof. Dr. Christine Boeckmann, Institute of Mathematics, University of Potsdam, Germany, aud. B-04
- **12.30 – 13.00**
  Coffee-break
- **13.00 – 13.45**
  "Photonic crystal fibers - A base for novel hybrid optical waveguiding structures", Prof. Dr. Markus Schmidt, Max Planck Institute for the Science of Light, Russell Division, aud. B-04
- **13.45 – 14.15**
  Closing Ceremony, Honor Price, aud. B-04
- **14.15 – 15.00**
  Lunch

Organizing committee

Prof. Dr. A.S. Chirtsov,	Dean of Physical Faculty of SPbSU
Prof. Dr. A.M. Shikin,	Coordinator of G-RISC in SPbSU
Dr. V. Yu.Venediktov,	Ass. Pr. of Physical Faculty of SPbSU
E.I. Spirin,	Dean-assistant of Physical Faculty of SPbSU
E.V. Serova,	Dean-assistant of Physical Faculty of SPbSU
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A.A. Popova,	G-RISC office in SPbSU

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Prof. Dr. G.A. Leonov,	Mathematical and Mechanics Faculty of SPbSU
Dr. N.V. Kuznetsov,	Mathematical and Mechanics Faculty of SPbSU

Heads of sections

A. Chemistry – Prof. Dr. Yu.S. Tver'yanovich, Chemical Faculty of SPbSU,
Prof. Dr. E. Rühl, Faculty of Chemistry, FU Berlin

B. Geo- and astrophysics – Prof. Dr. V.N. Troyan, Physical Faculty of SPbSU,
Prof. Dr. V.V. Ivanov, Mathematical and Mechanics Faculty of SPbSU

C. Mathematics and Mechanics – Prof. Dr. G.A. Leonov,
Prof. Dr. V. Reitmann,
Mathematical and Mechanics Faculty of SPbSU

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Physical Faculty of SPbSU

E. Applied Physics – Prof. Dr. A.S. Chirtsov,
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F. Optics and Spectroscopy – Prof. Dr. Yu.V. Chizhov,
Prof. Dr. N.A. Timofeev,
Physical Faculty of SPbSU

G. Theoretical, Mathematical and Computational Physics – Prof. Dr. Yu.M. Pis'mak, Physical Faculty of SPbSU

H. Biophysics – Prof. Dr. A.V. Lezov, Physical Faculty of SPbSU

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Invited reports

Thermodynamic Properties of Pure Ionic Liquids

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Germany

Recent studies concerns properties of ionic liquids – the modern direction of multidisciplinary research.

Ionic liquids are often moderate to poor conductors of electricity, non-ionizing (e.g. non-polar), highly viscous and frequently exhibit low vapor pressure. Their other properties are diverse: many have low combustibility, excellent thermal stability, wide liquid regions, and favorable solvating properties for a range of polar and non-polar compounds. Many classes of chemical reactions, such as Diels-Alder reactions and Friedel-Crafts reactions, can be performed using ionic liquids as solvents. Recent work has shown that ionic liquids can serve as solvents for biocatalysis. The miscibility of ionic liquids with water or organic solvents varies with side chain lengths on the cation and with choice of anion. They can be functionalized to act as acids, bases or ligands, and have been used as precursor salts in the preparation of stable carbenes. Because of their distinctive properties, ionic liquids are attracting increasing attention in many fields, including organic chemistry, electrochemistry, catalysis, physical chemistry, and engineering; see for instance magnetic ionic liquid.

Inverse ill-posed Problem, Regularization and Application in Aerosol Physics

Dr . Christine Böckmann
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Institute of Mathematics, University of Potsdam, Germany

In this lectures we first summarize some basic knowledge about ill-posed operators with noisy data as spectral theory and functional calculus of compact, self-adjoint operators in Hilbert spaces, Moore-Penrose generalized inverse operator, singular value decomposition of compact operators and the degree of ill-posedness. Second, we give some typical examples for those operators. Next, we introduce an abstract smoothness condition and define a regularization method as a pair of a continuous approximation operator and a parameter choice rule, e.g., Morozov discrepancy principle. Moreover, the general theory for linear regularization operators for linear ill-posed problems via filter functions will be given and some examples of well-known regularization methods will be investigated as truncated singular value decomposition, Tikhonov-Phillips method and Landweber iteration. Furthermore, we discuss briefly the order optimality of regularization methods. Finally, we show applications in Aerosol Physics concerning the retrieval of the aerosol-particle size-distribution function from retrieved optical backscatter- and extinction-coefficient profiles from noisy lidar signals. Both problems are ill-posed since the model equations form a Volterra or Fredholm integral system of first kind, respectively, which are compact and, therefore, ill-posed.

Rare-Earth and Actinide Compounds - Physics of Strongly Correlated Electrons

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Technical University, Dresden, Germany

The 4f-orbitals of the rare-earth elements lie inside the closed 5s and 5p shells which define the ionic radius. As a consequence, 4f-orbitals on neigboring atoms do almost not overlapp and maintain most of their atomic properties (particularly their magnetic moments) in the solid state. Electron hopping interactions between 4f and valence-states, however, become possible and lead in some rare-earth compounds to unusual material properties that vary sensitively as a function of composition ranging from magnetic order to magnetic screening via Kondo effect, mixed-valence, superconductivity and a breakdown of Fermi liquid behavior. Due to the localized character of the 4f-states the Coulomb-repulsion energy between two electrons at the same site is large. Proper handling of 4f-states in the framework of bandstructure theory is, therefore, not possible and other approaches as e.g. the Anderson model must be used.The 5f-orbitals of the actinides, on the other hand, are spatially more extended due to their orthogonality to the 4f-states and reveal, therefore, transitions from localized to itinerant behavior in solids. Angle-resolved photoelectron spectroscopy allows the most direct insight into the behavior of the f-states. Recent high-resolution data are presented and discussed in the framework of modern theories.

Bifurcation without parameter

Prof. Dr. Stefan Liebscher
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Institute of Mathematics, Freie Universität Berlin, Germany

We study dynamical systems with manifolds of equilibria near points at which normal hyperbolicity of these manifolds is violated. Manifolds of equilibria appear frequently in classical bifurcation theory by continuation of a trivial equilibrium. Here, however, we are interested in manifolds of equilibria which are not caused by additional parameters. In fact we require the absence of any flow-invariant foliation transverse to the manifold of equilibria at the singularity. We therefore call the emerging theory bifurcation without parameters.

Albeit the apparent degeneracy of our setting (of infinite codimension in the space of all smooth vectorfields) there is a surprisingly rich and diverse set of applications ranging from networks of coupled oscillators, viscous and inviscid profiles of stiff hyperbolic balance laws, standing waves in fluids, binary oscillations in numerical discretizations, population dynamics, cosmological models, and many more.

In this lecture we will give an overview of the behavior of flows near bifurcation points without parameters in comparison with classical bifurcation theory. We will discuss methods used in the analysis of these singularities and present applications.

Photoionization in Variable-Size Matter

Prof. Dr. Eckart Rühl
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Institute of Chemistry and Biochemistry, Physical and Theoretical Chemistry, Freie Universität Berlin, Germany

Photoionization of atoms, molecules, and macroscopic condensed matter is well-known since many years. However, much less is known about size-dependent changes of photoionization in variable size matter reaching from small clusters, via nanoparticles to microparticles. Photoionization by soft X-rays is known to be a process which probes the local surroundings of the excited site. Therefore, it is possible to distinguish different geometric sites in variable-size clusters. Size effects in photoionization are also observed in nanoparticles, where photoelectron imaging techniques indicate the location, from where the electrons originate. Complimentary are studies on charging single, trapped nanoparticles by soft X-rays, providing detailed information on the charging mechanisms as a function of photon energy. Moreover, short-pulse lasers in the infrared and visible regimes permit to study the dynamics of electron emission. Finally, recent results on single, trapped microparticles of aqueous solutions are presented, where cluster formation in droplets and charge-induced nucleation is discussed.

Photonic crystal fibers - A base for novel hybrid optical waveguiding structures

Prof. Dr. Markus Schmidt
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Max Planck Institute for the Science of Light, Russell Division,
Erlangen, Germany

Photonic crystal fibers (PCFs) consist of arrays of micrometer size hollow channels extendingalong the entire fiber length. Such fibers provide sophisticated waveguiding properties and found application in many areas of science and real world devices. In my talk, I'll introduce the basics of these microstructured fibers and discuss the several applications. Additionally, recent results on silica PCFs filled with noble metals, semiconductors or soft glasses will be presented.

A. Chemistry

X-ray Photoelectron Spectroscopy of Free SiO_2 Nanoparticles near the Si 2p Absorption Edge

E. Antonsson[1], J. Söderström[2], C. Nicolas[2], B. Langer[1], J. Meinen[3,4], S. Khasminskaya[3], M. Eritt[3], O. Sublemontier[5], X. Liu[2], C. Graf[1], G. Saidani[6], J.-L. Le Garrec[6], E. Robert[2], J. B. A. Mitchell[6], P. Morin[2], C. Reynaud[5], T. Leisner[3,4], C. Miron[2], and E. Rühl[1]

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Scientific supervisor: Prof. Dr. E. Rühl, Faculty of Chemistry, Freie Universität Berlin

The physical and chemical properties of nanoparticles are a subject of great interest. Their unique properties are often related to their high surface-to-bulk ratio. We study nanoparticles with X-ray photoelectron spectroscopy as a surface sensitive method. In order to study the intrinsic properties of nanoparticles free from interactions with any surrounding medium, we use aerodynamic focusing to form a beam of nanoparticles in high vacuum [1]. First results on X-ray photoelectron spectroscopy of free SiO_2 nanoparticles have been reported which were limited to the Si 2p and O 1s photoelectron peaks [2]. We have studied the photoemission from SiO_2 nanoparticles (98 nm and 214 nm diameter) over a wide electron-kinetic-energy range which reveals contributions from direct photoelectrons, slow secondary electrons, and Auger electrons as well as inelastically scattered electrons from the photoelectron and Auger electron channels. Furthermore, it has been shown that aerodynamically focused sub 10 nm nanoparticles can be studied by synchrotron radiation from a 3rd generation facility despite the low target density resulting from the small particle size [3]. This is accomplished by using pulsed particle injection into the ionization region which increases the signal-to-noise ratio and allowed us to measure photoelectron spectra near the Si 2p absorption edge of sub 10 nm SiO_2.

References

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2. E. R. Mysak, D. E. Starr, K. R. Wilson, and H. Bluhm // Rev. Sci. Instrum. 81, 016106 (2010).

3. J. Meinen, S. Khasminskaya, M. Eritt, T. Leisner, E. Antonsson, B. Langer, and E. Rühl // Rev. Sci. Instrum. 81, 085107 (2010).

Synthesis of monoliths layers and using its in TLC for determination of proteins

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In the present time, the analysis the proteins is the most important problems, because the amino acids are markers of various diseases including a brain. The major problem at their determination is insufficient efficiency of columns, high molecular weight of proteins and capacity is irreversible sorption on silica plates that complicates their qualitative and quantitative analysis.

Represented work is devoted to development of monolithic plates on the basis of monomers GMA-EDMA (glycidyilmethacrylate-ethylenglicoldimethacrylate) by a method photo initiated polymerization. In contrast to conventional packed beds, the main advantage of methacrylate-based monolith is their porous structure, which provides to all other fast division of a mixture.

In this work the possibility chromatographic separation on the polymeric layers of low-molecular substances (synthetic fat-soluble dyes) and high-molecular agents (proteins and peptides in the form of their fluorescing derivatives) is showed.

Effect of low-frequency sonication on ion-solvent interactions in solutions of copper (ii) salts

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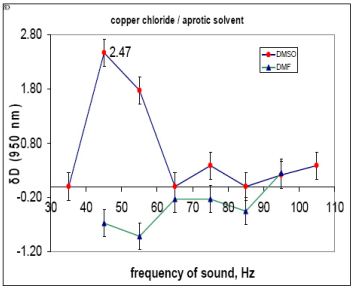
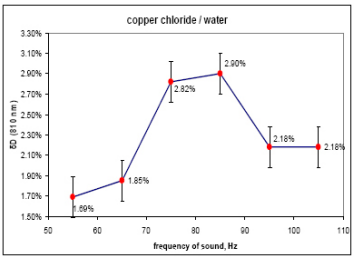
The effect of ultrasound waves on structure and properties of liquids was studied in details and has received an adequate theoretical explanation. At the same time the number of researches devoted to the action of acoustic waves of low-frequency range (20-120 Hz) is rather restricted. In this study some new data on the forms of manifestation of the effect of low-frequency acoustic field on the properties of solutions of copper (II) salts are presented and some possible mechanism is proposed. A number of the systems significantly different in such characteristics as solvation energy of ions, degree of hydrolysis of metal ion and structure of solvent were chosen for study.

The transformations initiated in the solutions were fixed by means of electron absorption spectroscopy and potentiometric determination of the acidity of a solution. Comparison of spectra of the solutions treated by acoustic waves within 45 minutes, and not irradiated these has shown a distinct difference in values of optical density in a maximum of absorption without displacement of the maximum. Hence, the constant position of absorption maxima in spectra and also the unchanged pH values of solutions enables us to conclude that the low-frequency acoustic field effect mostly on the interaction outside first hydration sphere of ion (interaction between molecules of bulk solvent and between coordinated and bulk solvent).





The comparison of the data for aqueous and non-aqueous solutions has shown that the effects for $CuCl_2$ – DMSO solutions are much more pronounced compare to $CuCl_2$ – DMF and similar to those observed for aqueous solutions. That is due to the degree of structuring of solvents. The individuality of solvent reflects in frequency values at which the highest effect is observed.

Russian Fund for Basic Research (project 09-03-00755-a) and Ministry of Education of Russian Federation (programme “Development of the research potential of higher school, project 2.1.1/1656) are greatly acknowledged for the financial support.

GeX_2-Ga_2X_3-Sb_2X_3 (X = S, Se) glasses for IR fiber optic

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Glasses of GeX_2-$Ga2X_3$-Sb_2X_3 (X = S, Se system) have been synthesized and studied for developing of materials for infrared fiber optics.

It was found that the increase of antimony chalcogenide in the relative content of glasses, leads to a sharp increase in glass-forming ability and crystallization stability, increase the density of glasses, increase in the refractive index, shift of the fundamental and phonon absorption edges to longer wavelengths. The optical transparency range of $71.4(0.16GaS_2 0.84GeS_2)28.6(SbS_{1.5})$ glass is about from 0.62 to 12 microns, refractive index is 2.254. The similar parameters for selenium base composition $71.4(0.16GaSe_2 0.84GeSe_2)$-$28.6(SbSe_{1.5})$ is from 0.83 to 16 microns and 2.749 respectively.

The researched glasses were used as a matrix for addition of Pr^{3+} ions in order to create active fiber optic infrared materials. Glasses contained 1.2 at % Pr were synthesized and investigated. The optical fibers of 80 microns diameter were prepared from the synthesized glass samples and their optical properties were studied.

This work was supported by program G-RISC and RFBR № 08-03-92 001 HHC.

Pulsed glow discharge time-of-flight mass spectrometry for direct determination of nitrogen in steel

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Quantitative determination of nitrogen in steels became one of the main problems in modern metallurgy because of intensive use of nitrogen as an alloy addition. For instance, it is extensively used in nitrided and superduplex stainless steel (SDSS) production. The presence of such additions is known to improve a number of characteristics of steel (pitting corrosion resistance, nonmagnetic behavior, strength and other). Both direct and indirect methods in use have many disadvantages and call for revision. The direct technique of nitrogen determination in steel on the base of pulsed glow discharge time-of-flight mass spectrometry is proposed. Gas mixture, consisting of argon (69,7%), helium (30%) and hydrogen (0,3%) was used as a discharge gas instead usual argon-hydrogen mixture. It is helium addition, that allows to ionize nitrogen at the extent sufficient to its quantitative determination (fig.1). Successful application of the method for steel samples with different nitrogen concentration was demonstrated. Dependence of nitrogen signal intensity as a function of repelling pulse delay was investigated, optimal delay time was obtained. Limit of detection for the proposed method was found to be 0,03%.

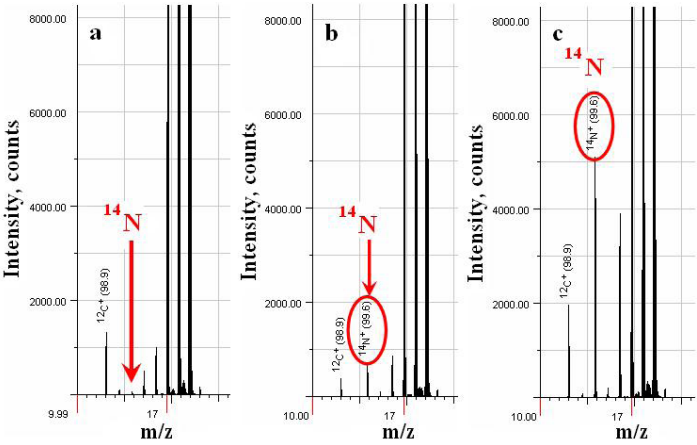

Fig. 1. Spectra of steel samples. a – nitrided steel (0,3% of nitrogen), argon-hydrogen gas mixture; b – non-nitrided steel, argon-helium-hydrogen gas mixture; c – nitrided steel (0,3% of nitrogen), argon-helium-hydrogen gas mixture.

Nanocrystalline titania-based photoactive coatings for photocatalytic decomposition of organic water contaminants in a flow-type reactor

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Scientific supervisor: Dr. Zvereva I.A., Faculty of Chemistry, Department of Chemical Thermodynamics and Kinetics, Saint-Petersburg State University

Heterogeneous photocatalytic processes using TiO_2 offer an attractive way of wastewater treatment especially with regard to very low concentrations of contaminants. The largest photocatalytic activity is shown by slurry reactors which utilize TiO_2 powder. However such systems require separation of the fine submicron particles from the treated milk-like water which decreases the economical viability of water purification. Therefore photocatalytic reactors with immobilized photocatalyst are preferred for practical applications. To increase the effectiveness of such photocatalytic reactors various ways of immobilizing TiO_2 particles, for example in thin film form, and different reactor configurations are investigated.

In this work we propose an effective, simple and cheap method to immobilize nanocrystalline titania on quartz glass. This method includes deposition from water suspension with a small amount of acetyl acetone and subsequent annealing at 450°C to form the titania coating. The morphology was examined by scanning microscopy (Carl Zeiss EVO 40EP and Zeiss ORION). The main advantages of our method are good keeping of fixed size and phase composition of initial titania nanoparticles, uniformity, continuity and stability under hydromechanical treatment of coatings.

Quartz glass coated by photocatalyst was loaded in a flow-type reactor to examine the decomposition of methyl orange dye and phenol as model organic water contaminants. The photocatalytic reactor of our construction can provide efficient exposure of the photocatalyst to light irradiation and a good contact between the reactants and catalysts.

The decrease of the dye concentration was detected using spectrophotometer Shimadzu UV-1650 PC. Different initial dye concentrations and average flow rates of water were used for the study of methyl orange decomposition kinetics. Finally, the first order apparent kinetic constants of methyl orange degradation were calculated. It was found that the presence of photocatalyst leads to an increase of the kinetic constant of methyl orange degradation at least by one order of magnitude. The main result of our work is the achievement of 99% conversion of methyl orange dye with initial concentration of 12-50 mg/l.

Synthesis, characterization, and surface functionalization of gadolinium-based nanoparticles as fluorescent and magnetic MRI contrast agents

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Scientific supervisor: Prof. Dr. Rühl Eckart, Faculty of Chemistry, Freie Universität Berlin

The aim of this work is the preparation and characterization of nanoparticles which can be applied as both fluorescent labels and T_1-weighted magnetic resonance imaging (MRI) contrast agents. Gd^{3+} ions with seven unpaired electrons provide the magnetic contrast and doping with other rare earth elements such as europium or erbium makes the particles fluorescent.

The work is divided into two parts. The first part is a study of whether the magnetism of Gd^{3+} ions in the particles changes when the particles are doped with fluorescent europium ions. This is achieved by X-ray magnetic circular dichroism (XMCD) measurements which were carried out at the Swiss Light source. In addition, these nanoparticles are characterized by fluorescence spectroscopy and transmission electron microscopy. In the second part, results on the functionalization of nanoparticles which contain Gd^{3+} and Er^{3+} ions with biocompatible, hydrophilic ligands are presented. Mono- and bivalent polyethylene oxide-phosphonate ligands are prepared and the bond between the ligands and the particle are investigated by infrared measurements. The ligand density is estimated by thermal gravimetric analysis. Moreover, the stability of the ligand-exchanged particles is studied by transmission electron microscopy and dynamic light scattering.

Preparation of Ordered Metallic Nanostructures for High Harmonic Generation

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Scientific supervisor: Dr. Christina Graf, Dr. Jürgen Plenge, Prof. Dr. Eckart Rühl, Institute of Chemistry and Biochemistry, Physical and Theoretical Chemistry, Freie Universität Berlin

In the common high-harmonic generation (HHG) process an atomic or molecular medium is exposed to a femtosecond laser pulse of sufficient intensity ($>1 * 10^{13}$ W/cm^2). The nonlinear HHG process leads to the formation of a comb of coherent XUV pulses of femtosecond to sub-femtosecond duration.

Instead of using high intensity laser pulses it has been shown that it is possible to generate high-harmonics by exploiting the local field enhancement induced by resonant plasmons within metallic nanostructures and so to decrease the required laser intensity [1].

Therefore it is necessary to prepare ordered patterns of highly anisotropic metal nanoparticles from which strong plasmonic effects are expected. Gold nanoparticles of different size and shape are prepared by colloidal chemistry and are arranged in ordered structures by self-arrangement on sapphire substrates. Self-organization of the nanoparticles is favorable because the nanoparticle approach yields structures with dimensions well below 100 nm on areas reaching up to square centimeters. This appears to be promising for the efficient generation of high-harmonics. For the formation of coherent ultrashort XUV pulses by ordered nanostructures a XUV-monochromator is needed. An experimental setup for detecting high-harmonics has been constructed and first experiments indicating that high-harmonics from rare gases are produced. Furthermore, first structures were used in the setup for the investigation of plasmonic effects during the interaction with femtosecond laser pulses.

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Synthesis of the Aurivillius phases using soft chemistry techniques

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Perovskite-like layered structures attract significant attention nowadays. This is due to the fact that many of them show a large variety of properties, including two-dimensional physical properties (magnetic and electric), catalytic activity and others. However, simple, affordable methods of synthesis of this class of compounds are still to be developed. Standard techniques of solid-phase synthesis demand high temperatures and long heating time, also a number of compounds cannot be obtained by such technique. Particles obtained by these methods are comparatively large and can not be used effectively as catalysts.

This paper presents the comparison of different methods to obtain the so-called Aurivillius phases $Bi_2AB_2O_7$ that are promising photocatalysts for water purification and hydrogen production. The cationic substitution, coprecipitation, molten salt and sol-gel techniques, as well as classical solid-state synthesis have been compared.

All techniques developed in the present work have been tested for the Aurivillius phase Bi_3NbTiO_9 as the representative compound, while other Aurivillius phases have been chosen for each technique depending on its peculiarities. The study of the formation processes was performed by thermogravimetric analysis and isothermal annealing-quenching followed by the X-ray diffraction. Particle size has been determined by means of scanning electron microscopy and analysis of the X-ray diffraction peaks broadening.

The use of the soft chemistry techniques results in the decrease of the heating temperature and synthesis time. The obtained compounds have smaller particle size. The photocatalytic activity of the obtained samples has been tested.

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Development of chromatographic and electrophoretic methods for determination of steroidal hormones in biological fluids

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Control of the trace amount of biologically active substances is an important task in clinical analysis. Fluctuations of concentration represent a number of pathological states. Thus, determination of steroidal endo- and exogenous hormones enables to find the cause of steroidogenesis derangements under different endocrine diseases.

The most commonly used techniques for determination of hydrophobic steroidal drugs and non-steroidal anti-inflammatory agents are chromatographic and electrophoretic methods. In the recent years the method of high-performance thin-layer chromatography with densitometric detection has been used besides reversed-phase high- performance liquid chromatography.

It is possible to reduce the detection limits by using off-line concentration methods, such as solid-phase extraction. On the other hand it is necessary to increase separation selectivity which is attained by application of various modifiers of stationary phase (β-cyclodextrin, sodium dodecylsulfate, cetyltrimethylammonium bromide).

Influence of thiophene incorporating on dipole geometry of liquid crystal molecules

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Low molecular liquid crystals (LC) widely used by modern industry in different sensors, indicators and liquid crystalline displays. Dipole geometry and total dipole value are the important characteristics that determine LC's behavior under the treatment of electric field as in the mesomorphic so as in the isotropic phase. The purpose of the present contribution was connected with the clearing of the influence of thiophene rings incorporating to the structure of carboxybiphenylene LCs on theirs dipole structure. In the framework of work the specificity of polarization of thiophene, bi-, three- and tetrathiophene have been considered, 4, 4'-bis(5-alkyl-2thienylcarbonyloxy)bithiopenylene has been studied experimentally by electrooptical Kerr effect and by the method of dielectric polarization in dilute solutions, and comparative analysis of experimental data and results received by quantum chemical semiempirical PM3 method have been done. The synthesis of experimentally studied LC have been realized at organic chemistry department of Free University of Berlin (Germany).

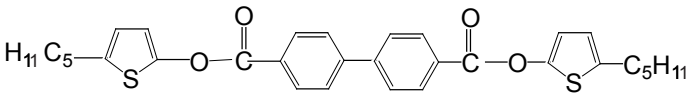

Fig. 1. Chemical structure of 4, 4'-bis(5-alkyl-2thienylcarbonyloxy) bithiopenylene.

Data of computer simulation on polarity and electrooptical properties of the compound under investigation have reveal good correlation and permit to explain its small in value and negative in sign electrooptical Kerr constant. The performed study has shown that thiophehe rings in the content of LC (fig. 1) are responsible for formation of total dipole strongly perpendicular to the longitudinal molecular axis. LCs of this type dipole geometry are of special interest as the materials for display technique [1].

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New perspectives in laser-assisted copper deposition from solution

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Current report represents the latest achievements in the field of laser-induced copper deposition on surface of dielectrics, which develops a process of creation of thin continual metal lines and structures.

The field of possible applications of the results is microelectronics: manufacturing of printed circuit boards, flexible monitors and keyboards.

Focused beam of the continuous-wave argon laser is used for the initiation of the deposition process. Photothermal chemical reaction leads to deposition of metal on the substrate with a high degree of adhesion. Motorized translation stage, being controlled by a computer, provides deposition of continual metal lines. While digital camera is used for on-line monitoring of deposition process on the computer screen [1].

The main chemical reaction in this process is authocatalytic reduction of copper by formadehyde. As the reaction takes place only in an alkaline solution, we need to use complexing agents (L) to prevent precipitation of copper in a form of hydroxide. The complexing agents decrease reducing potential of copper, preventing main reaction proceeding outside of the irradiated area. Therefore reduction of copper can only proceed in the area, heated by laser beam.

$$CuL^{(n-2)-} + 2HCHO + 4OH^- \rightarrow Cu^0 + L^{n-} + H_2 + 2HCOO^- + 2H_2O$$

In the latest experimental work our group have developed method of deposition of copper on a surface of Al ceramics. This result is very important, because previously we had succeeded in deposition of copper on amorphous materials, which is rarely applied in electronics.

We investigated dependence of deposition process results from laser power and composition of solution.

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Structural features and thermal stability of cation-ordered layered titanates $NdMTiO_4$ and $Nd_2M_2Ti_3O_{10}$ (M=Na, K)

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Layered perovskite-type oxides belong to the number of compounds perspective for creation of functional materials. They possess a wide spectrum of physical and chemical properties (electrical, optical, catalytic). Moreover cation-ordered oxides are attractive as precursors in soft chemistry roots for synthesis of new layered compounds. For the successful application of these materials it is necessary to have data on a temperature range of their stability.

In report we present results of the study on thermal stability of titanates $NdMTiO_4$ and $Nd_2M_2Ti_3O_{10}$ (M=Na, K) that belong to the Ruddlesden-Popper phases and built by the intergrowth of alternating layers – Perovskite type blocks and Rock-salt type slabs. Difference of the structure of these compounds consists in the thickness of perovskite layer formed by a two-dimensional net of octahedra TiO_6, which in $Nd_2M_2Ti_3O_{10}$ is three times more than in $NdMTiO_4$. Particularity of the structure of both compounds is full ordering of alkaline and rare-earth cations on structural positions in alternating layers (P and RS).

Thermal stability of layered oxides $NaNdTiO_4$ and $Na_2Nd_2Ti_3O_{10}$ has been investigated by isothermal annealing-quenching method followed by X-ray powder diffraction and SEM analysis and methods of the thermal analysis with constant speed of heating (TGA and DTA) in the range of temperatures 780 – 1100°C and 1100 – 1400°C accordingly.

The structure-chemical mechanism of the decomposition of layered structures and temperature intervals of phase transformations are determined. The structure of $Nd_2M_2Ti_3O_{10}$ oxide was found to be more heat resistant, and moreover it is the product of $NdMTiO_4$ decomposition parallel with oxides Nd_2TiO_5 and $Nd_2Ti_3O_9$. The decomposition of $Nd_2M_2Ti_3O_{10}$ occurs at higher temperature 1400°C and results in the appearance of $Nd_{2/3}TiO_3$ and $Nd_2Ti_2O_7$. The potassium-containing phases are less stable than sodium-containing ones.

The comparison of oxides stability is carried out in terms of crystal chemistry. The essential contribution in the phase transformations are brought by the effect accompanying change of the coordination environment of Nd^{+3} (C.N.= 9, 12, 6) and Ti^{+4} (C.N.= 6, 5) cations and considerable distortions of their coordination polyhedra. In case of $NdKTiO_4$ the tilting of TiO_6 octahedra results in decreasing of stability of structure in comparison with $NdNaTiO_4$. The difference in the length of M^+–O bond connecting P and RS layers results in the greater stability of $Nd_2M_2Ti_3O_{10}$ layered structure in comparison with the $NdMTiO_4$.

A new kind of acyclic diaminocarbene Pd complexes - high active catalysts in Suzuki reaction

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Pd complexes with acyclic diaminocarbenes (ADCs) are a new convenient catalysts in a wide range of cross-coupling reactions [1, 2]. They possess high chemical and thermal stability, low toxicity, and availability, due to possibility of their synthesis via nucleophilic addition of *N*-nucleophiles to coordinated isonitriles. Recently Luzyanin *et al.* reported that the carbene complexes Pd^{II} bearing incorporated sp^2/sp^3-N nucleophilic centers (in general, on benzophenone hydrazone $H_2N–N=CPh_2$) display high activity (TON *ca.* 900000) in Suzuki cross-coupling [3]. Obviously, the reason of such catalyst activity is due to high basicity of unchelated hydrazine part of the ligand. Inspired by these results, we synthesized another ADC complex with unhelated hydrazine fragment by a reaction between equimolar amounts of *cis*-$[PdCl_2(C{\equiv}NCy)_2]$ and $H_2N–NH\text{-}Ph\text{-}NO_2$ (having two N atoms with different nucleophilicity) and use this complex as a catalyst in cross-coupling.

At the initial experiments, we realized reaction between the *cis*-$[PdCl_2(C{\equiv}NCy)_2]$ and $H_2N–NH\text{-}Ph\text{-}NO_2$ in $CHCl_3$ at 20–25 °C. During 24h we observed appearance the carbene species *cis*-$[PdCl_2\{\underline{C}(N(H)N(H)\text{-}Ph\text{-}NO_2){=}N(H)Cy\}(C{\equiv}NCy)]$ **(1)** in good (95%) isolated yields. Complex is air- and moisture-stable in the 20–80 °C temperature range. Complex was characterized by ESI^+-MS, IR and ^1H, ^{13}C NMR spectroscopies.

We have investigated the new complex as catalyst in Suzuki reaction. We have chosen a reaction of 1,4-dibromobenzene with phenylboronic acid accomplishing *para*-terphenyl as a model system. The reason for our choice is interest to synthesis of polymer materials requiring use of aryl polyhalides as substrates. Conversion of 1,4-dibromobenzene is essentially complete after *ca*. 5 minuits in refluxing EtOH, furnishing the terphenyl product in *ca*. 98% yield. High yields were obtained even at catalyst loadings as low as 10^{-5} mol per mole of substrate.

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Synthesis of complex perovskite -like ferrites and study of the nonisovalent substitution Gd→Sr in the matrix of $Gd_2SrFe_2O_7$

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One of the important types of materials is the ferrite ceramics. It is using in electronics, such as memory devices, and as catalysts in the chemical industry. To develop the technology of the synthesis of complex ferrites with high yield and required properties it is necessary to ensure the crystal structure and stoichiometry of compounds. One of the most promising groups of ceramic materials is layered perovskite-like oxide materials. The oxidation state of transition metals in perovskite-like layered oxides is of high importance for the existence of outstanding physical and chemical properties.

The present study deals with:

- synthesis of polycrystalline solid solutions $Gd_{2-x}Sr_{1+x}Fe_2O_7$ (x = 0,1 - 0,6) by high temperature ceramic technology and sol-gel method,
- study of the oxidation state of iron in obtained solutions $Gd_{2-x}Sr_{1+x}Fe_2O_7$ by Mössbauer spectroscopy,
- investigation of magnetic susceptibility of $Gd_{2-x}Sr_{1+x}Fe_2O_7$ (x = 0 - 0,3).

Complex oxide $Gd_2SrFe_2O_7$ belongs to the class of layered perovskite-like compounds and built by blocks of perovskite and rock salt structural types. Solid solutions $Gd_{2-x}Sr_{1+x}Fe_2O_7$ were synthesized at atmospheric pressure using the method of isothermal "annealing-quenching" at a temperature of 1400 °C in the range of 48 -78 hours. X-ray powder diffraction confirmed the presence of single phase with perovskite-like layered structure only for the content $x \leq 0,3$. Investigation of magnetic susceptibility in the temperature range 4-300 K showed the presence of antiferromagnetic interactions in a layered perovskite oxide $Gd_2SrFe_2O_7$ not only between the iron atoms, but also between the atoms of iron and gadolinium. Similar results were obtained for solid solutions $Gd_{2-x}Sr_{1+x}Fe_2O_7$ ($x \leq 0,3$).

Mössbauer spectra of solid solutions differ significantly from the spectra of oxide $Gd_2SrFe_2O_7$. With a small Sr content, the iron atoms are in one state – Fe^{+3}, but in two fields of different symmetry. With the increasing of Sr concentration lowering of the symmetry of oxygen environment of iron atoms is observed and third type of iron atoms (Fe^{+4}) appears.

Synthesis of oxides by ceramic technology requires large energy costs (long-time synthesis and high-temperature calcination), but does not allow to get particles in nanoscale range. That is why, the one task of this work is to reduce the temperature and time of the synthesis using the sol-gel technology and thus to obtain submicrocrystalline samples with new features.

Ion exchange and hydration of layered complex oxides $NaLnTiO_4$ (Ln=Nd, La)

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Layered type solids are intergrowths of layers with different types of structures. Layered perovskites consist of two-dimensional perovskite slabs interleaved with cations or cationic-oxygen units. In recent years layered perovskites have attracted considerable attention because of their interesting physical 2D-properties.

Layered perovskite-type oxides $NaLnTiO_4$ (Ln=La,Nd) (Fig. 1) are of particular interest owing to high ionic conductivity [1] and prospect as an easily synthesized [2] precursors for obtaining a number of other layered compounds by ion-exchange and topochemical reactions.

The aim of this work was the investigation of the behavior of alkali-containing layered structures $NaLnTiO_4$ (Ln=La,Nd) in water solutions and ambient air.

In this work new compounds with general formula $H_xNa_{1-x}LnTiO_4 * yH_2O$ with H+ ions and water molecules in the interlayer space were obtained in water and acid solutions. The amount of water (y) and exchange degree (x) were estimated from TGA-data. Powder X-ray analysis was used to specify the structure of compounds. It was found that $NaLnTiO_4$ compounds readily exchanges interlayer Na^+ ions with water protons forming partially substituted hydrates $H_xNa_{1-x}LnTiO_4$ at pH>7 and fully substituted $HNdTiO_4$ without intercalated water at pH<5.

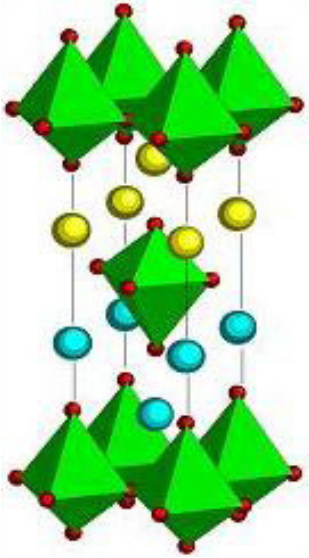

Fig. 1. Structure of $NaNdTiO_4$.

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Local Magnetic and Electronic Structure of Post-Synthesis Oxidized Iron Oxide Nanoparticles as Novel Magnetic Resonance Imaging (MRI) Contrast Enhancers

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Iron oxide (FeO_x) nanoparticles are applied in medical research as contrast agents in magnetic resonance imaging (MRI) where they reduce the spin-spin relaxation time (T_2 time) of absorbing tissues. Hence, control of their magnetic properties is essential for these applications. These properties strongly depend on the particle size, and shape, as well as the surface structure and the modification of the iron oxide core.

Therefore, monodisperse, spherical iron oxide (Fe_3O_4/Fe_2O_3) nanoparticles were prepared by a high temperature approach in organic solvents using iron oleate as a precursor. NEXAFS (Near Edge X-Ray Absorption Fine Structure) investigations showed that strorage over long time periods in an argon or ambient atmosphere induces changes of the local electronic structure of these particles which can affect their T_2 times. For a controlled simulation of these time-dependent effects the freshly synthesized particles are tempered in an oxygen- free or oxygen rich environment to improve their crystalline order and to change their magnetite to maghemite ratio.

Magnetic relaxometry measurements are carried out to evaluate, if these structural changes influence the spin-spin (T_2) and spin-lattice (T_1) relaxation time of the nanoparticles. NEXAFS and XMCD (X-Ray Magnetic Circular Dichroism) experiments were used to investigate local structural and electronic properties of the iron oxide particles before and after post-synthetic oxidative and thermal treatment. These results are correlated with relaxometry data

Solution – solid equilibria in systems $CuCl_2 – H_2O – S$ (S – 1,4-dioxane, tetrahydrofuran)

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Formation of solid phase in ternary saline water-organic systems and particularly generation of mixed water-organic crystallosolvates remains one of the insufficiently explored branches of chemistry of heterogeneous systems. In continuation of earlier systematic study of the effect of properties of organic solvent on the equilibrium solution - solid phase in the systems of $CuCl_2$ - H_2O - S (S - dimethyl sulfoxide, N, N-dimethylformamide, acetonitrile), the study of systems of $CuCl_2$ - H_2O - DX and $CuCl_2$ - H_2O - THF (DX - 1,4-dioxane, THF - tetrahydrofuran) was undertaken in this work.

Obtained results show that the solubility of the solvates $CuCl_2$ 2.5DX and $CuCl_2$ • THF is very low (0.03 mol/100 mol of solvent and 0.5 mol/100 mol of solvent respectively). This fact is due to two reasons. Copper ion in these compounds has a tetrahedral symmetry and the transition from distored octahedral aqua complexes to the tetrahedral ones always leads to a sharp drop in solubility. Low values of permittivity DX ($\varepsilon = 2.21$) and THF ($\varepsilon = 7.6$) also make for the decrement in solubility by reason of a strong association of ions in solution.

When the length of the branch of crystallization of compound $CuCl_2$ xS (S = THF, DX) is compared with the same characteristics of other organic solvates, it is the smallest in the case of DX. This fact is fully correlated with the minimum value of donor number of DX in this series of oxygen-donor solvents. The higher the value the donor number of solvent, D_N (S), the greater the length of the branches of the crystallization of the corresponding organic solvate on solubility isotherm, ΔN (S).

	$CuCl_2 \cdot 2DMSO$	$CuCl_2 \cdot 2DMF$	$CuCl_2 \cdot THF$	$CuCl_2 \cdot 2.5DX$
$\Delta N(S)$	0.628	0.558	0.27	0.10
$D_N(S)$,ccal/mol	28.9	26.6	20.0	14.8

It is apparently the solubility of copper dichloride in mixtures of H_2O - THF is much higher than in mixtures of water - dioxane. This is due to two factors. First, the dipole moment of THF (1.63 D) is much larger than the corresponding value for molecule DX (0.45 D). Moreover, in contrast to the molecule THF, which has only one donor site, molecule DX has two oxygen atoms, which may be coordinated to different central atom, i.e. DX can serve as a bridge or a ditopic ligand, and the formation of polymeric complex species should also reduce the solubility of copper dichloride.

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Dispersions of carbon nanotubes: perspectives of binary amphiphile stabilizers and mixed solvents

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A pre-requisite of carbon nanotubes (CNT) application is preparation of their homogeneous stable dispersions in media germane to the specific. We tackle providing time-stable CNT dispersions with fluidity of the medium spanning broad interval of sub-zero temperatures (down to -50 ^{o}C). To this end we study processing dispersions in a mixed solvent and addition of such components to the system, who upon binding with CNT surface, would ensure steric and charge stabilization of the suspension.

In first place we study micellar aggregation in the 3-component system, composed of anionic surfactant (sodium dodecylsulfate), cationic IL (one from the list: hexylmethylimidazolium chloride, hexylmethylimidazolium bromide, decilmethylimidazolium bromide,) and water. Employing three methods, viz., conductometry, titration calorimetry and fluorimetry we measured critical micellar concentration (CMC) in the said type of ternary systems. These data are complemented by molecular-thermodynamic model estimates (variant of Nagarajan-Ruckenstein model) of sizes and charges of aggregates for various ratios of binary amphiphile additives. Both experimental and calculation results indicate that there exists an interval of the surfactant/IL composition ratios, where the propensity towards aggregation grows by the order of magnitude(drop in the CMC and growth of micelles), whilst micelles retain 60-75% of the surface charges appropriate to the aggregates of the pure surfactant. This combination of circumstances casts in favor of the steric along with charge stabilization of CNT dispersions, given this sort of the binary amphihile is used as a stabilizer.

The second aspect of this study focuses on the issues of processing CNT suspensions in the mixed media. To warrant fluidity of the CNT dispersions at low temperatures we performed an initial series of experiments regarding CNTs in the ternary solution glycerol - ethanol - water with cetiltrimethylammonium bromide as a stabilizer. We give data on the properties of suspensions of multi-walled CNT in the proximity of the binary eutectic glycerol – water. A combination of relatively high viscosity owing to glycerol and low freezing temperature (around -50^{o}C) due to the addition of small amounts alcohol (2-5% wt) makes this medium a candidate for procuring properties of dispersions necessary for their usage as optical valve shutters. We illustrate this inference with data on the optical transmission in the gotten stable dispersions of CNT (for certain regimes of their processing: various powers and time expositions of ultrasonication and centrifugation).

B.Geo- and astrophysics

P-wave travel-time inversion in transversely isotropic medium

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The transversal isotropy is a typical approximation for models describing anisotropic formations. However, inversion for Thomsen-type anisotropic parameters in transversely isotropic media using surface seismic data proved to be a highly non-unique problem [1].

In this work we focus on estimation of information content for seismic signatures in 2D model with dipping reflector overlaid by homogeneous TTI medium. We assume that the seismic data we possess consists of surface seismic reflection data (CMP gather) and checkshot survey along the deviated well. In this study we consider both wide-azimuth and narrow-azimuth surface seismic data. The seismic signatures we use are NMO velocity, non-hyperbolic moveout and checkshot velocity measured along the well of arbitrary deviation. For analysis we apply singular value decomposition to a Frechet derivative in a weak-anisotropy approximation. In particular we show that for some combination of reflector dip angle and symmetry axis tilt angle the solution of inverse problem becomes unstable.

The results of this analysis can be used to suggest a specific acquisition design. Inversion of seismic data obtained from such acquisition should yield accurate estimates of anisotropic parameters.

Another question we consider in this work is VTI model building using TTI seismic data. While VTI model is often used to fit travel-times obtained for TTI media the question on how far obtained Thomsen parameters will move from their true values still requires investigation.

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Vertical motion of tail neutral sheet associated with the IMF Bx component: global MHD modeling results

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We use global MHD simulations to investigate the influence of the the interplanetary magnetic field (IMF) Bx-component on the the geometry, dynamics and location of the neutral sheet (NS). Contrary to existing opinion present study shows that the IMF Bx-component seriously affects the position of the tail neutral sheet (NS).

We provide results from two simulations (using BATSRUS code) with different Bx-values (Bx=-6nT, Bx=6nT) in which all other solar wind parameters were fixed, but only IMF Bz varied. We show large north-south shifts of the tail NS about order 2-3 Re from its steady position, whose direction depends on Bx (upward for Bx<0, downward for Bx>0). The magnitude of NS shift also depends on radial distance and increases in tailward direction. The most interesting and unexpected result is that amount of NS shift also strongly depends on IMF Bz, increasing a few times during time intervals of southward Bz-component compared to northward IMF case. To understand a physical origin of the NS vertical motion we compared the values of the total pressure in the northern and southern tail lobes $P_{tot} = P_m + P_p$, where P_m – magnetic and P_p – plasma pressure. Pressure difference about (5-10%) between north and south lobes observed under southward IMF is probably due to the difference of Ampere's forces in the northern and southern parts of the magnetopause. We also present some experimental test of the observed effect.

Application of the Gelfand-Levitan method for solution of the dynamic acoustic inverse problem in laterally homogeneous media

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The geophysical inverse problem is the problem of reconstruction of medium parameters like P-wave velocity V_p, S-wave velocity V_s, density ρ, etc. using data (displacement, pressure etc) recorded near the earth surface. The data contains information of interaction of the initial signal (shot) with the medium.

Today the geophysical inverse problem is mainly solved by seismic full-waveform inversion. One of main disadvantages of this procedure is strong requirement of a regular initial model which is often unreliable.

Otherwise, the geophysical inverse problem can be treated as a mathematical dynamical inverse problem. In this case there exist theoretically developed approaches for the solution. They do not require the initial model except for the medium parameters near the surface. This is main advantage of such methods. But the models they can afford are very simple (laterally homogeneous, smooth, etc) and that's main disadvantage.

The aim of a present work is to introduce the Gelfand-Levitan method for solution of inverse problem that can provide a simplified (laterally homogeneous and smooth) but more regular earth model. This regular model can be used further as initial for full waveform or any other type of inversion. The Gelfand-Levitan method for 1D acoustic equation was described by Blagovestchenskii [1]. The method is restricted to acoustic equation for media with lateral homogeneity. Also the constant density is used for more simple and clear equations.

The work consists of theoretical part and numerical investigation. The results of 1D numerical test prove the method to be accurate and useful. The method can be easily extended to 2D and 3D observations by Radon transform. Applicability of the method to real data is hampered by the fact that hydrophones and geophones do not record the lowest frequencies needed for a reconstruction method that uses a delta-function assumption. If the method can be successfully applied to real data, it can become a very important inversion tool in geophysics or in other disciplines. Further research will involve the investigation of applicability to real datasets as well as extension of the method to media with slight lateral variations.

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Ionospheric manifestation of the energetic plasma injections during substorm

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Motivated by recent comparisons of transient equatorward-moving auroral traces with short injections detected by Themis spacecraft [1] we analyze TV observations of 11 auroral substorm events (each showing a number of equatorward traces). For each event transient equatorward-moving auroral traces were compared with sharp increase in the energetic particle fluxes observed by LANL spacecrafts in nearby MLT sectors to understand - if there exists a distinct correspondence between two phenomena.

Geographical position as a function of time was defined for each trace. Using these data and standard magnetospheric model T96 all separate auroral traces and equatorward boundary of the auroral bulge were mapped to the magnetosphere and compared with LANL spacecraft energetic particle observations. In the electron (proton) fluxes dawnward (duskward) of the mapping region there was found clear enhancement. Near the mapping region the simultaneous enhancement in both electron and proton fluxes was observed. Drift trajectories for different energy particles were also calculated to define approximate azimuthal boundaries of dispersionless injection. The auroral structure mapping region was found within these boundaries for all events.

The electron precipitation boundary latitudes defined by NOAA satellites data were compared with equatorward auroral boundary. It was found that NOAA observes the intense precipitation containing a significant part of energetic particles above 30-100 keV energy (isotropic protons and anisotropic fluctuating electrons).

The first results of our investigation helped us to conclude that transient equatorward-moving auroral traces represent the ionospheric manifestation of the energetic plasma injection at geostationary orbit.

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The study of the buoyancy of thin flux tubes in the interior of the Sun

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Solar activity and dynamo problem pose significant challenge to researchers. One major achievement in understanding processes that drive solar activity was made by Babcock [1]. In Babcock's model initially poloidal field inside the Sun is transformed due to differential rotation into gradually increasing toroidal field, which becomes buoyant and then emerges to the Sun's surface as bipolar regions observed in wide range of wavelengths.

The present work is aimed to investigate the behavior of toroidally magnetized plasma in a star's interior in analytic and using numerical simulations. We use an approach to magnetohydrodynamics in which plasma is considered as a collection of thin flux tubes parametrized by frozen-in coordinates [2, 3] (a material coordinate along the flux tube and lagrangian time coordinate) and study the dynamics of a single flux tube inside the Sun. In this approach the motion equations turn out to be in the form of nonlinear string equations.

In general case of arbitrary tube with both nonuniform poloidal and toroidal field components there is no straightforward way to describe it's dynamics in external fields of gravity and pressure inside the Sun. The calculations are carried out assuming simplifications regarding symmetry of the tube.

The Lagrange function for a flux tube is derived and used to obtain effective potential energy of a tube in symmetric case. It has been shown in the work that a symmetric tube have two modes: pulsation in equatorial plane driven by buoyancy and maxwellian magnetic tension and floating up until surface is reached. The specific mode of motion depends mostly on the initial magnetic field intensity in the tube - result which is in accordance with the idea of Babcock's model.

The numerical simulations using two-step Lax-Wendroff schema reproduce two modes mentioned above for various values of initial parameters. The developed code may be used to study cases of perturbed symmetry.

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Line Profile Variability and Magnetic Field of Zeta Ori A

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Line profiles in spectra of OB stars are usually strongly variable. Both the stochastic line profile variability (LPV) which is connected with the formation of small-scale structures in the stellar wind and the regular LPV induced by the large-scale structures in the wind can be detected.

The existence of such structures in the wind can be explained if we accept that studied star possess the global magnetic field. Magnetic field can also regularize the structures in the wind, which are induced by the stellar non-radial pulsations. The recent measurements have shown that nine O and about of 5-10 % B stars have a weak magnetic field.

Kholtygin et al. [1] have proposed the program of searching the magnetic field of OB stars. Spectropolarimetric observations for eight bright OB stars were made in a framework of this program in 2005 – 2010. Up to the moment the magnetic field of B1Ib supergiant ρ Leo with the polar magnetic strengths of 250 G was detected. Recently Bouret et al. [2] has reported a detection of a weak magnetic field (50-100 G) of O9.5 supergiant ζ Ori A.

We report the results of a study of fast LPV in spectra of bright binary O supergiant ζ Ori A and searching its magnetic field. The observations were made in 2009 on February 11/12. The spectra of ζ Ori A was obtained in the Special Astrophysical Observatory (SAO). The regular short time-scale components of LPV in spectra of star with period P = 2.4-3^h have been detected. These components are probably connected with the non-radial pulsations of the primary component Aa of a binary system ζ Ori A. Presence of magnetic field reported by Bouret et al. [2] was not confirmed.

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Hierarchy of vibrational states sets for solution of the non-NTE radiative transfer problem in the 2.0 and 2.7 μm CO_2 bands in the Earth atmosphere

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The extended non-LTE model for the CO_2 infrared bands in the Earth atmosphere includes a set of 328 vibrational states of seven CO_2 isotopes [1]. To simplify solving the non-LTE problem of radiative transfer in the CO_2 bands, a procedure of reducing the amount of the vibrational states is formulated [2]. Influence of a number of accounted vibrational states and optical transitions of different CO_2 isotopes on results of solving the non-LTE CO_2 problem in the middle and upper atmosphere of Earth has been examined. A hierarchy of three models R1, R2 and R3, which are simpler than the extended model but provide a reliable accuracy of estimating non-equilibrium populations, is proposed. In the direction of decreasing accuracy, these simplified models include 226 and 136 states of seven CO_2 isotopes, and 80 states of five CO_2 isotopes, respectively. Solution of the non-LTE problem for 5 atmospheric models, 3 values of solar zenith angle and 2 profiles of the CO_2 volume mixing ratio has been obtained.

Even the simplest model R3 allows evaluation the populations of the lower vibrational states with a reasonable precision. For the values of non-equilibrium populations of the 10^01 state which gives rise for the fundamental vibrational (FB) transition of the 2.7 μm band of CO_2, an accuracy no worse than 0.002, 0.007 and 0.02 for the models R1, R2 and R3, respectively, has been found. For the 20^01 state giving rise to the FB transition of the 2.0 μm band of CO_2, the accuracy is no worse than 0.003, 0.004 and 0.017 for the models R1, R2 and R3, respectively.

Use of the simplest model R3 in evaluating the rate of net radiative heating in the both 2.7 and 2.0 μm bands of CO_2 gives errors which do not exceed 0,025 K/day above the stratopause.

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Regulrization methods in ray tomography

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Generalized model $\boldsymbol{Pv} + \boldsymbol{\varepsilon} = \boldsymbol{u}$ is considered, where $\boldsymbol{P}$ is an integral operator with the singular kernel, ν represents small smooth deviations of the field $\boldsymbol{\mu}$ of physical parameters of the media, and ε is the residual of the model and experimental data.

Regularized solution of the inverse problem is given by the formula

$$\hat{v} = D^{-1}P^{*}(PD^{-1}P^{*} + K_{\varepsilon})^{-1}u,$$

where $\boldsymbol{D} = \boldsymbol{I} - \boldsymbol{\Delta}$ in case of Tikhonov regularization and $\boldsymbol{D} = -\boldsymbol{\Delta}$ when "simplified" Tikhonov regularization is used. Regularization for model equations is represented in functional spaces, as in this case the algebraic analogs of these equations may be regularized independently on the dimension of the respective Euclidean space. The formulas for inverse problem solution are given in the operator form, but one can conclude that in matrix notation the element

$$(PD_{1}^{-1}P^{*})_{ij}$$

is equal to the energy of two threads-rays interaction (fig. 1) with corresponding to the type of regularization potentials (Coloumb or Yukava) charged with densities proportional to $\boldsymbol{\mu}$.

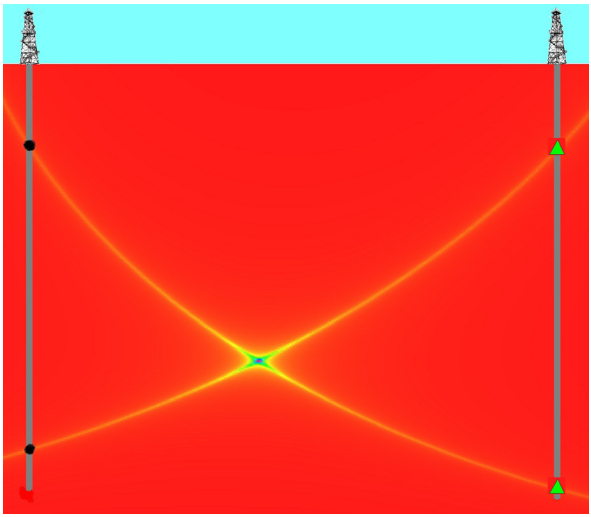

Fig. 1. Two "interacting" rays.

Different regularization methods in solving ray tomography problem are considered and a physical interpretation of algorithms suggested is given.

The application to the solution of the inverse problem in anisotropic case is discussed.

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Application of ground penetrating radar for river mouth processes investigation

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Hydrological processes in river mouth regions have many peculiarities that are not entirely investigated yet. One of the most unstudied phenomena in the mouth processes is the movement of the fresh water – saline water boundary – the halocline. Usually, traditional hydrological methods do not allow obtaining data with rather great spatial and time resolution, what is important in mouth regions with intensive flood tide - ebb tide oscillations.

Great difference in conductivity between fresh and saline water makes ground penetrating radar (GPR) an efficient method for detecting halocline.

The aim of the work was to develop the method of using GPR for fast halocline detection and to apply it for river mouth processes investigation.

In 2007-2010 the number of experiments was carried out in the mouth of river Keret (Loukhsky region, Karelia republic). The method of GPR application was developed and the conditions of its effective application were determined. The 3D image of the halocline structure during the ebb tide phase was obtained. Also the records of halocline depth variation during the flood tide – ebb tide cycle were acquired.

The experiment showed that application of GPR is effective for tracking processes in the regions of fresh water and saline water mixing. The fresh water – saline water boundary has complex time-dependent structure, which could not be analytically described yet. Spectral-time analysis of the data allows discriminating a number of halocline oscillation frequencies which can be associated with internal waves of different nature.

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Kink and sausage modes of flapping oscillations in the current sheet of the magnetotail

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Flapping oscillations observed in the current sheet of the Earth's magnetotail, represent rather slow waves propagating from the center to the flanks with a typical speed ~20-60 km/s, amplitude ~1-2R_e and quasiperiod ~2-10 minutes. The relevant model is based on double gradient of magnetic field: gradient of tangential (B_x) component along the normal (z) direction and normal component (B_z) along the x-direction [1]. Calculations were made for two different variants of initial disturbance.

In the framework of this model the rotation of the vector of magnetic field in the plane Z-Y as well as vector of plasma velocity is investigated to find differences between kink and sausage modes of the flapping oscillations. Were observed that rotation of the vectors don't depend from type of initial disturbance and it is also shown that the speed of the rotation of the vector (**v** or **B**) gives the fundamental parameters of the model including double gradient frequency.

The theoretical results are compared to the flapping oscillations observed by space mission Themis on 03.05.2008 in the morning sector of the magnetotail. The observed rotation of the velocity vector simultaneously on two spacecrafts of Themis mission corresponds to the kink mode of the flapping oscillations.

The results obtained show that data on rotation of **v** and **B** vectors can give important information about modes and characteristics of the flapping waves.

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Diffractor imaging with cross-well data

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Most of conventional imaging techniques are designed to locate the reflecting interfaces in the subsurface. Reflecting interfaces define basic features of geological model of the medium. However, besides reflecting interfaces at medium usually exists scattering objects (diffractors), for example, faults or salt vugs. These objects also may be of great interest for exploration. Scattering objects imaging may be useful for seismic data interpretation, production monitoring and reservoir characterization.

But the scattered wave amplitude may be so weak that it is difficult to see those objects in usual reflection images. The location of scattering objects requires then special data pre-processing and/or imaging. Several methods of pre-processing are based on diffracted wave enhancement (reflection suppressing) in the data: the plane-wave destruction filters, diffraction imaging by focusing-defocusing of reflected waves, filtering of reflected waves in different data domains.

There are also the modifications of migration excluding stacking of reflected waves. It is possible to enhance the diffractions by designing simple weight functions in the angle domain for Kirchhoff migration. We propose the technique of diffractor location with cross-well data. We use Kirchhoff migration with special weight functions. We have found that it is useful to employ all the components of the data to enhance valid signal, i.e. use the vector Kirchhoff migration instead of the scalar one. We considered several weight functions for both diffraction and reflection enhancement: limitation of the specular reflector dip at the image point and special selection of source and receiver sets. We verify the validity of reflectors and diffractors by building the Common Image Gathers (CIGs).

We have applied these techniques to synthetic data created for a fine-layered model with small diffractors. The diffractors, invisible with the conventional processing, were located with the weighted Kirchhoff migration.

Interaction of elastic waves with the one-dimensional nonlinear elastic region

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The interest arises recently to the detection of the objects having nonlinear properties.

This work is the example of solution of the simplest one-dimensional problems of elastic waves interaction with the nonlinear elastic medium. Processes of the reflection and refraction of the elastic waves on the boundaries of the linear and nonlinear elastic media and also their interaction with nonlinear elastic layer situated in the linear elastic medium are considered.

Posed problems are solved in the frames of five-constant theory of elasticity of Murnaghan. Linear elastic parameters are supposed to be continuous on the boundary between linear and nonlinear elastic media. Wave amplitudes depend only from one spatial coordinate (one-dimensional propagation).

The perturbation method is used to solve the nonlinear motion equation. Components of the displacement vector are presented as the sum of two items. First item is the solution of the linear homogeneous equation. Second item is built with the Green function of the linear equation.

Results of the numerical calculations are compared with analytical formulas for the case of the wave transmission through the region of the nonlinearity [1] and for the case of the interaction of the longitudinal wave with boundary of the linear and nonlinear media [2]. The solution of the problem of the elastic wave interaction with the region of the nonlinearity is compared with the results of finite-difference modeling.

Presented method can be applied to the other similar problems, in particular, to the solution of the nonlinear motion equation in the three-dimensional case more close to the real experiment.

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Magnetic Field of rho Leo

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Spectropolarimetric observations for eight bright OB stars were made during 2004 – 2008. From these observations Kholtygin et al. [1] detected magnetic field of rho Leo with polar magnetic field strength of about 250G. An analysis of spectra of the star showed presence of both short-term and long-term regular line-profile variations (LPV). The regular LPV can be connected with the co-rotation of large-scale structures (jets or disks) in the stellar wind. The existence of such structures in the wind can be explained if the studied star has global magnetic field. Magnetic fields can also regularize the structures in the wind, which are induced by the stellar non-radial pulsations. Recent measurements have shown that nine O and about of 5-10 % B stars have a weak magnetic field.

Schnerr et al. [2] made spectropolarimetric observations of many OB stars using the MUSICOS spectropolarimeter, mounted at the TBL, Pic du Midi, between December 1998 and November 2004. No definitive result about the possible magnetic field of rho Leo was obtained from their observations.

New spectropolarimetric observations of rho Leo were obtained during 11-14 February 2009 at the Special Astrophysical Observatory (SAO) using the 6m telescope and quartz echelle spectrograph in Nasmyth focus NES [3] with 2048 x 2048 Uppsala CCD. All spectra were obtained using a new polarization analyzer described by Panchuk et al. [4]. From these new observations we got two new measurements for the strength of the longitudinal magnetic field of rho Leo. Using previous measurements of the longitudinal magnetic field and the possible rotational period P=7.267d from [1] we determine the parameters of the global magnetic field in dipole approximation in a good agreement with [1].

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Guided waves propagation in a fluid layer sandwiched between different elastic half-spaces

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The low frequency oscillations of a fluid layer in elastic media are described by Krauklis [1, 3], Ferrazzini and Aki [2]. Such a wave (known as slow wave or fundamental mode) propagates along the layer with a velocity that approaches zero at low frequency, always exists and has larger amplitude than other waves. Dispersion curves of other modes are calculated by Ferrazzini and Aki [2] for case, when elastic half-spaces are the same. The aim of the present work is to consider asymmetrical case, when half-spaces have different material parameters, and investigate guided wave propagation in a fluid layer.

In order to derive dispersion equation the wave field, excited from a center of dilatation located at an arbitrary point in an isotropic media included a fluid layer sandwiched between two different elastic half-spaces, is constructed in terms of Lamb's method. The analytical and numerical analysis of real roots of dispersion equation is made. There is a phase velocity range in the asymmetrical case, for which dispersion equation has no real roots. Seismograms obtained by 3D axisymmetric finite-difference method are interpreted. The fact that the second mode, which is generalized Rayleigh wave analogue at low frequencies, has more intensive vertical component of amplitude than slow wave is established for some media parameters.

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The role of the meridional circulation of solar dynamo models

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This work is devoted to the analysis of kinematic model of solar dynamo, especially the role of meridional circulation in it behavior. The main components of this model are: differential rotation, meridional circulation, alpha-effect, turbulent diffusion, and magnetic buoyancy mechanism. Each of these components plays its own role in the whole «dynamo-orchestra».

Until a recent times it was a little known about the meridional circulation. Meridional circulation is a weak flow in meridional plane. It is directed toward the poles on solar surface. The relevance of this flow in different dynamo models is conventionally accepted [1]. The data of last years [2] have shed light on the behavior of the meridional circulation. It turned out that this flow changes during the solar activity cycle. Meridional circulation is faster in minima of solar activity and slower in its maxima.

The aim of the present work is to explore the dynamo behavior taking into account the real profile and approximate features of the flow. To investigate these features we created a model which may describe or at least illustrate such a phenomenon. We solve the standard equations for so-called alpha-omega dynamo problem [3]. All our calculations were done using the code SURYA modified for our purposes. The main results: the cycle duration, the strength of magnetic fields and solar activity, the form of butterfly diagram were obtained.

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Regular Line Profile Variability in Spectra of Star lambda Cep

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Line profiles in spectra of OB stars are usually strongly variable. Both the stochastic line profile variability (LPV) which is connected with the formation of small-scale structures in the stellar wind and the regular LPV induced by the large-scale structures in the wind can be detected. The regular LPV can be also connected with the co-rotation of large-scale structures (jets or disks) in the stellar wind. Several causes explain the formation of these structures. The large-scale structures can be explained by the hypothesis that hot stars possess global magnetic fields. Typically expected timescales for stellar rotation and pulsation in these stars are all in the range from a day to a week.

Kholtygin et al. [1] have proposed program of searching for regular and stochastic line-profile variability in the spectra of O stars. Spectropolarimetric observations of eleven bright O stars were made in a framework of this program in 1997 – 2009. Up to the moment the analysis of LPV of six stars have been made.

We report the results of our study of LPV in spectra of bright runaway `O6I(n)f` star λ Cep. The observations were made in 1997 and 2007. In 1997 the star was observed in the Special Astrophysical Observatory (SAO) of the Russian Academia of Science using the 6-m telescope and Lynx spectrograph. In 2007 the star was also observed in Bohyunsan Optical Astronomy Observatory (BOAO) with the 1.8-m telescope and the BOES spectrograph. The regular short and long time-scale components of LPV in spectra of star with period $P_s \approx 1\text{-}6^h$ (short) and $P_l \approx 0.6\text{-}3.4^d$ (long) have been detected. We suppose that these components are connected with the non-radial (short) pulsations and stellar rotation (long).

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Analysis of reconnection layer in the solar wind

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Different energy transformation processes have an essential role in plasma physics. Transformation of magnetic field energy into kinetic and heat plasma energy is often observed, for example in solar flares, magnetosphere substorms, solar wind-magnetosphere interaction. Magnetic reconnection is believed to be responsible for the most energy conversion processes, and many observational evidences were obtained in the magnetosphere and on the Sun. It is interesting that the most direct signatures of reconnection were recently observed in the solar wind at the fronts of CMEs. CME (Coronal Mass Ejection) can be considered as an object similar to magnetosphere as it has bow shock upstream, magnetosheath region with compressed hot plasma, and even reconnection events at the magnetopause (boundary) of CME. It has been shown by Gosling [1] that inside the reconnection layer in the solar wind, acceleration of plasma is clearly observed as well as density and temperature increase while absolute value of the magnetic field decreases, the length of reconnection line turns out to be 640 Re (Re is the Earth radius).

A database consisting of 113 events of solar wind reconnection was formed and analyzed. For every event the normal vector to the initial current layer at the front of CME, magnetic field vector, velocity vector, temperature, density, magnetic field shear angle were determined. Entropy was calculated as well. One of most important characteristic of a shock wave is entropy, and the increase of entropy has been observed in many cases of the solar wind reconnection from our data base. For example the event of solar wind reconnection happen on 2002 02 02 at 3:30-4:30 was examined in details. All reconnection-associated signatures which can be interpreted as transformation of magnetic energy into plasma energy, can be clearly seen in this event.

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Investigation of thermocline in freshwater lakes by GPR

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In the last decade GPR (ground penetrating radar) have been widely used to solve various geotechnical problems, in particular, they have shown its effectiveness in studies of freshwater reservoirs [1]. In homogeneous water column electromagnetic pulses propagate to great depths without significant distortion, which helps to obtain clear reflections from the bottom of the lake.

The main objects of GPR research is usually the bottom and silty sediments. Water column is usually considered to be homogeneous. However, the high sensitivity of modern GPRs allows to detect reflections from the boundaries within the water column caused by vertical changes in its physical properties (temperature and salinity). During field studies at freshwater lake in the Cape Kartesh, Karelia (these works were included in the program of student's geophysical practice) these additional reflections have been found.

Simultaneously with the radar survey, the temperature has been measured with the use of a portable bathometer and thermometer. It was found that the observed boundary is caused by the presence of vertical temperature gradient - such a boundary is called thermocline.

Evaluation of the reflection coefficient of the observed boundary showed that the variation in permittivity within the bounds of thermocline fits into the framework of well-known empirical relationship [2]. It gives the dielectric constant at the top of the water column equal to 80.4, while at the bottom it is close to 82.6, which is in good correspondence with georadar data.

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C. Mathematics and Mechanics

Oscillation control for pendulum with variable parameters

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Two problems of pendulum control are investigated: swinging pendulum by changing it's length (or gravity center position) and by changing it's suspension point position. An approximation to some invariant set in state space of system is considered as an objective of control. As an attitude to the problem solution high-speed gradient method is used.

The results obtained in the work allow us to find an area of initial conditions and parameters, where system possesses desired properties, and to select values of those parameters in practice.

Solution for elastic medium with infinite cylindrical borehole loaded with time-harmonic stress

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Investigated problem arose from practical engineering needs of improvement of modern jet technology for soil-concrete piles production. There are well-known solutions for static case [1]. Moreover, numerous integral representations of solution in dynamic case of arbitrary time-dependent boundary stress and various geometric axisymmetric configurations of medium are well-studied [2], but all of them have very complicated form, which is not suitable for direct numerical investigation of resonance properties of the system, required by engineers.

So the aim of this work was to derive new exact solution of mathematical problem, which models real complicated soil mechanics by isotropic homogeneous elastic medium with infinite cylindrical borehole loaded by time-harmonic normal stress with frequency ω, and main requirement for solution was ω-continuity. Due to the axial symmetry and harmonicity of stress, dynamic equation for displacements of elastic medium were written in cylindrical coordinates and solution was supposed to be harmonic in time. By means of differential substitution of the displacement functions to potential ones, differential operator of the system could be diagonalized. There was investigated class of potentials with Fourier-images satisfying Bessel's equations after the change of variables, as it lead to physically-correct divergent cylindrical waves. Corresponding differential substitutions were found and continuity properties on ω were determined. It turned out, that there exist only one unique longitudinal potential non-singular at ω=0, which satisfies given normal stress at the boundary. Then solution for tensions and displacements is represented by wave packets of divergent cylindrical waves from perturbation point. Prior numerical estimations indeed show resonance behavior of our solution. Also, our solution was checked to tend to static Lame one for the case of constant stress in the limit of vanishing perturbation frequency.

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Simulation of influence on regional development

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Formation of institutions of state power in Russia and its regions was a complex process. The aim of this work done for the project of the Association of Independent Centers of Economic Analysis, was an attempt to assess the impact of the Institute governorship on the socio-economic development of Russian regions.

For analysis, we chose two characteristics: the transition from election to appointment and the duration of stay in power of the head region. In the first case analyzed, influenced the transition to his appointment to the main indicators of regional development, in the second - how indicators of change in the region, depending on the duration of staying in power of the head region. Considered the following indicators – their own fiscal revenues in the region and investment in major capital.

Been hypothesized: significantly affect the transition to the appointment of governors did not have, socio-economic indicators worsened at the end of term with power, change of regional leaders is improve the socio-economic indicators. The analysis of data and preliminary calculations have shown that perhaps the first hypothesis is correct, while the other two - no.

We analyzed the data and build models based on production multiplicative functions, complemented by new factors. Models cross-section constructed for each year, and comparative analysis can reveal features of the influence of selected characteristics in different periods of time, во время экономического роста и во время кризиса. during economicgrowth and during the crisis

Analysis of the transition from election to appointment showed that the situation had not deteriorated, and when viewed in the dynamics, we can even note the positive changes. Regions, where in 2005 was appointed head in 2005 had incomes less than the average in 2006 - the average, in 2007 - slightly above average in 2008 - higher than average.

Analysis of the power shift has shown that it may have no effect on their own budget revenues. In the year of change of the head of the region's own revenues remained virtually unchanged in the first year in power they are slightly increasing, while the second fell a bit.

Analysis of the influence of the duration of stay in power was held by the different years separately and did not allow unambiguous conclusions. It is necessary to clarify the parameters and model.

Existence of the Global Attractor for the One-Dimensional Microwave Heating Problem

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The existence of the global attractor for the one-dimensional microwave heating problem is studied. The system under study consists of a damped wave equation (derived from two Maxwell's equations in one-dimensional case) and a nonlinear heat equation. The system describes microwave heating process of a one-dimensional region. The problem concerned is assumed to be autonomous and not to have a phase-change.

It was shown by H.-M.Yin in [1] that the system has a unique smooth solution. The dynamical system generated by this problem is constructed. The existence of an absorbing set is proved, which is the main prerequisite of the existence of the global attractor. Thus the results on decay of solutions given in [2] are extended.

Application of frequency domain method to the system is performed. Frequency condition is demonstrated to hold under an additional assumption. Assuring that this condition is true is the main component of proving absolute stability property of the problem.

Experimental results are presented.

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Heating problem solution by asymptotic series and power series methods

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We consider a one spatial dimensional heating problem which consists of the Maxwell's equations and the heat equation. Using special function spaces (Sobolev spaces) we introduce the weak formulation for the coupled equations which describe the generation of electromagnetic waves and the heat transfer in the material. In paticular we investigate biological tissues. Diseased cells are destroyed at high temperature, so it is important to investigate the behaviour of temperature profiles and to spare surrounding normal tissues. According to our assumptions we can show that all weak solutions are classical ones.

Our principal methods of research are the power series and the asymptotic series methods. We demonstrate the results of our experiments which use the analytical representation of solutions according to the above methods and two different forms of heating coefficient in the heat equation. In all experiments we show the structure of a two-phase system and the localization of the interface between the liquid and the solid phases

Almost-periodic Temperature Fields in the Microwave Heating Problem

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The problem of microwave heating in the presence of external Bohr almost-periodic in time perturbation is investigated. A coupled system derived from Maxwell's equations and the heat transfer equation for the one-dimensional case is considered.

For this system with perturbations a cocycle formulation is presented. Quadratic energy functionals of the Lyapunov type are constructed. Using these functionals some properties of the solutions (boundedness, stability) are shown. Under these properties the existence of almost-periodic solutions in the cocycle system is proved.

In the considered system the conductivity and the heat source according to Joule's law are nonlinear functions. Supposing that these nonlinearities are smooth and linearly bounded, and that the boundary and initial conditions are also given by smooth functions, the existence of solutions in the space of Holder functions is derived.

A model of hyperbolic space and the geodesic flow

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Hyperbolic geometry plays an important role in physics and mathematics. Introducing a model of hyperbolic geometry helps us to picture the geodesic flow on the unit tangent bundel of the hyperbolic space, called the Lobatchevsky's plane. We also will talk about the horocycle flow on the Lobatchevsky's plane and see its decomposition in a stable and unstable fibration.

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Bistability of Actin -An Elastic Network Approach

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We study the motion of actin via an elastic network model in order to understand the transition from G- to F-actin. The stability of actin is investigated to find possible further stable states that are indicated by experimental results.

Adaptive synchronization for delay-coupled networks of Stuart-Landau oscillators

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We consider networks of delay-coupled Stuart-Landau oscillators. As it was shown in [1] the value of the coupling phase is a crucial control parameter. By adjusting this parameter one can switch between different synchronous oscillatory states of the network. By applying the speed-gradient method [2] we derive an adaptive algorithm for tuning the coupling phase such that a desired synchronous state is obtained. We propose a goal function the minimum of which corresponds to different states of cluster synchronization. We demonstrate that the speed-gradient method allows one to find coupling phases for which the various states of synchronization, i.e. in-phase oscillation, splay state, or different cluster states, are stable.

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On two-phase microwave heating problem with monotone non-linearities

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We consider two-phase microwave heating problem in one-space dimension, consisting of Maxwell equations and the heat transfer equation.

We derive a week formulation of the heating problem using integral identities. It will be shown that the heating problem has a unique global solution in some function spaces. An important role in the mathematical investigation of the problem plays the property of maximal monotonicity of some non-linear operators. We provide numerical results concerning the temperature profile. In addition to this, we demonstrate the presence of two phases and interface between them.

Variational principles of PDEs

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It is well known, that the weak solution of certain evolution PDE could be obtained from the minimizer of some energy functional. In this talk, I will present a variational principle mostly developed by Nassif Ghoussoub, which allows the variational resolution for many non-Euler-Lagrange type PDEs.

To achieve this, the notion of the self-dual Lagrangians will introduced, yielding a principle for proving the existence of weak/mild solutions for many PDEs, e.g. the heat equation, the complex Ginzburg-Landau initial-value problem or the porous media equations.

On Mathematical Model of Thermo-Electrodynamics and the Solution Theory of Associated Evolutionary Problems

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We introduce a general class of linear evolutionary problems, which covers a number of diverse initial boundary value problems of classical mathematical physics and consider Thermo-Electrodynamics as an example and introduce Joule heating as a non-linearity.

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Non-Linear Response of Water Flux Through a Soil Column

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In order to understand the global water flow it is important not only to know the path the water takes, but also the dynamics: how fast and or to which amount it actually flows during the respective steps of the global water cycle. The paths are mainly known whereas the concrete dynamics are widely unknown.

Measurements of the noise characteristics show, that the white noise of rain results in $1/f$ noise in the water discharge of rivers. That fact implies a non-linear transport process, as linear systems are not capable of changing noise.

I analyzed a non-linear model of the water flow through soil which can be described by Burgers' equation. The non-linear problem can be transformed into a linear problem via the Cole-Hopf transformation. This transformation also acts on the initial and boundary conditions, als well as the driving. Especially the latter takes a very interesting form when solving the linear problem by means of Fourier series.

As the exact solution is not that simple some approximations are employed. Even fulfilling the conditions for these approximations the solution amplifies disturbances in excess of the physical constraints of the model. Therefore there are, however, hints that this model could even answer more questions of interest and should be investigated further. The response to a stochastic influx is of particular interest as this represents real rain.

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Decentralized target-capturing control of multi-vehicle systems based on inter-team range-only measurements

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Multi-vehicle systems have attracted an enormous interest during the last decade because of their potential in a variety of fields, ranging from exploration of unknown environments, surveillance and rescue operations and distributed sensor networks to biology and nano-technology. Different approaches and goals have been experienced in this field. A typical objective is to design a decentralized control law driving a team of vehicles to a pre-specified formation. Recently an extensive research was given to development of coordination control strategies that drive multiple vehicles to a capturing formation around a target. This type of maneuver is both interesting and significant because of numerous potential applications; see, e.g., [1-3]. However, nonlinear dynamics of real-life vehicles, their nonholonomic constraints, and sensing and actuating limitations were not much taken into account up to now.

We consider the problem of capturing a target by a team of autonomous Dubins-like vehicles. The objective is to drive all robots to the circle of a prescribed radius centered at the target and to uniformly distribute them over this circle. Considered are two scenarios where 1) every robot is aware of the team size and the angular velocity of the formation rotation around the target is pre-specified and 2) the robots do not know the team size and the above rotational velocity is not given, respectively. Unlike most papers in the area, we examine nonlinear vehicles with nonholonomic kinematic constraints, where the limitations on the driving velocities and restrictions on the robot's sensing capabilities are taken into account. Specifically, the robot-to-robot sensing capabilities of every vehicle are limited to only distances to the companions from a specific disk sector, whereas the entire target position in the robot relative frame is constantly available. A nonlinear decentralized control law ensuring achievement of the control objective is proposed and investigated. Mathematically rigorous proofs of convergence and stability of the proposed guidance law are presented. Extensive simulation results confirm the applicability and performance of the proposed guidance approach.

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D. Solid State Physics

DFT study of the atomic hydrogen adsorption on Ti_8O_{16} nanocluster

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Titanium dioxide is well known as one of the best photocatalyst. It is known that TiO_2 photoactivity can be increased by sensitization it to visible light and by reduction in size of the active particles (by nanoclusters formation). However, at the present time there is no uniform model to explain these processes. This is because the definition of structural and optical properties of the superdispersed materials is a very difficult experimental problem. Thereupon the molecular quantum chemistry research of such nanosystems is very actual.

This work is devoted to the simulation of adsorption of atomic hydrogen on Ti_8O_{16} nanocluster. This is the first step in theoretical study of the adsorption of atomic and molecular hydrogen, and also their ions on TiO_2 nanoclusters. Due to simplicity of simulation and availability of the broad experimental data supporting it, this reaction is a good verification of the offered approach. Moreover, at present time, the mechanism of the interaction of hydrogen with TiO_2 surface (in particular the nature of the adsorption centers and influence of hydrogen adsorption on TiO_2 electronic system) is incompletely clear and must be explained.

The calculations were done using the DFT method with B3PW91 functional. We used Hay and Wadt pseudo-potential for Ti atoms. For oxygen and hydrogen atoms 6-31G and 6-31++G** basis respectively was applied. The adsorption was simulated by approaching of one H atom to all O and Ti atoms in Ti_8O_{16}. The dependence of the total energy of the system on the distance between H and the adsorptive centers has been calculated. The calculation of electronic structure in valley of potential energy curves was obtained. As a result, 16 clusters with OH groups and 8 with TiH have been calculated.

Our calculations have shown that the adsorption of atomic hydrogen on oxygen atoms has the activation energy lying within 0.09-0.25 eV, what is in well agreement with experimental data about high-temperature adsorption of hydrogen on TiO_2 surface. The adsorption leads to the formation of stable Ti_8O_{15}-OH complexes. Desorption energy of hydrogen in this complexes lies between 2.57 and 3.61 eV. Also, the adsorption leads to the formation of a single half occupied energy level in the cluster's bang gap, which electronic density is localized on Ti atom. In this case it is possible to speak about formation of the active reduced titanium center. According to the calculations, the adsorption on Ti atoms is much weaker than on oxygen (desorption energy lies between 0.03 and 0.09 eV) and has no activation energy.

Adsorption of carbon atoms on the surface of silicon oxide

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Nowadays the interest to research of graphene (a monolayer of graphite) deepens. This interest is based on specific characteristics of this material, which allows using graphene in different areas of nanoelectronics [1].

At the moment several methods of graphene production are known, but there is no easy and predictable way of production of graphene layer on dielectric substrate.

The purpose of this research was study of possibility of production of carbon film, which is formed as a result of atom adsorption, on a substrate with dielectric characteristics. Silicon with 600Å-layer of SiO_2 was chosen as a substrate. During the research the emitter producing a beam of carbon atoms was invented. The emitter works in the following manner: carbon atoms vapour from heated graphite cylinder and move through the aperture, then they reach the substrate and form a carbon film on it. Heating of the graphite cylinder is achieved by electronic bombardment.

The research was pursued with Auger-electronic spectrometer with cylindrical-type analyzer. Vacuum in the system was at least 10^{-7} Pa. The surface of the substrate was cleaned by high-temperature heating.

Behavior of peaks of basic elements in the film (carbon, oxygen and silicon) was researched. Data analysis has shown that after the film forms serious decrease of height of peaks corresponding to silicon and oxygen takes place. This implies that a carbon layer appears on the substrate. Warming the substrate up to 900°C caused some changes in the form of carbon Auger-peak: this peak took the form, typical for graphite [2].

The results of the research point to possibility of forming desired structures of carbon film by choosing processing mode of the system.

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Low temperature luminescence of bound exciton in $CuGaSe_2$ crystal

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$CuGaSe_2$ is a member of I-III-VI_2 group of semiconductors, which are isoelectronic and structural analogs of II-VI compounds. All I-III-VI_2 compounds can be mixed with each other in various proportion, forming solid solutions with a smoothly varying bandgap. On the basis of $CuGaInSe_2$ mixed crystals, elements for solar cells with very high efficiency are developed. So these semiconductors has attracted much attention. Studying the exciton and impurity states in $CuGaSe_2$ allows to understand its unique properties more accurately.

The crystals have been grown by method of iodine transport [1]. Exciton luminescence of CuGaSe2 has been investigated at temperatures of 5-40K. Luminescence spectra were obtained with continuous excitation of second harmonic of neodymium solid-state laser Melles Griot company. We have investigated luminescence in 1.65-1.73 eV region,. where free exciton and bounded exciton interacted with quasilocal oscillation [2] have appeared. The interaction of bounded exciton with quasilocal oscillation changed depending on the quality of crystal in excited area. At the batter quolity points, with more marked free exciton structure, less Stokes shift has been observed.

We have made calculations of luminescence spectra. The best coincidence to experimental curves has been reached at following parameters:

Point №	Eq, eV	S	w, eV	wq, eV
1	0.0037	1.20	0.0025	0.0023
2	0.0037	1.44	0.0026	0.0026
3	0.0037	1.84	0.0029	0.0027

E_q – quasilocal oscillation energy, S – Huang-Rhys factor, w – bounded exciton half-width, w_q – quasilocal oscillation half-width.

With this parameters short-wave and long-wave parts of spectra coincided well, but in the middle small difference has been observed. We suppose an additional structure in this area. This assumption is confirmed by temperature dependence of bound exciton. The various reasons of this phenomenon are considered.

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The investigation of the t_{1u} resonances in the X-ray absorption spectra of free, clustered and solid SF_6 molecules

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The SF_6 molecule is a high symmetry molecular compound where the electronegative fluorine cage surrounds the central sulfur atom, so that the inner well and out well states are distinguished [1]. The core-level excitations of the sulfur atom in the free, clustered and solid SF6 molecules have been examined both experimentally and theoretically in detail [2, 3]. But the x-ray absorption spectra of the SF_6 molecules near fluorine K ionization threshold also have a character behavior that have not completely explained jet [4].

Core-to-valance transitions near fluorine K ionization threshold in the SF6 molecule, where the molecular units are either bound in free variable size van der Waals clusters or in the solid are examined and compared with the excitations in gas phase. The special emphasis is put on X-ray absorption spectra of free, clustered and solid SF_6 molecules recoded for the F 1s → a_{1g}, t_{1u}, t_{2g} regimes. Their comparison shows that there are no visible changes in the position and line shape of the F $1s^{-1}a_{1g}$ and $1s^{-1}$ t_{2g} resonances, whereas the line shape of the F $1s^{-1}t_{1u}$ resonance in the clustered and solid SF_6 molecules signally different from the free SF_6 molecules.

In assumption that the core-level F 1s excitation reduce the symmetry of the SF6 molecule the fit analysis of the F $1s^{-1}a_{1g}$, F $1s^{-1}t_{1u}$,$1s^{-1}$ t_{2g} resonances was realized. It was shown that the triply degenerate t_{1u} molecular orbital was splitted on the none degenerate orbital and double degenerate orbital. The value of splitting of the t1u molecular orbital equals 1.85±0.05 eV, 1.25 ±0.05 eV, 0.45±0.05 eV for the free, clustered and solid SF6 molecules respectively. We assume that the triply degenerate t_{2g} molecular orbital also will be splitted on the none degenerate orbital and double degenerate orbital, but the resolution of the experimental set up does not allow to see it in the experimental data.

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Shape resonances and multielectron excitations in X-ray absorption spectra of clustered SF_6 molecules

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Above the core ionization thresholds both shape resonance and multielectron excitations play a dominant role in X-ray absorption in molecules, clusters and solids. Shape resonance is complicated process associated with temporary trapping of the outgoing photoelectron by a finite-size potential barrier and subsequent tunneling of the photoelectron through the barrier into the core ionization continuum.

In the present work special emphasis is put on X-ray absorption near the S 2p edge in the SF_6 molecule, where the molecular units are bound in free variable size van der Waals clusters. The energy position and lineshape of the molecular $2t_{2g}$ and $4e_g$ shape resonances near S 2p ionization threshold are discussed in more detail.

The spectroscopic study of SF_6 in the S 2p energy region [1] evidences that shape resonance and unoccupied valence orbitals dominate in formation of F^-, S^- and SF^- fragments. The double barrier optical potential (DBOP) model with imaginary part [2, 3] is applied to study and compute the multielectron excitations effects on the shape resonance formation near S 2p ionization threshold in clusters. Imaginary part of DBOP describes energy dissipation of the photoelectron going through the cluster environment. The performed calculations demonstrate additional broadening and upward energy shift of shape resonances in free and clustered molecule SF_6 due to multielectron excitations effects.

Also in this work the asymmetry lineshape of the $4e_g$ shape resonance is discussed in detail. Different fitting methods and interpretation of asymmetry profile are introduced.

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$SrTiO_3$ as a high-k dielectric for future generation memory devices

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Recently, much work are focused on the development of high-k dielectrics and metal gates for high-performance logic Complementary Metal–Oxide–Semiconductor (CMOS) field effect transistor (FET) made from silicon. The minimum feature size in a transistor decreases exponentially each year. But the scaling cannot go on forever.

The most serious problem in logic circuits is now the FET 'gate stack', which is the gate electrode and the dielectric layer between the gate and the silicon channel. The scaling of CMOS has led to the silicon dioxide layer, used as a gate dielectric, being so thin (1.4 nm) that its leakage current is too large. It is necessary to replace SiO_2 with a physically thicker layer of oxide of higher dielectric constant *(κ)*. Recent researches show that the most promising candidates to *SiO*2 replacement in development of new semiconductors devices are *HfO_2, ZrO_2, TiO_2, Al_2O_3*. Nowadays there is a great interest to $SrTiO_3$ structure as a high-k dielectric that can be also used in mass storage memory devices. The attractive properties of $SrTiO_3$ thin films include a high dielectric constant (100) with a high breakdown strength, and good chemical stability but it has a too low band gap (3.2 eV) and this is a considerable defect for its application in semiconductors devices.

The current study is focused on the consideration of the track of solution of the problem of SrTiO3 high-k dielectric, specifically on the analysis of conditions, affected to the value of dielectric constant of $SrTiO_3$ film (the crystalline structure and thickness of the film), and also on the possibility of expansion of the band gap, by introduction of special buffer layer.

The discussion of experimental methods for the most effective analysis of $SrTiO_3$ films is also carried out. As will be shown the methods of the X-ray reflection spectroscopy and X-ray photoelectron spectroscopy (XPES) are more suitable methods. XPES is a technique commonly used for surface analysis and allows in principle to carry out a quantitative chemical analysis of the sample. X-ray reflection spectroscopy is a non-destructive in-depth characterization tool of the local atomic crystalline structure of material. Combined using of these methods provides in-depth characterization of $SrTiO_3$ structure.

The detailed analysis of above mentioned peculiarities of $SrTiO_3$ (STO) films on silicon has a great interest from the fundamental and the technological point of view.

Resonant Cu $L_3M_{4,5}M_{4,5}$ Auger electron spectra of CuI at the Cu$2p_{3/2}$ absorption edge

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Quasimolecular approach based on an assumption about existing of localized states at the bottom of conduction band (CB) of the CuI@SWCNT composite was able to explain qualitatively well the atomic structure changes of the CuI filler due to its encapsulation inside the tubes [1]. Resonant Auger spectroscopy (RAS) is well known technique for identifying of states in the valence (VB) and conduction bands spatially localized near the core-excited atoms [2]. Present work is aimed to identify the localized states in the VB and CB of CuI by RAS.

All measurements have been performed at the Russian-German beamline at the BESSY [3]. Thin (20-25 nm) CuI layers were prepared in the preparation chamber by evaporation of CuI powder from a Knudsen effusion cell onto a polished stainless-steel plate. NEXAFS spectrum at the Cu $2p_{3/2}$ edge was obtained in the total electron yield mode by detecting a sample current. The photon-energy resolution of the monochromator at the Cu $2p_{3/2}$ edge was about 300 meV. Resonant Auger spectra were measured in integrated normal emission mode with total energy resolution of about 0.5 eV.

Analysis of RAS spectra for CuI has resulted in a conclusion that there are practically no empty localized states having Cu 3*d* character near the bottom of the CB in accordance with formal valency of the Cu^+ ion having the $3d^{10}4s^0$ electron configuration in CuI. At the same time it was found that Cu $L_3M_{4,5}M_{4,5}$ spectra of CuI can be interpreted as a superposition of at least 3 resonating and nearly linearly dispersing spectator Auger signals and normal Auger. Corresponding spectator electron states are connected with ones at the bottom of CB of CuI localized near the absorbing Cu^+ ion and which have mostly Cu 4*s* symmetry. Energy positions of these states correspond well to the energy position of Γ_6, L_6, $X_{7,6}$ characteristic points of Brillouin zone in the relativistic KKR band-structure calculations for CB of CuI [4].

This work was supported by the Russian Foundation for Basic Research (project no. 09-02-01278) and the bilateral Program "Russian-German Laboratory at BESSY".

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The investigation of the reaction NO + CO + hν → N_2 + CO_2 on nano-sized TiO_2 (Hombifine N) under irradiation in 300 – 440 nm spectral region by means of kinetic mass-spectrometry and thermo-programmed desorption spectroscopy

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Titanium dioxide is widely used as photocatalyst in environmental catalysis, because it is highly active in degrading of many organic and inorganic pollutants. Earlier it had been shown that the photoreaction CO+NO+hν → N_2 + CO_2 (1) on TiO_2 (Degussa P-25) under UV (λ < 400 nm) or VIS (λ > 400 nm) irradiation takes place [1]. The UV activity is caused by interband electron transitions while the activity under VIS light is due to the light absorption by surface and/or bulk structure defects (oxygen vacancies, Ti^{3+} ions) [2]. The course of the reaction (1) was divided into two stages [1]. The first stage is characterized by NO photoadsorption and requires the electron type centers, whereas the second one is distinguished by an increase in N_2 pressure up to a half of the initial NO pressure and needs a hole type centers. CO_2 was found to remain on the surface. The same behavior of reaction (1) on TiO_2 (Hombifine N) superfine powder was observed.

The aim of the present work was to perform a preliminary investigation of the spectral dependence of photoreaction (1) on nano-sized TiO_2 (Hombifine N, anatase, S = 320 m^2/g, mean particle size d ~ 6 nm) in 300 – 440 nm range at constant initial CO+NO amounts by means of kinetic mass-spectrometry and thermo-programmed desorption spectroscopy. The emission lines λ = 303-313, 365, 404 and 436 nm of the high-pressure mercury lamp DRT-120 equipped with a set of glass filters (LOMO) were used as light source. The experimental technique and procedures are the same described in [1].

It is found that the maximal effectiveness of NO photoadsorption is under irradiation at λ = 365 nm whereas the second stage has an effectiveness maximum at λ = 404 nm. Such difference in spectral maxima could be explained by various electron-hole processes occurring under irradiation in the region of absorption band (3.4 eV) and near its edge (3.07 eV). The lowest effectiveness of both stages at λ = 436 nm is due to low light absorption in this region.

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Magnetic-Dichroism Study of Cobalt Silicides Formed at the Co/Si Interface

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In the past decades, formation of thin cobalt silicide films on silicon has drawn much attention because this field involves interesting science and promising applications. The renewed interest to the system is stimulated by studies of magnetic Si-based heterostructures and the mechanism of interlayer exchange coupling through nonmetallic spacers in Co/Si multilayers [1]. However, in contrast with Fe/Si system, Co/Si heterostructures have been much less studied. In particular, very little is known about ferromagnetic ordering of the Co/Si interface at initial stages of its formation. The aim of the present work is to study the evolution of phase composition, electronic structure, and magnetic behavior of the Co/Si interface in a course of deposition and annealing of ultrathin metal films on the Si(100)2×1 surface.

The experiments were carried out in UHV using the Russian-German beamline at BESSY. The phase composition and the electronic structure of the interface were studied by high-resolution photoelectron spectroscopy. The magnetic properties of interface structures were analyzed by magnetic linear dichroism in Co□ *3p* core-level photoemission. The use of these surface sensitive techniques in the frame of a single experiment allows us to reveal specific features of the evolution the system and establish correlations between its phase composition and magnetic properties.

It is shown that in-plane ferromagnetic ordering of the Co/Si(100)2×1 interface has a threshold nature and arises after the deposition of ~ 6 Å Co. At this coverage the ultrathin nonmagnetic layer of interfacial silicide becomes covered by a continuous film of a Si solid solution in cobalt. Subsequent deposition of Co (up to 16 Å) results in the growth of ferromagnetic Co film over the Co-Si solid solution. Annealing of the film leads to thermostimulated solid-phase reactions starting at ~ 250°C. The first synthesized phase is the ferromagnetic Co_3Si, which gradually transforms to the nonmagnetic ε-CoSi and $CoSi_2$ at temperatures above 350°C and 500°C correspondingly.

The work was supported by the Russian Foundation for Basic Research (project no. 10-02-00632) and the Russian-German Laboratory at HZB BESSY.

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Dislocation networks in silicon: energy levels in the band gap and dislocation conductivity

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Direct Si wafer bonding is an industrial technique that can be used to form well controlled dislocation networks (DNs) compatible with CMOS technology. The exceptional properties of such DNs can be used in various applications highlighted in [1] and are as follows: dislocation luminescence with maximum intensity at 1.55 μm that can be used for optical on-chip interconnects, and enhanced conductivity along the dislocations that can result in ultra-fast Si transistors [2]. Although the investigations of DNs have been carried out for relatively long time the exact origin of dislocation luminescence and conductivity is still unclear. The aim of this work was to study DN related electrical levels which could be responsible for DN-conductivity.

We studied n-type doped Si crystals bonded hydrophilically with small twist misorientation angle ranging from 1 to 5 degrees. DNs were formed at the distance of 200 nm from the surface. Au Shottky contacts were sputtered on top of the structure for the electrical measurements.

We used deep level transient spectroscopy (DLTS) and minority carrier transient spectroscopy (MCTS) as a main tool to study energy levels of the DN. The shallow and deep levels were found in both halves of the Si band-gap. One deep electron trap (DET) appearing in the spectra of all the specimens exhibited strange behavior. DET level had unusually low cross section of 10^{-20} – 10^{-22} cm^2 and its signature (activation energy and cross-section) changed drastically while changing the contact diameter or applying different voltage. Some of these features were similar to those observed in Si/SiGe/Si quantum wells [3] with lateral diffusion along the thin SiGe layer. According to this work theoretical model of the band-like structure with lateral diffusion beyond the contact area was proposed for the DET level. This assumption makes it a favorable candidate for a level responsible for DN related conductivity. In order to verify our hypothesis mesa-diodes were prepared on these structures and extra measurements were carried out. Unfortunately results still remain ambiguous.

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Intracenter Mn^{+2} luminescence in II-VI group nanocrystals

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Diluted magnetic semiconductors (DMS) are the promising materials for application and the model objects for the optical and magnetic studies. The most popular DMS are the II-VI semiconductors with the partial substitution of II group element with the iron group element (for example, $Cd_{1-x}Mn_xTe$).

The compound under consideration $ZnS{\cdot}MnO{\cdot}(CH_3)_2SO$ which contains Mn^{2+} ions has some similar optical properties as compared to DMS. The Mn^{2+} ion shows the bright near 2 eV due to the nonfilled 3d electronic shell.

We have studied the intensity dependence of the Mn^{2+} 3d-luminescence on the excitation power, the luminescence being exited with 2nd harmonic Nd^{3+} IAG laser (2,33 eV).

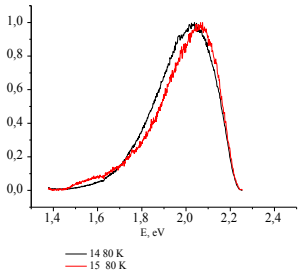

Fig. 1. Intracenter luminescence of Mn^{2+}

The red emission band in $ZnS{\cdot}MnO{\cdot}(CH_3)_2SO$ luminescence with the maximum at 2,1 eV originates from $^4T_1 - {}^6A_1$ transition in 3d-shell (fig. 1). The main characteristics of this band is not sensitive to the excitation level, but a deviation the integral intensity versus the excitation power from the linear dependence takes place within the range 0,15 – 10 W/cm^2

The data analysis at 77 and 300 K leads to the conclusion that the shape of the emission band is governed by the $^4T_1 - {}^6A_1$ transition with a weak inhomogeneous broadening, which indicates the low fluctuations of the ligand field and its insignificant change within the wide temperature range. The saturation of 3d-luminescence under the increasing excitation power is probably related to the two-step transitions in the Mn^{2+} ion (the excitation of the Mn $^{2+}$ ion which is already in $^6A_1$ state).

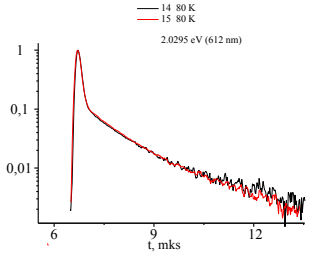

Fig. 2 The kinetics of the 3d-luminescence.

The kinetics of the 3d-luminescence at 77 and 300 K have been under consideration. The decay curves demonstrate very clear two characteristic lifetimes (fig. 2). The origin of the both fast and slow components is discussed.

Electronic structure of titania nanoclusters doped by fluorine and nitrogen: DFT calculations

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Titanium dioxide is well known as one of the best photocatalyst. Pure TiO_2 is active under ultraviolet. The most accessible and non-polluting light source is the Sun. To sensitization TiO_2 to the sunlight the doping may be used. Also, the activity of titania increases by size reduction of the active particles to several nanometers (by nanoclusters formation). The definition of structural and optical properties of those superdispersed materials is a very difficult experimental problem. Thereupon today the molecular quantum chemistry research of such nanosystems is very actual.

The aim of the present work is to study electronic structure of titania nanoclusters Ti_8O_{16} doped by fluorine and nitrogen. Doping modeling was occurred at replacement in titania nanocluster of oxygen atoms on fluorine or nitrogen atoms. After this procedure, a full geometry optimization was carried out. These calculations were done using the DFT method with B3PW91 functional using GAUSSIAN03 package [1]. During calculations it became clear that small doping for our case is more effective.

According to calculations the band gap of Ti_8O_{16} is 4.171 eV, what corresponds to the ultraviolet absorption spectrum.

Our calculations have shown that the fluorine doping (n - type) leads to the formation of occupied defective levels in the band gap in direct ratio to the number of doped fluorine pairs. Electronic density of these levels is localized on Ti atoms. This level lies on 2.091 eV lower the bottom of conduction band. The nitrogen doping (p – type) leads to the formation the vacant defective level, which electronic density localized on N atoms. This level lies on 1.508 eV higher the top of valence band. At higher degree of doping the band-gap narrowing was observed.

According to the calculations in case of mixed p–n doping an electron transport from fluorine on low-lying nitrogen level was observed. Also the band-gap narrowing from 4.171 eV (to Ti_8O_{16}) to 2.515 eV is occurred. Thus the shift of the long-wavelength cutoff to visible area should be expected.

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Temperature behaviour of photoluminescence in CdTe/ CdMgTe heterostructures with various quantum well widths

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Lower dimensional systems are widely applied now in electronics. Thus the optical investigation of these systems is very important.

The behaviour of exciton photoluminescence from CdTe/CdMgTe heterostructures CdTe/CdMgTe heterostructures with various quantum well (QW) widths in the temperature range 5 – 160 K have been studied. The samples contains four CdTe QWs with the thicknesses 31, 16, 8 and 4 monolayers (ML), the wide gap barrier is built by CdMgTe. The wavelength of the excitation laser has been 530 nm.

Fig.1 a) and b) show the structure of the luminescence spectra at the temperatures 5, 70 and 100 K.

This spectrum exibits four bands, which are correlated with the energy of the excitons in the QWs with different widths: 31 ML E=1.63 eV, 16 ML E=1.71 eV, 8 ML E=1.88 eV, 4 ML E=2.08 eV.

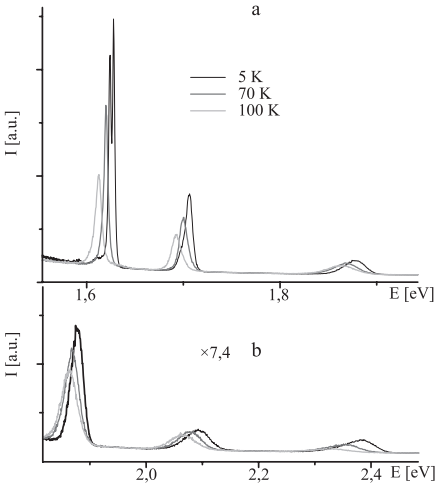

Fig. 1. The structure of the luminescence spectra.

The fifth peak belongs to the barrier exciton (E=2.38 eV). The first and the second bands which correspond to 31 and 16 ML QWs show clearly double peak and the structure of other bands is also noticeable. The sample heating from 5 to 160 K initiates the band energy shift to the low energy side. The low energy peak in each double structure relatively decreases with the increasing temperature, this process being more significant for the narrow QWs.

These properties of temperature behaviour of CdTe/CdMgTe heterostructures are discussed in details.

Ab initio study of stacking and stability of Mg/Ti and Mg/Nb thin films - hydrogen storage materials

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During the last decades hydrogen has attracted worldwide attention as an energy carrier. MgH_2 is one of the most promising materials for hydrogen storage due to its high hydrogen uptake (up to 7.6 w%), large reserves and low cost. However, the potential for practical use of MgH_2 is severely limited because of its high temperature of hydrogen discharge, slow desorption kinetics and a high reactivity toward air and oxygen. Nevertheless, the transition metals (TM) doping of Mg greatly enhances the kinetics of hydrogen uptake and release.

Recently a series of new hydrides Mg_7TiH_x and $Mg_{6.5}NbH_x$ of Ca_7Ge type structure has been synthesized [1, 2]. The hydrogen desorption properties have been found to be better than for pure MgH_2. However, as the metals do not form any alloy, the structures are hold together by the presence of hydrogen and no binary compound exists after released hydrogen. Nevertheless, such metal combinations can exist as thin films and recently Mg-Ti thin films were synthesized [3]. Moreover, up to now, the structure of interface border of magnesium with TM nanoparticle additives still remains unexplored. From this perspective, simulation of thin films could be also helpful to determine the interface structure existing in Mg-TM nanocomposites and to study the influence of TM additives on the hydrogen sorption process.

In this contribution we report on the results of our *ab initio* modeling of Mg_n/Ti and Mg_n/Nb_m thin films. The electronic structures of thin films were calculated within the DFT full-potential linearized augmented plane-waves method. Our theoretical studies of Mg_n/Ti and Mg_n/Nb_m thin films have revealed that the Ti containing films are very unstable due to a strong repulsion between Mg and Ti layers. However, stability of those Mg_n/Ti thin films increases with the number of Mg layers. Despite that all calculated films including Mg_7/Ti exhibit positive heat of formation, a film stacking reveals less unstable than a bulk compound of Ca_7Ge type structure. For both Nb_2/Mg_6 and Nb_4/Mg_4 thin films it was found that when deposited on a Nb-(011) surface, Mg layers keep the bcc stacking mode.

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Effects of chemical bonding on the resonant F KVV Auger electron emission from fluorinated multi-walled carbon nanotubes and polytetrafluoroethylene

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Nowadays carbon nanosystems (CNS) are very popular objects of investigation. An activation of such systems for increasing of range of application is one of the important problems. In this respect, the fluorination of CNS is of special interest because it decreases the chemical inertness of the initial systems. In spite of great interest in fluorinated CNS, their atomic and electronic structures have been studied by using a limited number of experimental techniques up to now. The aim of this work is to obtain information about features electronic structure and chemical bond for fluorinated CNS (fluorinated multi-walled carbon nanotubes [F-MWCNTs]) and fluorinated polymer (polytetrafluoroethylene [PTFE]) based on the analysis of the absorption spectra and resonant F *KVV* Auger electron spectra.

All measurements have been performed at the Russian-German beamline at the BESSY [1]. A sample of F-MWCNTs (10 wt. % of fluorine) was prepared in air by rubbing its powder into the scratched surface of a clean stainless-steel plate. The PTFE sample was prepared with a sliding technique [2] which involved sliding (several times) a bar of PTFE over the surface of a flat silicon substrate covered with a ~ 1μ thick gold layer. Its thickness was in the range from ~ 10 to 30Å. Absorption spectra were measured using total electron yield. Photoelectron and resonant F *KVV* Auger spectra were collected in the angle-integrated mode using Phoibos 150 electron analyzer.

Owing to the analysis of the Auger emission spectra of PTFE and F-MWCNTs near the F1s-edge it was found that main Auger lines in resonant F *KVV* spectra excited with photon energies in the vicinity of the first absorption peak in the F1*s* spectrum are shifted to higher kinetic energy as compared with normal Auger spectrum. This effect is associated with strongly localized hybridized character of electronic states at the bottom of conduction band. The high-energy shift in F *KVV* spectra differs in value for various compounds and therefore can be used for characterization of chemical bonding in fluorinated compounds and CNS.

This work was supported by the Russian Foundation for Basic Research (project no. 09-02-01278) and the bilateral Program "Russian-German Laboratory at BESSY".

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The influence of valence excitations on spectral distribution of vibrational excitations associated with C 1s photoionization in the CO molecule

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Inner-shell photoionization of a molecule is accompanied by both vibrational and rotational excitations. In the present work the main attention is paid to the vibrational excitations of CO molecule. Intensity of those has been believed to produce Franck-Condon distribution $|\langle v'|0\rangle|^2$. Taking shape-resonance into account results in the following expression for vibrational distribution function: $f_{v'}=|\langle v'|0\rangle|^2\, J_{v'}(\nu)$, where $J_{v'}(\nu)$ is interferential factor.

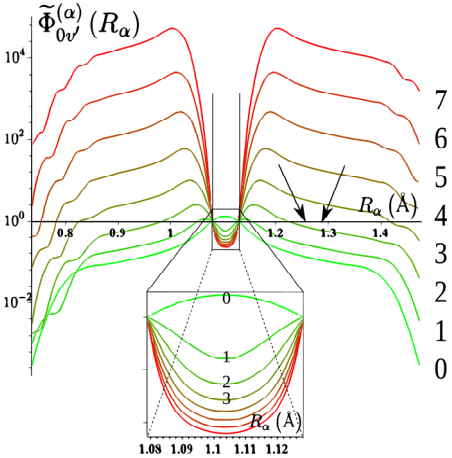

Fig. 1. The coeffitients Φ^α comptuted as a function of R_α for v'=0...7 [1]. The scale of Φ^α is logarithmic.

When the incident photon energy is enough to ionize the molecule into a shake-up state, e.g. $^2\Sigma^+_u$, which has $2\sigma^{-1}1\pi^{-1}2\pi^1$ electonic configuration, such a state can participate in the photoionization process as an intermediate state:

$CO \rightarrow CO^{+}{}^{*} \rightarrow CO^{+}$ instead of direct channel $CO \rightarrow CO^{+}$.

The life-time of this intermediate state is believed to be much greater than the molecular vibrational period. Such an assumption leads to the formula expressing the distribution function: $f_{v'} \approx |\langle v'|0\rangle|^2\, R_{v'}(\nu)$, where $R_{v'}(\nu)$ is a factor depending on energy $h\nu$ and internuclear distances of the initial, intermediate and final states:

$R_{v'}(\nu) = 1 - \Sigma_\alpha\, (\sigma_\alpha(\nu)/\sigma^+(\nu))^2\, (1 - (\Phi^\alpha) / |\langle v'|0\rangle|^2)$.

Dependences of Φ^α on R_α for $v'=0...7$ are plotted in fig. 1. Positions of two $^2\Sigma^+_u$ shake-up states taking part in process are indicated by means of arrows.

The way, how a direct shake-up state can influence on distribution functions of final vibrational state, is shown in the work. Dependence of the Φ^α-factor on the position of intermediate state R_α is investigated in detail.

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The investigation of the NO +CO photoadsorption on nano-sized TiO_2 (Hombifine N) and forming intermediate products by means of kinetic mass-spectrometry and thermo-programmed desorption spectroscopy

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Titanium dioxide is widely used as photocatalyst in environmental catalysis, because it is highly active in degrading of many organic and inorganic pollutants. Earlier it had been shown that the photoreaction $CO+NO+h\nu \rightarrow N_2 + CO_2$ (1) on TiO_2 (Degussa P-25) under VIS ($\lambda > 400$ nm) irradiation takes place [1] due to the light absorption by surface and/or bulk structure defects (oxygen vacancies, Ti^{3+} ions) [2]. The course of the reaction (1) was divided into two stages [1]. The first stage is characterized by a decrease in NO concentration to nearly zero, appearance of N_2O and N_2 (~5-8 % of NO) after the light was switched on. The reaction second stage is characterized by a decrease in CO and N_2O pressures in the gas phase and by an increase in N_2 pressure up to a half of the initial NO pressure. Produced CO_2 was found to remain on the surface. The mechanism of reaction was proposed [1]. The same behavior of reaction (1) on TiO_2 (Hombifine N) superfine powder was observed.

The aim of the present work was to investigate the kinetic features and adsorbed species forming during of the first stage (NO photoadsorption) of reaction (1) on nano-sized TiO_2 (Hombifine N, anatase, S = 320 m^2/g, mean particle size d ~ 6 nm) at various initial CO:NO ratios by means of kinetic mass-spectrometry and thermo-programmed desorption spectroscopy (TPD). The experimental technique and procedures are the same described in [1].

It is found that the kinetic of NO photoadsorption strongly depends on the CO amounts in reactor indicating the transitional photoinduced processes of electron-type sites formation occurring on the TiO_2 surface in CO presence. The analysis of adsorbed species after reaction first stage by means of TPD reveals the desorption of CO (weakly bonded), N_2O, NO and CO_2. The correlations between intermediate adsorbed products and initial NO and CO amounts were obtained. The mechanism of intermediate products formation is proposed.

This work was supported by RFBR under grant 09-03-00795-a.

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The vacuum arc technology of removal of scale from metals

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The purpose of this work was to investigate the possibility to develop the technology of removal of scale alternative to the one, based on acid etching of a surface of hot-rolled steel and of other metal details. At the basis of technology of removal of scale is the principle of the vacuum arc discharge with the cold cathode (the pattern to clean). Such technology is ecologically clean and allows to process the alloys you can't etch.

The main problems were to discover special features of the arc on cathodes of different metals and to elaborate the equipment for vacuum arc scale removal.

The investigations were held in the vacuum camera "Bulat" with different residual gas pressure, different discharge currents and cathode materials (different steels and special refractory alloys, molybdenum, niobium).

We have found out that non-metallic layer on the cathode surface is destroyed first due to different electrical and mechanical properties, as well as the presence of transient electrical resistance between the base and the scale. Arch plasma forms more intensively on scale, than on pure metal (because of easier ion detachment from scale [1, 2]), and removes scale layer-by-layer from a metal surface, baring the original structure of a surface, including defects from rolling and it's own structure. It is established also that at small currents (~ 20 A) arch plasma is formed steadily on scale, doesn't interact with pure metal, and spontaneously switches off after clearing, leaving metal intact.

Because of the interaction of arc current with its own magnetic field, the field of current in the cathode and external fields cathode spot randomly moves on the cathode surface at high speed ($>10^3$ m/s [2]), providing uniform destruction of a blanket with the speed depending on properties of scale and metal, and also an arch mode. Using external magnetic field allows providing regular scanning the sample by cathode spots, instead of chaotic.

Using the X-ray diffraction analysis, it was established that the phase structure of the surface layer of the cleaned metal is similar to the initial structure of the basic metal.

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Quantum-size phenomena in pseudomorphic layers of copper on W(100)

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The difference in physical properties of thin metal films compared to the bulk material has been the key motivation for the extensive research devoted to the thin metal films for more than 20 years. These differences are due to the reduced dimensions or a crystalline structure different from the equilibrium structure. A nonequilibrium crystalline film structure may arise when the lattice constant or symmetry of film and substrate material are different. An example of such a situation is the pseudomorphic growth. In the initial stage the film tends to adopt the crystal structure of the substrate and, thus, will have properties different from that of its bulk. Generally, if the differences between film and substrate cell parameters are not significant, pseudomorphic growth takes place only for first monolayer and then film grows with structure corresponding to its bulk. System Cu/W(100) attracts interest because two monolayers of copper perform pseudomorphic growth. Deposition beyond the critical coverage results in the formation of$(11\bar{2}0)$ oriented hcp islands [1, 2]. Several investigations were devoted to the growth of copper layers on W(100) [1-3], nonetheless, quantum states of such a system has not been investigated intensively by now. Thus, the present work is devoted to quantum phenomena in pseudomorphic films of copper synthesized on the W(100) substrate.

Using angle-resolved photoelectron spectroscopy (ARPES) we explored the electronic structure of this system. The appearance of the discrete valence electron states, so called quantum-well states (QWS's), in such double layered structure was successfully disentangled. These states are formed by the copper valance electrons which are captured between two potential barriers at the surface and the interface with W(100). To explore their nature in details we took series of PE spectra changing the photon energy and the angle of the emitted photoelectrons. Apparently, those states reveal the properties similar to that reported for the experimentally studied Shockley and Tamm surface states that allows to describe QWS's in the corresponding manner.

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Investigation of system Ge/C_{60} by field-effect in electrolyte methods

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The interaction of fullerenes with different solid surfaces has been widely investigated over the last few years [1]. But with all of interest to such structures, the system Ge/C_{60} was poorly investigated. Our work can help with filling of this gap. In terms of applied physics formation of passivating C_{60} films on the Ge surface and possibility of another technological applications of the Ge/C_{60} system are quite interesting too.

Present research was based on capacitance-voltage (CV) and current-voltage characteristics, surface conductance-voltage dependence (σ-φ) measuring and infrared spectroscopy. CV, current-voltage characteristics and σ-φ measuring was carried by using field-effect in electrolyte methods. IR-spectrums were measuring on spectrophotometer "Specord M80". IR-spectroscopy can give information about C_{60} condition on Ge surface.

The germanium surface was cleaning by etching in concentrated H_2O_2 or piranha acid (H_2SO_4:H_2O_2). The C_{60} films were deposited on Ge from solution C_{60} in hexane or chloroform. Film's thickness differs from 30 nm to 200 nm. We use p-Ge with doping level ~10^{14} sm^{-3} and surface orientation (111). CV and current-voltage characteristics measuring was carried by pulse method with τ=1 mks. The surface conductance-voltage dependence measuring was carried on variable signal with frequency 23 Hz. Surface potential values was varying from -0,7 V to 0,6 V, which allows us, particularly, obtain information about electron states distribution on the Ge/C_{60} interface.

We developed techniques of C_{60} deposition on the Ge surface, obtained preliminary results about modification of surface states spectrums of the Ge surface. IR-spectroscopy data showed changing symmetry of C_{60} on the Ge surface.

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Determination of the microtopography and chemical composition of Pt clusters in Pt/polymeric matrix nanosystem

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Work is directed onto the search for the optimal conditions of the deposition and studies thin polymeric films containing nanoparticles of platinum. The solution of this problem will make it possible in turn to solve the extremely important problem of creation of the water-soluble polymer-inorganic nanomaterial required for development of pharmaceutical industry, petrochemical syntheses, membranous technology and in numerous special areas of instrument-making and electrical engineering. At present the scientific groups around world work on its solution.

The work was organized on determining the morphology and chemical composition of the Pt\PDMAEMA nanosystem after removing the polymer by way of thermal annealing in air and etching treatment.

At the beginning was organized the study of PDMAEMA-polymer film topography on natural silicon oxides before removing organic matter. Further for removing organic layers was used thermal anneal at 300ºC and 500ºC for hour in air. As a result it was discovered that after thermal annealing average size of globule decreases from 250 up to 60 nm.

Then study of the chemical composition Pt/polymeric sample was organized by means of XPS method. Also for removing organic layer etching treatment by ion Ar was organized for 5 minutes under accelerating voltage 3 kV and current of 20 mkA. This made it possible to reveal clusters of platinum.

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Charge transfer X-ray transitions in Mg L2,3 emission bands

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A shape of characteristic X-ray emission band (XEB) reflects an energy distribution of partial and local valence electron density of states (PLDOS) in the vicinity of emitted atom in accordance with dipolar selection rules. It seems clear an intensity of XEB must directly close correlates with a number of corresponding angular momentum valence electrons localized in atomic sphere. This gives possibility for direct estimation of the local partial occupancy of the emitted atom (partial effective charge) as an alternative to nondirect estimation of the effective charge via usual core level chemical shift measurement. The aim of this work was a detailed theoretical study of the XEB shape and intensity formation in one-electron model.

The plane wave pseudopotential method based on density functional theory (DFT) is used to calculate the shape and intensity Mg $L_{2,3}$ XEB in Mg metal and in MgH_2, MgO, MgF_2 and MgB_2. For the calculation X-Ray transition $L_{2,3}$ amplitudes and probabilities one need to estimate matrix elements between core atomic states and band wavefunction. The main problem is to reconstruct so-called "all-electron" crystal orbital from the band pseudo wavefunction in the core region. This is done by two different methods. The first method is based on the Blochl transformation between all-electron and pseudo crystal orbitals. In the second method the band pseudo wavefunction is projected into the space of atomic pseudo orbitals and then atomic pseudo orbitals are replaced by the all-electron atomic wavefunctions. Comparison between the results obtained by these methods give a possibility to estimate the error introduced by the reconstruction procedure.

A good agreement are obtained between the theoretical and experimental Mg $L_{2,3}$ XEB in Mg and its compounds. The theoretical XEB is divided into two s- and d- components. It is found that in Mg compounds, the contribution of the d- component is drastically large in comparison to Mg metal. We assume the reason of this effect is a contribution of the ligand wavefunctions "tails" in the vicinity of Mg atom (so-called cross transitions or charge transfer transitions). To confirm this hypothesis we projected band wavefunctions into the space of atomic orbitals and calculated transition probabilities from the ligand valence states to 2p-state of atom Mg. We also calculated Mg $L_{2,3}$ XEB integral intensities in Mg compounds normalized to the intensity of Mg metal. Unfortunately, theory does not coincide with experimental results. Understanding of this discrepancy is now in progress.

Sampling Depth for NEXAFS spectroscopy near Si L2,3 absorption edge in SiO_2/Si system

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Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy, also known as X-ray Absorption Near Edge Structure (XANES) spectroscopy have proven itself as one of the most usable techniques of research in modern solid state physics science. However, despite the long history of its application, there are still questionable points, such as Sampling Depth (SD), usually associated for this technique with Electron Escape Depth (EED). Being not so important for the research of thick layers, the precise determination of SD becomes especially crucial when less than 10 nm thick layers are studied.

The main object of this work was the determination of sampling depth for NEXAFS spectroscopy at SiO2/Si system example near Si L2,3 absorption edge and the investigation of SD dependence on grazing angle of photon beam.

Si L2,3 NEXAFS spectra of SiO2/Si samples of different dioxide thickness (<20 nm) at fixed grazing incidence angle and of the same dioxide thickness at different angles were studied. Calculations of EED within the framework of the point model [1] were conducted using the obtained angular spectra dependences. All of the measurements have been carried out in RSM-500 and RSL-1500 x-ray spectrometers-monochromators, in which the bremsstrahlung from the tungsten anode of the x-ray tube was used.

In contrast to the known value meanings of SD of 5 nm [2], the dependences measured show that for the studied SiO2/Si system the information in NEXAFS spectra is obtained from the depth up to 13 nm. The calculations carried out in the framework of the point model didn't show sufficient coincidence with the measured values. This can be explained by the fact that the point model doesn't consider the contribution of the movement of secondary electron, which significantly affect the value of quantum yield and increase the meaning of SD, and thus needs further rectification.

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Atomic mobility in nanostructured liquid Ga-In alloy

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Nuclear spin relaxation and Knight shift for the ^{71}Ga, ^{69}Ga, and ^{115}In isotopes were studied by NMR in liquid gallium-indium alloy confined to porous glasses. Drastic spin relaxation acceleration under nanoconfinement was observed for the three isotopes. Quadrupole and magnetic contributions to spin relaxation were separated for gallium and indium isotopes using the experimental data obtained which allowed, in particular, the evaluation of correlation times of atomic mobility. The strong decrease in the correlation time was found for the confined alloy which evidenced a remarkable diffusion slowdown. The effect of changes in atomic mobility on NMR line broadening was also discussed.

The mean pore size of matrices 5 and 200 nm was determined using mercury intrusion porosimetry. The filling of the pore volume evaluated by weighing the samples was about 70 % for both of them. Bulk Ga-In alloy of the same composition was also studied to make a comparison.

Nuclear spin-lattice relaxation, the lineshape, and Knight shift for both gallium isotopes, ^{69}Ga and ^{71}Ga, and for ^{115}In in the melted gallium-indium alloy were measured using Bruker Avance400, Avance750, and MSL500 pulse spectrometers. The inversion recovery procedure was applied to observe longitudinal spin relaxation. Measurements were performed at room temperature at which the bulk alloy and the alloy in the pores are completely molten.

Studies of the lineshapes and spin-lattice relaxation time revealed a significant acceleration of nuclear spin relaxation for two gallium isotopes and indium in the alloy within the pores compared to the bulk alloy. The results of measurements showed that relaxation acceleration depends on the pore size. Data obtained in different magnetic fields from 9 to 17 T, together with data for the Knight shift showed that this acceleration is due to the increase of the quadrupole contribution to relaxation, while the magnetic contribution remains practically unchanged. The rate of quadrupole relaxation was evaluated for three isotopes under study for the alloy in the porous glasses with pores 5 and 200 nm. It was obtained that the rate of quadrupole relaxation increases with decreasing pore size. The well-known relations for quadrupole spin relaxation in liquids were used to calculate the correlation time of atomic motion. The correlation time was found to increase with decreasing pore size and exceed by more than an order of magnitude the correlation time in the bulk alloy. This result evidences a strong slowdown of atomic mobility in the indium-gallium alloy in confined geometry.

Features of the electronic structure of graphene on different substrates

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Investigation of the graphene monolayer have attracted considerable interest in recent years due to its unusual electronic structure (linear "photon-like" dispersion of electron states near the Fermi level in the region of the K-point of the Brillouin zone) and related to this its unique transport properties. So far the only feasible route toward large-scale production of graphene is epitaxial growth on a substrate. The presence of the substrate will, however, influence the electronic properties of the graphene layer. The main aim of our work was investigation of principal features of electronic properties which appear as the result of the interaction of the graphene layer with different substrates.

In the present work the electronic structure of such systems as 1ML graphene on top of Ni(111), SiC(0001), Cu/Ni(111) and Au/Ni(111) was studied [1]. All this data was compared with each other and with electronic structure of bulk monocrystalline graphite. Systems were investigated by angle-resolved photoelectron spectroscopy (ARPES) with the application of synchrotron radiation.

The analysis of dispersion relations of graphene on top of intercalated Au and Cu layers shows that hybridization of d states of Au and Cu with π states of graphene takes place. This hybridization leads to modification of dispersion relations in the region of crossing of these states. Gaps of dispersion relations and the bonding and the antibonding (d - π) states above and below gap are formed. For graphene formed on top of Ni(111), covalent interaction of π states with d states of Ni substrate is stronger. It leads to the shift of π states about 2 eV in comparison with those of bulk graphite [2]. Antibonding π* states are located above Fermi level and only bonding π states are occupied, therefore the interaction of graphene with Ni(111) substrate is very strong.

In some systems besides covalent interaction ionic bond is existed, i.e. charge transfer from atoms of metal to graphene monolayer takes place. For instance, for systems MG/Cu/Ni(111) and MG/SiC(0001) there are partial occupation of antibonding π* states at Fermi level near the K point of the surface Brillouin zone of graphene.

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Comparative analysis of x-ray absorption spectra of ligand atoms in cyanide complexes of transition-metal atoms

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Cyanide complexes of transition atoms are popular objects of theoretical and practical studies, since they have a whole set of interesting physical and chemical properties. The main aims of the present work are (i) to measure and to analyze the absorption spectra of carbon and nitrogen atoms for the complexes $[Ni(CN)_4]^{2-}$, $[Pt(CN)_4]^{2-}$ and $[Pt(CN)_6]^{2-}$ and (ii) to clarify the differences in the chemical bonding between atoms of nickel and platinum with the carbon atoms in complexes under study.

All measurements were performed at the Russian-German beamline at the BESSY II synchrotron radiation facility. [1] Samples for measurement were powders of $K_2[Ni(CN)_4]$, $K_2[Pt(CN)_4]$ and $K_2[Pt(CN)_6]$ rubbed into the scratched surface of pure copper plates. The NEXAFS spectra were obtained in the total electron yield mode by detecting a sample current.

All the spectra obtained were considered within the framework of a quasi-molecular approach with the use of the method of molecular orbitals [2] for complexes under study. In the first stage of the analysis, detailed interpretation of the quasimolecular structure Ni $2p_{3/2}$, N1*s*, and C1*s* absorption spectra was performed for $[Ni(CN)_4]^{2-}$. As a result, the symmetry, the composition and relative energy positions of the free electron states in this complex were determined. Then differences observed in the NEXAFS spectra of C and N atoms in similar square-planar complexes of nickel and platinum were discussed. They are attributed to the peculiarities of the valence 5*d*-orbitals of the Pt atom in comparison with the 3*d*-orbitals of the Ni atom – to more spatial delocalization and the nodular character of the 5*d* wave functions, which provides the difference π-interaction in the $[Pt(CN)_4]^{2-}$ complex. Finally, the spectra of $[Pt(CN)_4]^{2-}$ and $[Pt(CN)_6]^{2-}$ are compared.

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Investigation of hydrogen transport through a nickel membrane using the electrochemical diffusion membrane technique

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The material of interest is supposed to be used as a membrane in a double electrochemical cell with the EDM-technique. The method was developed by Devanathan and Stachurski [1] in 1962. They have submitted the so-called "time-lag" method for a diffusion coefficient determination:

$$D=d^2/6T$$

D – diffusion coefficient, d – membrane thickness, T – time lag.

The EDM-method has sufficient advantages in comparison with the others, i.e. a simple realization, an opportunity to observe the hydrogen diffusion in real-time mode, an applicability at room temperature, an opportunity to obtain other parameters of the membrane, associated with hydrogen penetration.

The basic concern of the work is the elaboration of a new way of EDM-method use. Recently hydrogen transport through a membrane has been observed via the registry of the hydrogen oxidation current, arising on the opposite side of the membrane during its anodic polarization in potentiostatic mode [2]. However, the opposite site of the membrane also is being oxidized during anodic polarization.

The distinction of the method, discussed in the work, incorporates the measurement of the variation of the electrode potential of the opposite side of the membrane, occuring when hydrogen is gating from the opposite side of the membrane after being injected to its enter side via its cathodic polarization in galvanostatic mode.

This method has the following advantages in comparison with the others:

1) an additional cover of the membrane opposite side is not required;

2) higher sensivity to the hydrogen appearance on the membrane opposite side.

This variation of the EDM-method has been successfully experimentally tested, yielding the diffusion coefficient of hydrogen for nickel at room temperature equal to 2.2×10^{-8} cm^2/c. Also the diffusion coefficient dependence of the applied current has been investigated.

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Magnetic ordering of iron and vanadium moments in small clusters: ab initio calculations

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At present nanoscale intermetallics can be grown in various forms, ranging from finite-size clusters to overlayers, multilayers and alloys. Their magnetic properties, which strongly depend on the both size (cluster size or film thickness) and composition of a nanoscale system, are object of interest in many different fields [1, 2]. Iron-vanadium small clusters provide an example of such a system.

Bulk vanadium is a nonmagnetic metal. But in small clusters and thin films its magnetic properties are changed: vanadium atoms gain magnetic moments up to $1\mu_B$. Besides, in Fe-V systems vanadium atoms have induced magnetic moments [1-3].

In this work we report on the theoretical results of the magnetic ordering study in small Fe_nV_m clusters. The electronic structure, atomic magnetic moments and spin density distribution have been calculated within Density Functional Theory using the Gaussian03 package. To choose appropriate exchange-correlation functional and basis sets the formation energy and the bond length in vanadium dimmer V_2 have been calculated. BPW91 functional and 6-311G basis set provides the best agreement with experimental data [4], and have been used for further calculations of the V_m, Fe_m (m=2, 3), FeV, Fe_2V and FeV_2 clusters.

It has been obtained that in all considered Fe-V clusters magnetic moments of iron and vanadium atoms are antiparallel. Furthermore, magnetic moments of vanadium atoms in V_3 are coupled antiferromagnetically.

The results of this work, combined with our previous calculations of magnetic properties of thin films [5], can be used for modelling of microstructure in alloys $Fe_{1-x}V_x$ and interlayers of Fe_n/V_m thin films.

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The Spectra of Raman scattering of GaAs and AlGaAs nanowires

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Interest in self-standing semiconductor NWs ranges from fundamental physics of their growth, transport and optical phenomena to many promising applications in nanoelectronics and nanophotonics [1]. Due to their ability to accommodate strain in two dimensions, NWs are promising for monolithic integration of dissimilar semiconductor materials [2]. Study of Raman spectroscopy of III-V NWs is important for a better understanding of their structure as well as applications. It is well known that, depending on the growth conditions and diameter, the crystal structure of GaAs NW can be either cubic ZB or hexagonal WZ or 4H polytype . In most cases, the crystal structure is not stable and highly faulted ZB/WZ mix-ups exist [3].

The analysis of NW's crystal structure by Raman spectroscopy is the aim of this work.

Raman scattering, or more generally inelastic light scattering is a standard nondestructive contactless characterization technique of materials, which allows to access mainly the phonon modes at the Γ point and in some cases to the dispersion [4].

In this work, we have investigated Raman spectra of GaAs NW's, which were grown on substrates GaAs(111) and Si(111), and AlGaAs NW's on substrate GaAs(111), containing GaAs quantum dots . The growth of GaAs NW's was carried out by molecular beam epitaxy. In Raman spectra of all investigated NW's there was revealed the frequencies, corresponding to cubic or hexagonal modification of GaAs. The analysis of a Raman-spectra of AlGaAs NW's containing quantum dots GaAs made it possible to define concentration component Al and Ga in a solid solution from a frequency shift of longitudinal and transverse optical modes.

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Comparative NEXAFS and resonant photoemission study of nickel and cobalt phthalocyanines

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The 3*d*-metal phthalocyanines (MPc's) show interesting properties and are widely used in technological applications. The NiPc and CoPc are suitable objects for comparative study because their electronic configurations differ only in one additional 3*d* electron in NiPc. The main aims are (i) to get new information about the nature of occupied and unoccupied states of NiPc and CoPc (ii) to get further insight into effects of 3*d*-3*d* electron interaction on decay processes of Ni 2*p* and Co 2*p* core excitations.

The measured high-resolution X-ray absorption (XA) and resonant photoemission (Res PE) spectra for NiPc and CoPc are presented. All measurements were performed at the Russian-German beamline at the BESSY II synchrotron radiation source [1]. The NiPc and CoPc samples were prepared *in situ* by thermal evaporation. The NEXAFS spectra were obtained in the total electron yield mode. The photoelectron spectra were collected in the angle-integrated mode.

The M 2*p* XA spectra probe the unoccupied electron states with the M 3*d* character. The drastic differences observed between M 2*p* XA spectra of NiPc([Ar]3d^8) and CoPc([Ar]3d^7) point to the essential influence of the 3*d* shell filling and 3*d*-3*d* exchange interaction on the energy disribution of Co 2*p* exitations. All features of Ni 2*p* and Co 2*p* spectra can be understood within the framework of a quasimolecular Ni(Co)N_4 approach. The strong spatial localisation of the core exitations within the quasimolecule is confirmed on the basis of analysis of the enhancement effects in Res PE spectra measured in the vicinity of the M $2p_{3/2}$ absorption edges. Moreover, the occupied states with 3*d* character near the Fermi level are defined. The enhancement effects are different for Res PE spectra of NiPc, CoPc. Therefore the strong influence of 3*d* electron configuration on formation and decay processes for M $2p_{3/2}$ excitations in MPc is clearly shown.

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Resonant Spin Amplification as an efficient tool for a spin dynamics study in nanostructures

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Nowadays, investigation of spin dynamics in quantum structures is an actively developing area in physics. The most interesting structures are those with long spin relaxation times of electrons and holes (tens of ns) because they are potential candidates for information storage. A sensitive method for the investigation of spin dynamics is the well-known Pump-Probe method, which is based on the detection of the photo-induced magneto-optical Faraday effect [1]. One of the modes of this method is the Resonant Spin Amplification technique (RSA). RSA is an efficient tool for studying the lifetime of resident carriers spin orientation if it is much longer than the repetition period of the pumping laser pulses. Experiments demonstrate a large variety of RSA profiles with complex shapes of the RSA peaks which depend on structure studied and experimental conditions used. To extract information about spin dynamics from the data, good understanding of the mechanisms behind RSA-signal formation is required. Although a basic theory of RSA signal formation has already been developed [1], several questions remain. How far can the theory be extended to studying different systems and where are the limits of its applicability? What effects influence the RSA signal and what might be a possible model for their description? How will nuclear effects influence the RSA signal?

The main direction of my research was the theoretical analysis of the effect of spin precession of trions on the long-living spin dynamics of resident carriers. For that I analytically obtained the formulas describing the behavior of the polarization projection to the direction of observation. For further calculations and simulation of the RSA signal I wrote a program, which utilized these formulas and gave a good agreement with the published experimental data. Finally the analysis showed that, for the observation of a RSA signal, it is necessary to have a long spin relaxation time of the resident carriers and a low-power excitation. The simulation results also indicate that the consideration of the trion precession leads to a significant deformation of the RSA signal. This analysis allows us to describe the experimentally observed RSA signals quantitatively and to determine the electron and hole relaxation times. Also, it is found that large fluctuations of the magnetic field due to the fluctuations of nuclear spin polarization make the observation of RSA in quantum dots impossible.

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Photon driven O_2 adsorption/desorption processeson nano-sized self-sensitized TiO_{2-x}

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Titanium dioxide is widely used as photocatalyst in environmental catalysis. Photocatalysis proceeds thanks to surface electrons and holes being highly reactive chemical species (Ti^{3+}, the reducer, and O^-, the powerful oxidizer, respectively). The band gap of TiO_2 is 3.2 eV, so only UV light i.e. ~3% of solar radiation is active while visible part (more than 40%) is not. To extend the absorption into visible region, sensitization is used, traditionally being achieved by introducing dopants or forming hetero-structures. However, it was found [1] that pure nano-sized TiO_{2-x} is already self-sensitized due to presence of colored anion vacancies (F-centers) and is capable of photocatalysis upon visible irradiation. Further reducing TiO_{2-x} by annealing in vacuum strengthens visible light absorption. Being an important stage in photocatalytic cycle, the interaction of irradiated TiO_{2-x} with gaseous oxygen is of great importance.

The aim of present report is to investigate the mechanisms of oxygen photoactivation on nano-sized TiO_{2-x} particles. The kinetic mass-spectrometry and TPD were used for to analyze the processes in gas and adsorbed phase. A high-pressure xenon lamp with glass color filters was used for irradiation.

It was shown that TiO_{2-x} irradiated in vacuum emerges oxygen, creating anion vacancies. However, oxygen adsorbs upon UV or visible irradiation of TiO_{2-x} in gas oxygen. Photoadsorption leads to formation of atomic adsorbed species.

The use of nonequilibrium isotopic mixtures of oxygen additionally revealed the photoactivated substitution of adsorbed molecules by gas molecules without their dissociation and in addition active atomic ions O^- on the surface. Thus the UV-VIS irradiation permits to change the amount of adsorbed oxygen species as well as the concentration of surface anion vacancies and to create chemically active oxygen species.

This work was supported by RFBR under grant 09-03-00795-a.

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Combining formula for calculation of quantum network S-matrix

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Structurally a quantum network consists of quantum dots connected with each other by quantum wires. As a charge carrier can scatter both in a dot, and in a wire site, it is convenient to introduce functional definition: *quantum network* is set of branches and junctions. *Branch* is functional network unit in which a charge carrier does not scatter. *Junction* is functional network unit in which a charge carrier scatters.

For calculation of transport properties of a quantum network it is necessary to find its *scattering matrix* (*S-matrix*). In the present paper the calculation scheme of quantum network S-matrix on the basis of known S-matrixes of its junctions is offered. The suggested approach consists in the following: having chosen any network site of two neighboring junctions (fig. 1) to find its scattering matrix by the *combining formula*:

$$S^{[\mathbb{J},\mathbb{L}]} = \begin{bmatrix} S^{[\mathbb{J},\mathbb{K}]\mathbb{J}\mathbb{J}} & O^{\mathbb{J}\mathbb{L}} \\ O^{\mathbb{L}\mathbb{J}} & S^{[\mathbb{K},\mathbb{L}]\mathbb{L}\mathbb{L}} \end{bmatrix} + \begin{bmatrix} S^{[\mathbb{J},\mathbb{K}]\mathbb{J}\mathbb{K}} & O^{\mathbb{J}\mathbb{K}} \\ O^{\mathbb{L}\mathbb{K}} & S^{[\mathbb{K},\mathbb{L}]\mathbb{L}\mathbb{K}} \end{bmatrix} \times$$

$$\times \begin{bmatrix} -S^{[\mathbb{J},\mathbb{K}]\mathbb{K}\mathbb{K}} & \exp\left(-iK^{\mathbb{K}\mathbb{K}}A^{\mathbb{K}\mathbb{K}}\right) \\ \exp\left(-iK^{\mathbb{K}\mathbb{K}}A^{\mathbb{K}\mathbb{K}}\right) & -S^{[\mathbb{K},\mathbb{L}]\mathbb{K}\mathbb{K}} \end{bmatrix}^{-1} \begin{bmatrix} S^{[\mathbb{J},\mathbb{K}]\mathbb{K}\mathbb{J}} & O^{\mathbb{K}\mathbb{L}} \\ O^{\mathbb{K}\mathbb{J}} & S^{[\mathbb{K},\mathbb{L}]\mathbb{K}\mathbb{L}} \end{bmatrix}$$

$$K^{kl}_{mn} := \kappa^k_m I^{kl}_{mn}, \quad \kappa^k_m := \sqrt{\varepsilon - \lambda^k_m}, \quad A^{kl}_{mn} := a^k I^{kl}_{mn}$$

where $S^{[*]}$ is extended scattering matrix of junction $\Omega^{[*]}$, I is unitary matrix, O is null matrix, ε is energy of a charge carrier (electron or hole), λ^k is dimensional quantization energy of a charge carrier in k-th branch, a^k is length of k-th branch; here all quantities are dimensionless. As a result this site can be considered, as new network junction with known S-matrix. It allows to reduce formally number of junctions by 1. Therefore, consistently applying the formula obtained in given work, it is possible to find a scattering matrix of any quantum network in terms of its junctions S-matrixes

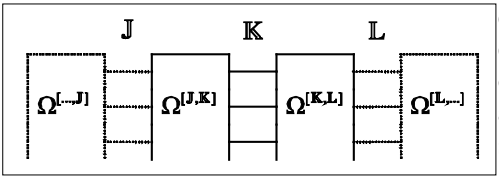

Fig. 1. The scheme of elementary network site $\Omega^{[\mathbb{J},\mathbb{L}]}$: firm lines are internal junctions ($\Omega^{[\mathbb{J},\mathbb{K}]}$, $\Omega^{[\mathbb{K},\mathbb{L}]}$) and branches (their numbers: $\mathbb{K} \subset \mathbb{N}$), dot lines are external junctions ($\Omega^{[...,\mathbb{J}]}$, $\Omega^{[\mathbb{L},...]}$) and branches (their numbers: $\mathbb{J},\mathbb{L} \subset \mathbb{N}$).

Spin-polarized auger electron spectroscopy of surface of invar alloys

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The surface of $FeNi_3$(110) crystal with iron films on it was studied by spin-polarized auger electron spectroscopy (SPAES).

Excitation of sample was made by non-polarized electron beam. Electron energy analysis was made by means of specially designed 2-pass cylindrical mirror analyzer. [1] For polarization measurements the compact Mott-detector was used. [2] Both devices were created in our scientific group.

Before every measurement the $FeNi_3$(110) sample's surface was cleaned by consecutive cycles of ion bombardment and annealing.

Iron films of different thickness were deposited on sample's surface. Secondary electron polarization curves were observed to be hysteresis loops. It was shown that on some minor iron film thickness the hysteresis loop "wing" splitting occurs.

SPAES measurements show that upon iron film deposition Fe auger-peak polarization remains positive and constant at observed film thicknesses. But Ni auger-peak polarization significantly improves in area where secondary electron polarization hysteresis loop shows splitting effect and is negative in such circumstance.

Reason of registered negative Ni auger-peak polarization is probably invar transition on surface of sample because of iron film deposition. In invar state surface sublattice of nickel shows anti-ferromagnetic alignment in relation to substrate's volume.

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Simulation of time-resolved Hanle effect in a quantum dot

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Spin dynamics in semiconductor are investigated by optical methods for many years. In particular, it is studied by observing the Hanle effect – depolarization of an electron spin in transverse magnetic field. Modern achievements of growth technologies and experimental technique allow one to observe phenomena, which cannot be explained by basic theory [1].

In this paper, we consider a quantum dot (QD) with one resident electron. An angular momentum of the electron is from time to time oriented along *z* axis by circularly polarized photons. Our system is placed in external magnetic field directed along *x* axis. The electron spin and nuclear spins interact with each other and with the external magnetic field. The Hamiltonian of the system is

$$\widehat{H} = \sum_k A_k \left(\hat{\vec{I}}_k \cdot \hat{\vec{S}}\right) + \frac{\mu_B g_e}{\hbar}\left(\hat{\vec{S}} \cdot \vec{B}\right) + \frac{\mu_N}{\hbar}\sum_k g_N^{(k)}\left(\hat{\vec{I}}_k \cdot \vec{B}\right), \qquad (1)$$

where the sum runs over all nuclei in the QD.

Here we propose a new approach for simulations of processes in the electron-nuclear spin system. This approach is based on assumption that an electron spin interacts with one nuclear spin only. We consider other nuclear spins as one big angular momentum, which just precesses in the external magnetic field and by-turn creates its own effective magnetic field (Overhauser's field) acting on the electron spin. The electron spin feels the sum of external and nuclear magnetic fields. We also suppose that all the nuclei in QD are equivalent (box-model). So we come from Hamiltonian (1) to the Hamiltonian

$$\widehat{H} = A\left(\hat{\vec{I}} \cdot \hat{\vec{S}}\right) + \frac{\mu_B g_e}{\hbar}\left(\hat{\vec{S}} \cdot \left(\vec{B} + \vec{B}_N\right)\right) + \frac{\mu_N g_N}{\hbar}\left(\vec{L} \cdot \vec{B}\right), \qquad (2)$$

where $\vec{L}$ is a big angular momentum of the nuclear system. At the moments of electron spin orientation, angular momenta $\vec{L}$ and $\vec{I}$ are summarized.

The main advantage of this approach, to contrary to microscopic approach [2], is that it allows one to simulate spin dynamics in the large time range and for arbitrary number of nuclei. This model also explains the dynamic polarization of nuclear spin system via interaction with the polarized electron spin.

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E. Applied Physics

The Research of Chernobyl's Nuclear Pollution in Leningrad Region

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The Chernobyl disaster that occurred on 26 April 1986 was a nuclear accident of catastrophic proportions. As a result more than 30000 PBq of radioactive isotopes were thrown out into the atmosphere. Long-lived isotopes Sr-90 and Cs-137 were among them. Later on this isotopes were spread on a significant distances and then returned to the different areas of the earth surface as atmospheric precipitations. They can be assimilated by the plants from the soil and later the isotopes penetrate inside the human body, causing an extra radioactive irradiation. Sr-90 is mostly accumulated in the bones and Cs-137 in the muscles. Both isotopes have a long radioactive half-life period, about 30 years. Cs-137 also emits gamma quantum, except of its β-radiation, so this is possible to carry out the research using gamma-spectrometer.

Areas with soils polluted by Cs-137 were also found in the south-east of Leningrad region. It is supposed that the pollution is connected with Chernobyl disaster. There was a research made in 1991 which estimates the quantity of pollution of the soils by Cs-137 as 1-5 Ci/km^2 [1]. We supposed that specific activity of the pollution had reduced to a second since 1986 because of the radioactive decay and the wash-out of the soil. With the lapse of time radioactive isotopes also go deeper in the soil.

In 2010 we carried out the research of estimation of quantity of Cs-137 in the soil samples which were taken from Kotelsky village. The village is situated in the polluted area of Leningrad region. The research was carried out on the semiconductor gamma-spectrometer. The efficiency calibration was made by the method of the "effective center of the detector" [2].

As a preliminary result we obtained the quantity of specific activity A=2896 Bq/ kg. It's about 2 times of the ordinary value.

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The determination of electrolyte characteristics in aluminum industry by X-ray diffractometer "Difrey 401"

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The knowledge of the electrolyte characteristics (such as the cryolite ratio, CaF2 and MgF2 contents) is necessary in aluminum industry for the electrolyte modification to reduce the power cost and to increase the yield. One of the techniques used for this purposes is X-ray diffraction. The main problems of these characteristics determination by X-ray diffractometer "Difrey 401" are discussed.

Application of image reconstruction from projections in MRI

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Research for the internal structure of objects and processes has been always put forward as a major problem in various fields of human knowledge such as medicine, chemical technology, physics of the Earth and atmosphere, astrophysics etc.

To obtain an undistorted image of internal macroscopic structure of an opaque object became possible after the computing tomography appeared. Its foundations were laid in the paper by Radon. He suggested the inversion formula of the integral transform making it possible to recover the original function if it's transform was known [2]. Radon transform is a base of the method of image using in X-ray and Positron Emission Computer Tomography and other imaging techniques.

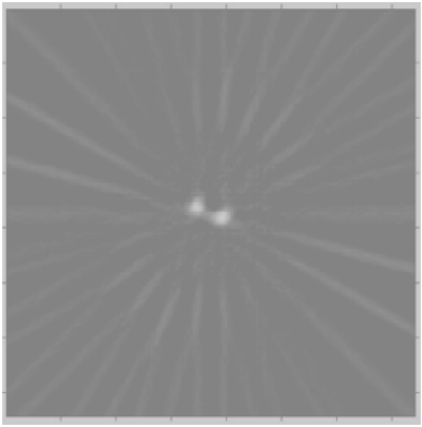

Fig. 1. Experimentally obtained image.

But the technique is not typical into nuclear magnetic resonance imaging projections reconstruction is useful to certain applications. The message presents the experimental results of reconstruction by projections in NMR and its comparison with images simulated previously [1].

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Parallel realization of Monte-Carlo algorithm for solving systems of linear algebra equations on many-core computational systems

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Necessity for solving large systems of equations arises in many physical problems. It's not always necessary to get all solution for many problems but often only some components of the answer are to be revealed. Consequently, there is a necessity to search for the components of the answer without full solution of the overall system of equations. For such cases, there is the Monte Carlo method for finding the component-wise solutions of linear algebraic equations form:

$$x = A\,x + f.$$

On the base of the current trends towards multi-core and parallel computing applications we have developed the parallel implementation of the algorithm, which allows to find quickly the components of the solution.

In this work we consider solving large systems by the Monte Carlo method and estimate the efficiency of the parallel implementation on many-core systems.

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Molecular specificity of bithiophenesilane dendrimers: experimental and PM3-modeling data

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Poly- and oligomeric thiophenes are objects of interest as the materials for modern organic electronics. The representatives of these compounds are utilized for manufacturing of conducting and photosensitive thin films in such practically important areas as solar cells, organic light emitting diodes, dye lasers and others optoelectronic devices. Present contribution is devoted to novel thiophene derivatives – bithiophenesilane dendrimers (fig. 1) which synthesis have been developed not far ago [1]. Molecular properties of these compounds have not been studied yet in details. Experimental investigation of electrooptical and spectral characteristics of different generation bithiophenesilane dendrimers using orientational Kerr effect and UF-VIS spectrophotometry was the first goal of our study. The second goal was connected with a comparative analysis of optical polarizability parameters of linear and dendritic analogues having the same number of thiophene rings in their structure by means of computer simulation using quantum chemical semiempirical method PM3 in the frame work of HYPERCHEM program.

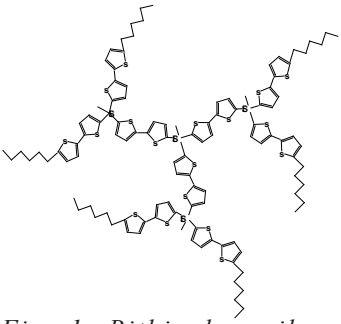

Fig. 1. Bithiophenesilane dendrimer of the second generation.

Based on results of the study it was concluded that dendrimers have molecular peculiarities which are in contrast to linear polythiophenes. Electrooptical properties of linear analogues are determined by the length of correlation (near 8 thiophene rings) in their chains when the same properties of dendrimers are independent on generation or total number of thiophene rings in the molecules. Spectral study has shown that Silicon atom does not support a conjugation in the branches of dendrimers. At the same time the central Silicon containing fragment of these macromolecules may be characterized as the dominative species responsible for electrooptical and spectral properties of novel thiophene derivatives.

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Strong magnetic field influence on discharge dynamics of small magnetoplasma compressor

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The influence of strong magnetic field onto the dynamics of discharge of small magneto-plasma compressor (MPC) was investigated in experiment. Small MPC was comprised by the discharge system with coaxial geometry and external diameter 9 mm. The diameter of inner cathode is 3 mm. The magnetic field was created using the multiturn solenoid, surrounded by the cast iron bandage to avoid its destruction. Duration of pulses was 800 μs; their amplitude was up to 20 T. The discharge of 2850 μF capacity battery was carried out via the serially connected solenoid and MPC.

The record of discharge current and the video record of the discharge space were carried out. The current curves without a magnetic field (MPC was placed outside the solenoid) and with magnetic field (MPC inside the solenoid) are presented. The application of the magnetic field has resulted in the reduce of maximal current and of the current increase rate. The current curves' analysis has provided the dependence of the current reduce measure upon time.

The application of magnetic field has resulted in increase of the flash intensity and shortening of the shine period after the discharge due to the faster plasma emission. Focusing of plasma torch was also detected.

Development of multi-media descriptions for laboratory sessions with a usage of the femtosecond laser

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Nowadays it's usual situation when laboratory sessions for students includes work with modern expensive devices and actually difficult operations on it. They are scanning-probe microscopes, atomic-force microscopes, high-pulse lasers and so on. Knowledge about working with such units is the necessary part of good-qualified specialist's education. That's why it's important to make up a new way of organisation such sessions. In case of difficult-operated equipment traditional text descriptions are not very useful: they include a lot of new terms and titles of device's blocks (which are not studied in traditional Bachelors courses) but are not able to make a real conception about a real device. Moreover not every block of the unit can be adjusted by students or even seen by them because of its high sensitivity and high cost. However it's necessary to know the equipment's structure. Therefore the idea of creation new types of descriptions comes. Certainly in includes the traditional text but not only.

This new type of description includes three-dimensional models of the equipment carried out according to the real device in a software 3ds Max. Using these models, photos of the equipment and flash-technologies animated lectures are made. They describe the structure of the device using audio and video perception. Besides these parts there are also video-files which show real operating with the device and activities which can't be made with this device. There is also a computer training simulator which allows to "push buttons" on the device, to adjust it or even to make forbidden activities. The final part of the description is test for student's self-control which includes a number of questions about the device, its structure and operations with it. It's also very important such descriptions are useful not only for students but also for non-specialists in some area who have to carry out their experiment on this equipment.

As in follows from the title the aim of this work was to create multi-media descriptions for laboratory sessions with a usage of the femtosecond laser "PULSAR 50-10". 3D-models and animated flash-lectures of all blocks of the laser (oscillator, stretcher&compressor, amplification block and pump laser) was made. The next step is the laser simulator.

Magneto-Plasma Compressor for investigation of hypersonic plasma jets

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Magneto-Plasma Compressor (MPC) is a coaxial discharge system that generates hypersonic plasma jet. MPC has six bar anode placed around cone cathode. The effective outlet diameter is about 14 mm. MPC operates in residual gas regime (RGR) under pressure 10-30 Torr. It generates compressed quasi-stationary flow with the following typical parameters: velocity 5-20 km/s, duration 60 μs, density 10^{17}-10^{18} cm^{-3} [1]. The discharge current is 20kA and energy spending is 15-20 J/pulse [2].

MPC has several possible applications: it is considered to be useful for hypersonic flow control as a plasma actuator or as micro engine, also it can be used for advanced materials processing (surface hardening or creation of silicon submicron structures) [3].

The present work is dedicated to investigations of plasma jet generated by Magneto-Plasma Compressor: theoretical review of plasma flow behavior, including analysis of viscous effects and magnetic pressure; observation of new experimental data.

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Theoretical estimation of two types of CO_2 gas analyzers

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The global mean CO_2 concentration in the atmosphere is about 0.04 %. The maximum permissible concentration of CO_2 in the workplace is 0.5 %. A concentration of 10% can cause respiratory paralysis and death within a few minutes. It is the cause of the acute need of the effective CO_2 gas analyzers. A nondispersive infrared sensor [1] is a simple spectroscopic device often used as a CO_2 gas detector. A typical scheme of this analyzer is shown in the fig. 1.

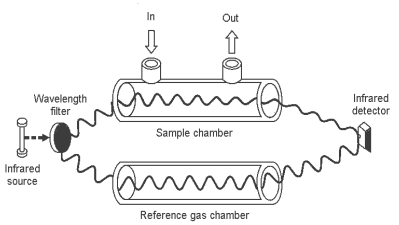

Fig. 1. Analyzer with a black-body source.

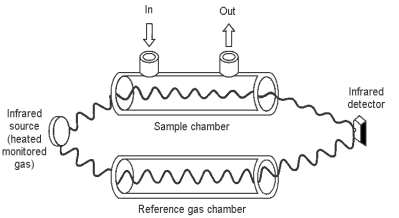

Fig. 2. Analyzer with a heated gas source.

The main components of the gas analyzer are an infrared source, similar to the black-body, a wavelength filter, and an infrared detector. The radiation goes simultaneously through two chambers, one with a portion of sample gas and another with an enclosed reference gas, typically nitrogen (fig. 1). The filter eliminates all wavelengths except those at the domain of CO_2 gas molecular absorption. A vibration-rotation band consists of a set of narrow lines, and it seems that the use of the heated CO_2 gas as an infrared source without a wavelength filter (fig. 2) would be more effective. The theoretical estimation of the efficiency of these two types of gas analyzers is performed in this work.

The calculations demonstrate that the use of the heated gas infrared sources has both advantages and disadvantages in comparison with the black-body sources with optical filters. The main advantage is an appreciable growth of the sensitivity, and the disadvantage is the decrease of signal-to-noise ratio due to the decrease of the initial beam intensity. The results can be applied to the engineering of new types of gas analyzers.

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Evaluation of delta-electron yield in heavy ion NA61 experiment

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Nowadays, a large number of experiments whose aim is to study nucleus-nucleus interactions at high energies has been accomplished using heavy ions beams of Super Proton Synchrotron at CERN. A great interest in such interactions is caused by the possibility of onset of a new phase of strongly interacting matter – the so-called quark-gluon plasma (QGP) in relativistic collisions of nuclei. The main objective of the NA61 experiment, started at CERN two years ago, is to study the properties of the phase transition of strongly interacting matter from the state of the hadron gas to QGP state.

NA61 experimental setup is a large acceptance hadron spectrometer. The main track detectors are four time-projection chambers (TPC). In the fixed-target experiments (like NA61), there is a possibility of that ions from the primary beam do not interact with the target and pass through an air gap separating the right and left half of the TPC. Delta electrons produced by the interaction of relativistic heavy ions with gas atoms may get into the TPC operation volume and create additional background, which complicates the track reconstruction. It is assumed that special upgrades may reduce the yield of the delta-electrons and thus suppress that background.

This goal can be reached by putting a beam pipe filled in light gas, such as helium (instead of air) in the air gap of each TPC, and by connecting the consecutively arranged time-projection chambers with an additional beam pipe.

In this article we present GEANT simulation of delta electrons produced by the passage of relativistic ions at 10 and 160 GeV per nucleon through the NA61 vertex time-projection chambers. An average number of electrons produced by the passing of one ion through the gas-filled beam pipe has been calculated. Based on these data the following conclusions have been done:

- It is possible to reduce significantly the delta electron background (comparing with air gap) by using helium-filled beam pipe.
- A presence of an air gap between the first and second TPC leads to generating of large number of delta-electrons, which may reach the operation volume of second TPC.

The excitation of cymbal's oscillations by electromagnetic impulse

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It's known that discharging an electronic flash unit near a cymbal will produce a sound from the cymbal. But well-known phenomena often don't have well-known explanation [2]. The research was started due to the preparation to the Young Physics Tournament' 2008, was presented at finals of the AYPT' 08 and the conference "Physics and Progress - 2008 ".

In our research we perform theoretical and experimental analysis of the probable reasons for the cymbal's sounding.

Our conclusions:

- The main reason of the cymbal's sounding is a very fast deformation of the cymbal, caused by the absorption of the light and rapid heating.
- Very sort time of the impulse is one of the main conditions for the sounding.

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Extension of oil and gas isothermal open-source simulator BS-Eagle to thermal simulator

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Recent years are characterized, on the one hand, by the significant deterioration of the oil and gas resources structure, on the other hand – by the development the fundamentally new technologies in the fields of the deposits investigation and simulation, of the wells drilling and injection, the use of the fast computers for the complicated computations and hydrodynamic simulation. At the present time, almost all deposits development is carried out using the simulation, because simulation allows to plan the deposit development and the oil, gas and water extraction process optimal from economic and resource saving point of view.

Models of thermal filtration are used to describe processes of oil extraction by different heat transfer agent (hot water, vapor, in-situ combustion). Generally these technologies are used for the extraction of viscous oil and bitumen. In this case we consider a model of thermal filtration, properties, composition of fluids and permeabilities depend on temperature. Therefore, to close the system of equations it is necessary to add one more equation – law of energy conservation.

There are two methods of creation simulator of thermal model. First way is to create new simulator of thermal model. In some sence it's easier because we can design and implement simulator for thermal simulation from the beginning. And this design and implementation will be suitable for thermal model. But it takes much more time and other resources. At present there are available oil and gas simulators of isothermal model. Some of them are open-source and ready for extension. For example, BS-Eagle. We can use existing isothermal code and extend it to thermal. In this report we describe one possible way to do it.

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F. Optics and Spectroscopy

The possibility of capacitive discharge with using one external electrode for measuring nitrogen admixture to argon

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Calculations show that the lifetime of the metastable atoms in technical argon at atmospheric pressure is about 100 microseconds. This estimation is a lower limit, since it does not take into account the processes of populating the metastable levels.

Let us consider an electric discharge in a stream of argon. Plasma, leaving the discharge region, quickly "lights-out", but there still remain the metastable atoms, which for 100 μs, in average, at a velocity of 30 m/s fly 3 mm.

To test this theory, we have furnished the setup. In a fused silica capillary through a metal tube was fed a stream of argon. The tube represents the first electrode. The second electrode is an external one – it is a metal ring around the capillary. The high-frequency voltage supply is connected with the electrodes. In the Fig. 1 is shown the discharge in the absence of gas flow, and in the Fig. 2 - with the flow, the velocity of flow through the pipe was 30 m / c.

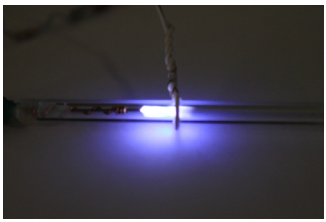

Fig. 1 Glow without flow.

Measurements of emission spectra has shown that, as expected, the integral intensity of the second positive nitrogen system with respect to an integral luminosity of argon lines in the visible region was higher, approaching in some areas of the discharge to the intensity of argon luminescence. This makes it possible to determine the concentration of nitrogen in argon without using interference filters or dispersive elements.

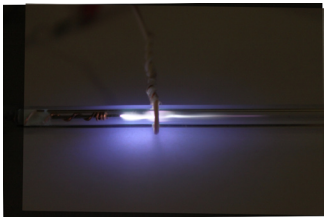

Fig.2. Glow with flow velocity 30 m/s.

The kinetics of the processes occurring in the discharge plasma in its various fields is of a great interest, and this is the subject of further study.

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Acetic acid complexes in solution and in the gas phase. Experimental study of v(OH) band

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Studying systems with hydrogen band in the gas phase make possible to define spectral and thermodynamic complexes' properties when there is no disturbing by interaction with environment. Particularly those data are necessary to clear out spectral lines broadening after v(OH) band foundation. At that time general number of publishing about spectroscopy studying hydrogen band in gas phase are rather few. Limited numbers of subjects having high enough vapor tension near the room temperature, experimental hardship, at first time substances adsorption are main factors making this researching difficult. Acetic acid was made such matter for us.

After recording the spectra we have compared them with spectra obtained in early experiments of other authors in this research area [1, 2]. We were looking for how spectrum transforms when we changed acetic acid to trifluoroacetic acid and acetone to heavy acetone (completely deutereted).

Complexes diethyl ether and acetone with acetic acid in solution were studied also. We have recorded spectra and have obtained some experimental data for trifluoro- and trichlor- acetic acid`s complexes also. Comparison spectra of complexes in the gas phase and in solution can give information about physics of interaction between molecules. We have recorded spectra complexes of acetic acid with diethyl ether and acetone, have obtained some value such as zero and the first reduced moment, half-width v(OH) band for acetic acids complexes and have given some explanation for seeing.

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The anomalous isotope shifts in vibration spectrums of the low-temperature molecular liquids

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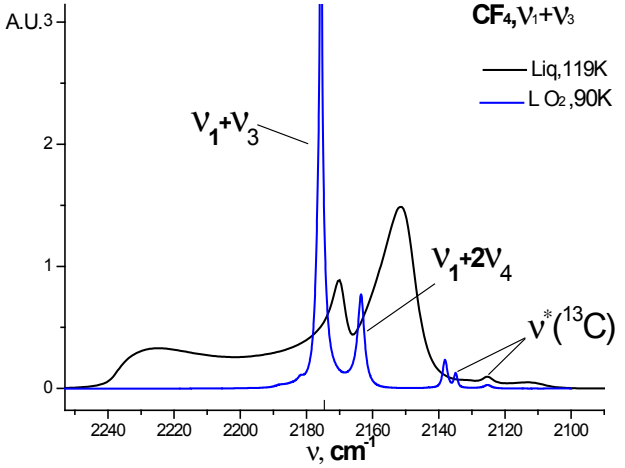
Isotope shifts for molecules CF_4 (on frequencies $2\nu_3$, $\nu_1 + \nu_3$), COS, $NF_3(\nu_1+\nu_3)$, CF_3Br, CF_3Cl (ν_1, ν_4, $\nu_1 + \nu_2$, $\nu_2 + \nu_4$) at various low temperatures were investigated. Appropriate spectral moments in solutions (O_2, Ar) and liquids have been discovered. Also were counted the spectral moments of bands in considered frequency regions. The significant variance of isotope shifts in different solutions and liquids was received. The obtained results could be explained with a resonance dipole-dipole interaction between isotope replacement and surrounded molecules. Using earlier obtained data from the published articles [1] and consideration of various spectrums has given possibility to observe watch correspondence between calculations and experiment.



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The possibility of oil type determination, based on absorption spectra

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Today the foodstuff control is to a large extent based upon analytical methods. Optical spectral methods play a major part in these studies. Quality control can measure the quantity of admixtures and, moreover, the correspondence of product to some of the classes (its classification). Complicated structure of such foodstuff production, which is the mixture of numerous different compounds, requires application of the statistical methods to their study involving the pattern recognition algorithms [1].

For our research we have chosen vegetable oils that are the mixture of complex organic compounds. Such physical and chemical diversity of similar products makes it possible to test our method on a wide variety of similar objects.

In our research we have used statistical pattern recognition methods for class identification of vegetable oils, based on oils' absorption spectra in visible, near-IR and UV ranges of spectrum.

Spectra were obtained with spectrophotometer «SF — 56». We have measured the spectra of 25 vegetable oils with 1 nm step from 300 to 1100 nm.

With the purpose to distribute the vegetable oils among classes we have used the statistical pattern recognition method that concludes with determining class borders on a plane of principal components, corresponding to different types of vegetable oils. Due to a very large dimension of statistical space (801), the method of principal components [2] was used for pattern recognition.

Borders determination for each kind of vegetable oil is based on estimation of parameters of two-dimensional Gaussian distribution on the major constituent's plane. Borders are calculated numerically by splitting the major constituent's plane into elementary cells.

The results were as following: (1) 25 types of vegetable oils were analyzed, therefore statistically significant data for further research was accumulated; (2) preliminary analysis was conducted and it has proved the possibility of oil classification using simple optical methods.

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The research on ability of identifying gas condensate by their absorption spectrum in close IR-area

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Nowadays gas condensates are becoming more and more important throughout the world due to wide usage of those in the fields of chemical manufacturing and energy production. In the area of their possible applications for various petroleum products, the undisputed interest is caused by the search capabilities of optical methods: particularly, of the research in the IR range, limited by transparency range of quartz and alumina (Al_2O_3).

The mission of this work is to make research on ability of identifying gas condensates by their absorption spectrum in close IR-area (i.e. in the wavelength range of 1500 to 2500 nm).

It's rather noticeable that we cannot distinguish individual absorption band on the obtained spectra. The highest absorption for all the condensates is observed at the wavelength of 1700 nm and at the wavelengths greater than 2300 nm. The light transmission for different condensates varies greatly both in magnitude and in the form of the transmission curves.

Let's consider the method of principal components [1] applied to samples of the gas condensates. It may be noted that high proportion of the mixture can be formed either by high relative concentration of heavy fractions or by high relative concentration of heavy and medium fractions. Nevertheless, the spectra of these substances have certain characteristic features that allow us to mark them out in a separate group.

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Output radiation of an optical lightguide in absorbing media

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Optical methods are widely applied in solving various problems of fundamental and applied character. One of such methods is refractometric method of analysis the substances, convenient for research strongly absorb substances.

The method is based on effect of total internal reflection (TIR) violation in lightguide in which result light partially leaves from lightguide in the absorbing medium. The object of the refractometric studies of liquid mixtures of complex compounds is very convenient was such a mixture as engine oil.

As part of the work was to measure the spectral dependence of the intensity of transmission of the U-shaped fiber optic refractometer, immersed in oil with known characteristics.

During the experiment, when light refractometer, immersed in oil, there was a bright blue-green light (side radiation). In order to explain the nature of side radiation, we studied the scattered radiation measurement.

In the simplest model all the radiation losses are explained by a violation of TIR. Thus, measuring the intensity of the emergent radiation from the cell and making a correction for absorption should have an initial range. The simple theory does not explain the loss of light.

Radiation losses in optical lightguide refractometer explains the behavior of radiation at the material refractometer and the environment. In absorbing medium, even under the conditions of TIR, the reflection occurs from the loss of intensity. Thus, the loss of radiation during the passage of light along the optical fiber immersed absorbing medium, cause the one hand, the output radiation of the interface due to breach of TIR, and on the other hand, losses due to the presence of absorption in the external environment under the conditions of TIR. Mechanisms for loss of intensity during the passage of light along the lightguide include refraction, absorption with the nonradiative relaxation, fluorescence and scattering. Quantifying the role of these phenomena is the subject of further work.

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Studies of two-photon property of intensely luminescent metal-organic complexes

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We have measured the two-photon absorption (TPA) cross-section of some dissolved organic molecules using the two-photon induced fluorescence method. We used molecules with two types of fluorescence. The first type is fluorescence from first excited singlet state to ground state $S_1 \rightarrow S_0$, and the second type is fluorescence from first excited triplet state to ground state $T_1 \rightarrow S_0$.

The number of molecules (R) promoted to the excited state during laser pulse (dt) in volume $dldxdy$ in consideration of two-photon absorption is written like:

$$R = \frac{1}{2}\frac{1}{(h\nu)^2} N\sigma_{2p} dl I^2 dtdxdy \qquad (1)$$

Here I is intensity of laser irradiation, $h\nu$- quantum energy, N- molecular concentration, dl- length of absorbing layer, σ_{2p}- two-photon absorption cross-section. Number of photons (W) emitted after laser pulse from volume $dldxdy$:

$$W = qR \qquad (2)$$

Here q is a quantum yield. In experiment we compare intensities of fluorescence for observable (x) and reference (re) matter. After cell replacement all geometric factors are invariable. Then from (1, 2) we get equation for

$$\frac{W^x}{W^{re}} = \frac{q^x}{q^{re}} \frac{\sigma_{2p}^x}{\sigma_{2p}^{re}} \frac{N^x}{N^{re}} \qquad (3)$$

Finally we obtain equation for the two-photon cross-section

$$\sigma_{2p}^x = \sigma_{2p}^{re} \frac{W^x}{W^{re}} \frac{q^{re}}{q^x} \frac{N^{re}}{N^x} \qquad (4)$$

Number of photons is calculated by integration of fluorescence spectrum (fig. 1).

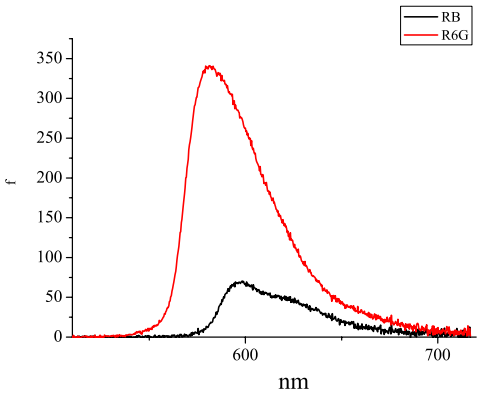

Fig. 1. Fluorescence spectrum of rhodamine 6G and rhodamine B.

Investigation of possibility to use the phenomenon of Raman scattering to determine the concentration of aromatic hydrocarbons in complex mixtures

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One of optical methods of detecting the presence of benzene in mixtures is connected with the phenomenon of Raman scattering. There was a task to consider the possibility of application of Raman spectroscopy of liquid mixtures of complex hydrocarbons in order to develop a method for determining the concentration of benzene in mixtures of complex compounds.

Measurement of Raman spectra of mixtures have been carried out in gasoline-benzene mixture with different ratio of substances in the mixture. To observe the Raman scattering the CW neodymium laser with a wavelength of 532 nm was used. During the work the peak of anti-Stokes components of benzene, received in a mix of gasoline with addition of 15 % of benzene, has been recorded. After the analysis it is possible to conclude that the lowest concentration of benzene which can be registered with the use of the thus used setup on anti-Stokes component is about 5-10 %. At the same time there is a real possibility of modifying the registration system, which, in our opinion, would bring the sensitivity to a value not exceeding 1%.

Also the Stokes component of Raman scattering of benzene in a mixture of gasoline, benzene, at a concentration of 5% was recorded. Limiting concentration, which can be registered, is at the best 2 %. Based on the progress of the experiment and evaluations, we can conclude that this method is enough suitable for measuring the concentration of benzene in gasoline at concentrations of less than 1% of the largest anti-Stokes components. For measurement of the concentration of benzene in gasoline, according to the Stokes components at the level less than 1 % it seems to be reasonable to use the laser with the lines of generation lying in yellow and red area of a spectrum. In this case the intensity of fluorescence of gasoline can be significantly lower and it is possible to reliably measure of the concentration of benzene in quantities of less than 1%.

Geometries of OHO Hydrogen Bonds Probed by H/D Isotope Effects on Nearest Carbon Chemical Shifts

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Interpretation of NMR spectra of OHO hydrogen bonded complexes in terms of geometry is often ambiguous: the only magnetically active nucleus directly participating in H-bond is proton, which usually lacks *J*-couplings with other nuclei and tends to be engaged in exchange processes which lead to signal averaging. Alternatively, one could analyze chemical shift of neighboring carbon atom, $\delta(^{13}C)$ is determined mainly by the chemical nature of the molecule and only to a little extend by the H-bond geometry.

Here we propose to use H/D isotope effect on $\delta(^{13}C)$ instead of its absolute value. In this differential quantity the contributions of the molecular skeleton are the same for H and D isotopologs and the value of the isotope effect reflects mainly the changes of the H-bond geometry upon deuteration. To establish correlations between H/D isotope effects on $\delta(^{13}C)$ and the H-bond geometry ([1, 2]) is the long-term goal of this work.

In this paper we focus on intermolecular H-bonded complexes formed by ^{13}C-labelled acetic acid with tetraethylammonium (TEA) salts of 4-nitrophenol-^{13}C and 2-chloro-4-nitrophenol-^{13}C (see fig.1) in solution in CD_2Cl_2 at low temperature. Labeling of the molecules with ^{13}C increases the sensitivity, while reducing the temperature to ca. 170 K suppresses the intermolecular proton and deuteron exchange, allowing one too see separated signals from complexes of various stoichiometry and isotopic composition.

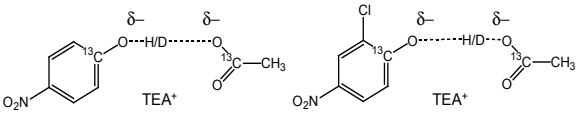

Fig. 1. Structures of complexes of 4-nitrophenol/acetic acid, 2-chloro-4-nitrophenol/acetic acid.

We demonstrate that both studied complexes exhibit short strong anionic OHO hydrogen bond, subject to some proton tautomerism. The main difference between complexes is in the average proton position (on different sides of the H-bond center), the information which could be extracted from the signs and values of the H/D isotope effects on nearest carbon chemical shifts.

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Prototype of the Parallax-based Relative Position Measurement System

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The Relative Position Measurement system based on parallax effect was developed. The demand for this system is caused by wear factor of existing sheaves-and-ropes measurement concept used in flaw detector cars, where it is applied for metering the position of railcar's bogie against its body. Nowadays, precision and performance of this concept isn't satisfying anymore.

New concept consists of three self-luminous ranging marks attached to the bogie, which are observed by three cameras attached to the body's bottom, so that each mark is continuously observed by its own camera. The market of modern CMOS and CCD cameras was explored; special lens systems were developed, as well as appropriate ranging marks design was chosen.

The main problem in designing this system lies in sophisticated nature of dependence between sought quantities (three Euler's angles and three inline offsets of the bogie against railcar's body) and quantities to be measured (six observation angles of ranging marks against cameras). These variables are bounded with a system of non-linear polynomial equations, whose amount varies from 9 to 15 depending on the method of mathematical model's formulation.

The request of real-time imaging of the railtrack's geometrical parameters requires determination of this system of equations on-the-fly for each set of values measured. As finding system's general solution is unlikely due to its complexity, we are going to determine its computational solution after each measurement with the help of Seidel method. This approach leads to tremendous amount of computation, hence, the Seidel method will be incarnated in a FPLD to offload evaluator's CPU and to assure real-time mode.

Expected sensibility of the system is about 0.5 millimeter for inline offsets and about 1 angular minute for Euler's angles.

In order to check the system's realizability, a laboratory prototype was constructed. Exploration of this model has shown that chosen cameras, as well as our original lens systems, survive severe conditions of railtrack flaw detection quite well. Besides, the evaluator architecture was planned, and its hardware development was started.

Structure modification mechanisms in As_2S_3 under the laser irradiation

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Laser writing is the local process of structure modification in optical materials. Such changes in structure lead to changes in optical properties. Recent investigations have demonstrated that light influence can produce prominent modification in such optical materials like glasses, crystals and polymers [1]. In the present work, we report photoinduced modification phenomena in chalcogenide glasses (based on the chalcogen elements S, Se, Te).

Chalcogenide glasses are rather attractive material for laser writing, because one of their properties is lability of glass structure to laser irradiation. We have investigated two main processes of laser modifications in calcogenide glasses: linear and nonlinear writing (it depends on one or two photon absorption accordingly). Nonlinear laser writing was realized with Ti:sapphire femtosecond laser with parameters: wavelength = 800 nm, repetition rate = 80 MHz and duration of laser pulses = 100 fs. We created waveguides at different writing parameters [2]: geometry of laser writing, translation rate of object and scan regime. Linear laser writing was realized with semiconductor laser wavelengh (660 nm) and CW YAG:Nd laser (532 nm).

The advantage of femtosecond laser pulses is the possibility of depositing energy into material during a short period that allows making structure modifications inside an object. It makes possible to create waveguides for integrated optical elements and lab-on-a-chip for express analyses in chemistry, biology and medicine, nonvolatile memory could be realized. The wavelength should be chosen according the glass band gap, as a result one could get stable or reversible modifications.

On the basis of Raman Spectra Analysis we could conclude the bond switching which occurred under the laser irradiation. We solved the thermal conductivity equation and obtained temperature distributions in the laser-affected area. Using microphotos and computer simulation, the conclusions of the laser-induced mechanisms were made.

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Hyperfine structure in alkali metal dimers: Improved analysis

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Excitation spectra of alkali metal dimers measured in the optical-optical double resonance (OODR) technique often exhibit partly resolved hyperfine structure [1, 2]. The analysis of this structure is able to reveal the mechanisms of the intramolecular interactions and bring out the quantities of the interaction parameters. We have found that the earlier model of the hyperfine effects proposed in Ref. [2] was unable to describe some of the details of the observed spectra and needed improvements. We have explored the mechanisms, which can influence the experimental data, and corrected the method of Ref. [2] by including those mechanisms into it. Then we have applied the improved method to the analysis of the spectra of K_2, Na_2.

This work was supported by the Russian Foundation for Basic Research, grant No. 10-03-91151.

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Investigation of the relaxation time of free carriers in GaAs quantum wells under femtosecond laser irradiation

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Low-Temperature (LT)-grown semiconductors such as GaAs present very interesting optoelectrical properties that could lead to many potential applications in the domain of ultrafast optoelectronics [1].

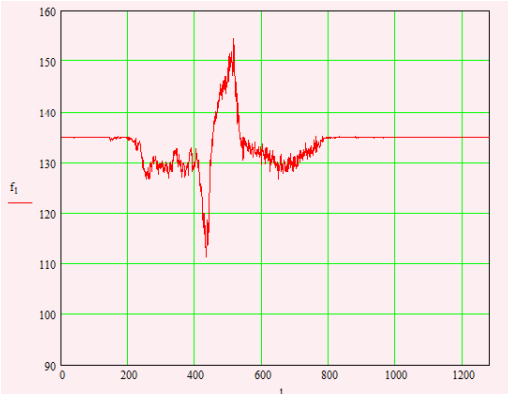

Fig. 1: Time variation of the reflection coefficient in relative units.

This research is an experimental study of the relaxation time of free carriers generated by emission of femtosecond laser at a wavelength of 790 nm in the semiconductor GaAs system with quantum wells.

By the experiment two beams (pump and probe pulse with lower intensity) converge on the sample GaAs, intersecting at a slight angle so that their wave surfaces are found on the sample surface only on one line, while in other places either pumping or probe pulse is delayed (depending on the delay). Reflection of probe pulse was recorded near the Brewster angle to reduce the background from the pump.

In this paper we obtain a set of tracings, on which by subtraction of two different signals the pump and probe pulses, separated by a time period of 600 fs, we determine relaxation time of reflection. Between the two pulses signal of relaxation is visible, the time of its fall is just obtained about 600 fs.

Obtained results are essential for research of effectiveness of fast optoelectronics based on nanocomposite GaAs semiconductor.

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Laser-assisted local metallization of dielectrics and semiconductors

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Since the very beginning the laser-assisted methods have become of critical importance for the metal deposition. Various laser techniques allow metal precipitation on the different kinds of the materials. One of them is the Laser-induced chemical liquid phase deposition (LCLD), which is considered among the others to be the most promising and efficient. Indeed, the LCLD method offers convenient way of the metal precipitation with rather high uniformity of the morphology and good electrical properties of the deposits. In spite of the achieved high quality of the metal structures the ongoing attempts are undertaken for the improving of the deposition efficiency and the quality.

In the LCLD method the laser initiates the chemical reducing reaction and the laser focal volume determines the volume of this reaction what results in the localized submicron metal deposition. Also this method permits controlling width, morphology and resistance of metal structure as a result of variation laser power, temperature of solution and other parameters of deposition. The laser-assisted photothermal chemical reaction yields deposition of the structures on the substrate with high degree of adhesion. This method is characterized by technological efficiency, chemical safety and low-price equipment.

Up to now the LCLD method was successfully realized for precipitation of such metals as Cu, Ni, Pd, Ag on several kinds of semiconductors and insulators such as Si, Ge, GaAs, polymers and so on. But a question about alloys deposition using this method has been never risen.

In the present work the possibility of alloy precipitation was investigated. The deposition process was carried out from metalloorganic complexes witch consist of the $[Au_6Cu_6]$ clusters 'wrapped' in the $[Au_3(diphosphine)_3]^{3+}$ triangles [1]. Possibility to change Au-Cu ratio in the initial solution allow controling composition of the deposited metal structure. This metallization technology can be successfully used in the microelectronics industry for the creation of the electrodes the metal conductors on the microchips, in the display technologies for the production on flexible polymer monitors and keyboards, creation micro thermocouples and so on.

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2D correlation analysis of IR spectroscopic data of ethylene ozonolysis on the amorphous water ice surface

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At lower troposphere as well as at stratosphere the complex processes involving ozone such as an ozone interaction with organic molecules are very ecologically important. Snow and icy aerosol atmospheric particles are active participants involved in processes occurred in the Earth's atmosphere. Ice surface may concentrate a broad variety of organic pollutants and thereby promotes chemical and photochemical heterogeneous reactions with them.

In our work, the ozonolysis of ethylene adsorbed on amorphous water ice film at 77 K [1] was chosen as a model reaction. This study has shown that the part of ethylene molecules form π-complexes with OH-groups of ice. The behavior of superficial ethene significantly differs from that of the bulk ethene molecules.

2D correlation spectroscopy method [2] was used for more detailed analysis of the data obtained. It provides better access to information not readily observable in conventional spectra. The splitting of ethylene IR bands was proved. Also products of this reaction (primary ozonides, secondary ozonides, and acetaldehyde) were identified.

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Luminescence and absorption of acridine hydrogen bonded to carboxylic acids and alcohols

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Protonation of acridine by strong acids results in a characteristic extension of its absorption spectrum, intensity increase and shift to longer waves of its luminescence spectrum [1]. A considerably more challenging task today is elucidation of the structures of complexes of acridine hydrogen bonded to weaker acids, when the formation of hydrogen bond complexes of acridine with proton transfer are unlikely, especially in non-polar solvents.

Absorption and luminescence spectra of acridine with chloroacetic and acetic acids in the di-chloromethane in equal concentrations showed that the taken concentration is sufficient to form a complex with proton transfer only in the case with chloroacetic acid. This observation might indicate that acetic acid cannot donate the proton to acridine in a low polar solvent. In contrast, at a higher acetic acid concentration proton transfer takes place in other composition than 1:1, which are presented in the solution. [2]. The absorption spectrum of acridine in ethanol resembles the absorption spectrum of acridine in di-chloromethane. The same is true for the luminescence except a dramatical increase of its intensity. For the system of acridine – hexafluoropropanol (pK_a=9,75) in di-chloromethane an increase of the luminescence intensity is accompanied by a small long-wave shift of the spectrum.

The most important preliminary result is that the positions of the luminescence maxima correlate with the pK_a values of the proton donors. The stronger is the proton donor the stronger is the long-wave shift of the luminescence as compared to free acridine. The shift is accompanied by a progressive increase of the luminescence intensity. Thus, both the intensity and the shift of the luminescence of acridine upon hydrogen bonding can be potentially used to estimate the geometry of the forming bonds.

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Fundamental absorption band in the spectrum of the CF_4 low-temperature liquid

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Purpose of the present paper is to obtain the ν_3 fundamental band shape, intense in the IR absorption, for the CF_4 liquid spectrum at temperature T~80 K. The path length *l* should be of order micron to record the absorption spectra of low-temperature liquids in the fundamental region. Since this condition is difficult to accomplish, here the absorption band shape was found by using the experimental reflection band shape of liquid CF_4 in the same spectral region. To record the reflection spectra the new cell equipped with BaF_2 window was elaborated and constructed. The cell was cooled with cold nitrogen vapors. Additionally, the model calculations were performed at several values of the absorption coefficient χ (χ = 1, 0.5, 0.1) and different profiles (Lorentzian profile, shape of the combination band).

Two-photon decay of excited levels in hydrogen: The ambiguity of the separation of cascades and pure two-photon emission

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In our work we demonstrate the ambiguity of separation of the «pure» two-photon contribution in ns-1s transition in hydrogen. This problem became important in connection with role of the two photon transitions in hydrogen in the cosmological recombination.

During recent years the two-photon decay processes in hydrogen have attracted special attention due to new and very accurate observations of the cosmic microwave background temperature and polarization anisotropies. In view of these observations, it becomes important to understand the hydrogen recombination history with high precision. In the early universe, the strong Lyman-alpha 2p-1s transition did not permit the atoms to remain in their ground states: each photon released in such a transitions in the one atom was immediately absorbed by another one. However, due to very weak 2s-1s two photon decay process the radiation could finally decouple from the interaction with matter and thus, permit a successful recombination. This problem becomes more complicated in case of ns-1s ($n>2$) transitions due to presence of cascades. Since the cascade photons can be effectively reabsorbed, the problem of separating the «pure» two-photon contribution from the cascade contribution arises. An interference between the two decay channels, i.e. «pure» two-photon decay and cascade, should also be taken into account.

In our work the two-photon 4s-1s transition probabilities with all the cascades taken into account was calculated. The interference contribution is also presented.

Use of methods of pattern recognition for the quantitative analysis of liquid mixes of complex connections

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The primary goal of given work, consists in estimating possibility of application of the given method of pattern recognition for the componential, quantitative analysis of liquid mixes of complex compounds on absorption spectra in visible area. As object of research the solution of paraffin in gasoline has been chosen. The given choice is caused by following reasons: Paraffin is one of the impurities which concentration is supervised in the course of manufacture of various oil products. Gasoline and paraffin are transparent in visible area of a spectrum and practically have no characteristic spectral feature.

For production of transmission spectra of investigated mixes the spectrophotometer SF-56 was used. For experiment carrying out special solutions of paraffin in gasoline have been prepared with following concentration: 1%, 3%, 5%, 9%, 17%, 23 %, 42 %, 59 %, 79 %. And also we used pure gasoline and paraffin. Transmission spectra of the all given mixes were measured in a range from 300 to 400 nanometers, and It is found out that even the small additive of paraffin in gasoline leads to strong change of the transmission in this range of lengths of waves. For processing of the received spectra we used a so-called principal component analysis. A main objective of the given method is simplification of data presentation and revealing of signs on which the data concerning various objects, differs to the greatest degree. Such method allows us to arrange pattern of the objects in space of the principal component, with possibility of the subsequent representation of these results as calibrating plot.

In this work, we demonstrated the possibility of applying the method of principal component in quantitative analysis of liquid mixes of complex compounds, using data from an optical absorption method. The results obtained allow us to determine the mutual concentrations of these substances with sufficient accuracy.

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G. Theoretical, Mathematical and Computational Physics

Scaling in the theory of critical phenomena: calculation of renormalization group functions without using the renormalization constants

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Nowadays renormalization group approach is generally recognized as the method of the second order phase transitions and critical phenomena research. It allows to justify critical scaling and to calculate critical exponents in form of ε-expansion. The main technical problem, which one needs to resolve, is the calculation of renormalization group functions. Commonly it is made by means of calculation of so-called renormalization constants [1]. These constants are singular by parameter ε. This fact makes difficulties for their numerical calculation. In this paper these functions expresses through renormalized Green functions, not singular by ε, so it gives the possibility to make direct computation by means of computer programs. Critical exponents in φ^3 and φ^4 models were calculated in the second degree of ε-expansion.

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Screened vacuum polarization correction to the hyperfine splitting in highly charged ions

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Investigations of the hyperfine structure of highly charged ions are motivated by a possibility to test quantum electrodynamics in extremely strong electric and magnetic fields. In order to eliminate the uncertainty of the theoretical prediction due to the nuclear structure effects simultaneous study of hydrogenlike, lithiumlike and boronlike ions with the same nucleus is required. While the one-electron quantum-electrodynamic correction to the hyperfine structure was evaluated to high enough accuracy the screening effects on it were calculated in effective potential approach only.

The aim of the present work is to evaluate the inter-electronic interaction effects of order 1/Z on the vacuum-polarization correction to the hyperfine structure of highly charged lithium and boronlike ions within the rigorous QED approach. These calculations were accomplished so far only in the Uehling approximation for the vacuum polarization potential.

The significant progress in the present research has been achieved. Wichmann-Kroll contributions calculation has been carried out, and electric and magnetic vacuum-polarization loop Wichmann-Kroll corrections evaluation has been finished by now. These corrections have already been calculated before, but it was important to repeat them, improving numeric technique and testing Green functions for different nuclear charge distributions. For magnetic loop and light-by-light scattering diagram only analytical approximate Green functions for shell model of nuclear charge distribution were used before.

Now electric and magnetic vacuum-polarization loops have been calculated employing numerically-generated Green functions for arbitrary nuclear charge distribution model.

Now it is already possible to compile the most precise theoretical values for screened vacuum-polarization correction to the hyperfine splitting, employing the discussed Wichmann-Kroll contributions, as it has been done so far in the Uehling approximation only.

Two more contributions are to be calculated to complete the investigation - the Wichmann-Kroll part of light-by-light scattering diagram and the light-by-light scattering diagram with a magnetic vacuum-polarization loop. The latter has never been considered before, and according to the Furry theorem its Uehling part is equal to zero, but Wichmann-Kroll part is not, and it is going to be the final calculation for my PhD-research. A couple of articles is planned to be published up to the end of the discussed research.

Conservation laws for classical particles in AdS-Beltrami space

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In this work we will consider the conservation laws for classical particles in AdS_4. At first we will parametrise geodesic line and construct conserved quantities with the use of analog of five dimensional Minkowski space $M^{(2,3)}$. In the result we receive it in a form of parametrized vectors. The conserved quantities are written in Beltrami coordinates.

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Extensions of the random phase approximation in the microscopic theory of electric and magnetic nuclear excitations

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To explain a large amount of experimental data in nuclear physics, one has to use quantum many body theories. The first theory of the finite Fermi system was developed by Migdal on the base of the Landau Fermi liquid theory. Afterwards, some extensions were developed to consider more complicated cases.

In the present work we have provided some extensions of the widely-used random phase approximation (RPA). Originally, in this approximation one studies the linear response of the system on the weak external field. With the help of Green functions technique one can obtain RPA equations and solve them in a self-consistent way. But there are some problems.

Firstly, spectroscopic information could be obtained only for transitions between ground and excited states in the standard RPA framework. But in some cases one needs in characteristics of transitions between excited states, for example, in studies of the r-process nucleosynthesis. This problem could be solved in the Thermal RPA (TRPA) extension. We have performed it in the present work by introducing the new temperature parameter, which has been included in a self-consistent way into the energy levels occupation numbers of the Fermi system. Corresponding equations were derived and numerical calculations within TRPA were performed in the present work. We have obtained an interesting dependence between excitation energy and temperature, which turns out to be similar to the Fermi gas result with box boundary conditions.

Secondly, in some cases RPA equations are too complicated, but important integral spectroscopic characteristics could be obtained with the help of very useful tool referred to as the sum rules. The sum rules are the equations for the moments of the so-called strength function obtained in some approximation. There are some well-known sum rules for electric excitations in RPA, but for magnetic excitations there are the results only for some cases. We have derived equations for the sum rules for magnetic excitations within the RPA and calculated their numerical values, which for some cases could be compared with known experimental data. Finally, we have found that our formulas for the sum rules give the numerical results in complete agreement with direct calculations of the RPA moments.

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Generation of many-loop Feynman diagrams in critical dynamics

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Feynman diagram technique is useful in applying to various problems of critical dynamics. An example of such problems is kinetics of order parameter fluctuations near the phase transition. As an order parameter one may consider density (in liquid-vapor transition), magnetization(near Curie point), etc. Application of perturbation theory to these problems starts with construction of set of Feynman diagrams. And the number of diagrams for high order of perturbation theory is really high. For this reason process of generation should be computerized.

The essential idea of considering method is "growing" higher order diagrams from lower order diagrams by adding vertices and edges. The generation of φ-3 and φ-4 models diagrams was provided with relatively small time. The main adventure of considering method is slow growth of generation time in dynamical case, when different types of fields appear and diagrams includes different types of lines.

On the theory of supercritical droplet growth at isotermal binary condensation

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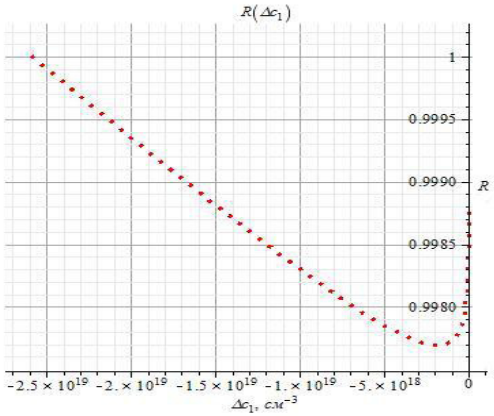
The aim of this work is the study of the diffusional growth of droplet in case of binary condensation. General relationships for dynamics of size and composition of a supercritical droplet in a binary vapour mixture obtained in [1] are analized in frame of ideal solution approximation. For a particular but practically important case of a droplet growth in a mixture of water and sulfuric acid vapours the numerical analysis is given. Numerical computations for droplet radius dependence on a deflection of the concentration of acid in droplet from its stationary value and the evolution of the concentration in time are completed. The results of these calculation shows that as well as in linear theory [2] a monotonous tendency of composition to a certain stationary one takes place. However radius of droplet may have nonmonotonous behaviour in time depending on initial composition of droplet. The figure shows a droplet radius R dependence on a deflection Δc_1 of the volume concentration of acid in droplet from its stationary value. R is taken in units of initial radius.



Behaviour of concentration is monotonous in time, so one can consider this graph also as illustration for time dependence of a droplet radius. If the initial concentration of acid solution in droplet is below a certain value then droplet gradually goes from evaporation to the stationary growth.

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Calculation of graphs with higher-spin particles exchanges

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In this paper the author suggests a method to obtain analytic expressions for Feynman diagrams, containing higher-spin boson particles. The author uses an effective Hamiltonian, containing an arbitrary polynomial of fields and its derivatives in arbitrary high order and power. Rarita-Shwinger representation was used to represent higher-spin particles. The method is founded on systematical arranging of factors, included in the diagram expression and implying several rules, formulated in the paper. These rules are written as theorem, and readers can apply them in a very easy way. The author believes, this is a technique, but not a formula. That means one can apply the technique to make his expression more easy-looking, but he can't obtain the final easy form of this by some function of diagram parameters. The author supposes that if it is possible to obtain a formula, it is the next step of the investigation. The advantage of such approach is obtaining the angle-depending expression for a diagram, and some routs of that are known from theorems included in the technique. The application of this may be different: from calculating the mass shift in renormalization to attempts of obtaining new special summation rules in perturbative scheme in QFT models.

Cross-section of two-electron capture by bare heavy nucleus

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We investigate two-electron capture by a bare nucleus followed by emission of a single photon. The total cross-section of the process is calculated relativistically within the framework of QED.

Process of the two-electron capture is investigated experimentally [1, 2] and theoretically [3, 4]. The recent experiment [2] shows necessity of more detailed theoretical investigation of the two-electron capture. The process of two-electron capture is explained by the interelectron interaction. In the present calculation the interelectron interaction is taken into account partly to all orders of the perturbation theory. We calculate the cross-section with employment of the Line profile approach (LPA) [5, 6]. The results are compared with available experimental and theoretical data.

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Fukui Function in Extended Koopmans' Approximation

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Fukui functions measure the change of electronic density which is connected with the attachment and removal of the electron. In principle this can be done by separate calculation of the neutral, cationic and anionic states of the electronic system [1]. Using the extended Koopmans' theorem within the many configuration approximation we express the one electron densities of the cationic and anionic states via two-electron density of the neutral state function. These calculations indicate the local reactivity (electro-negativity and chemical hardness) of the system.

This algorithm for calculations of the Fukui functions is illustrated for molecules LiH and HCl.

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Fluctuations of a number of wounded nucleons and binary NN collisions in nucleus-nucleus interactions for NA61/SHINE experimental setup in CERN

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One of the most important experiments in the CERN on SPS of NA61/SHINE detector is measurement of fluctuations for finding the critical point of phase transitions from hadrons' gas and quark-gluon plasma for strongly interactive matter [1]. One of the problems of experimental detection of that point is to separate the signal from the background. In order to do that we need to calculate the background fluctuations.

In this work the author simulates Pb-Pb collisions with Monte-Carlo method using C^{++} - language in conditions of that experiment (collision with fixed target at energy $\sqrt{s_{NN}} = 17.2\ GeV$). On the experiments one receives data on quantity of scattering nucleons in a projectile nucleus, but doesn`t know anything about target after collisions. The author has solved the problem of definition of target`s characteristics. As a result the plots for fluctuations of a number of wounded nucleons and binary NN collisions in nucleus-nucleus interactions have been received. Also the analysis of calorimeter`s indications with different fixed errors and errors, which take into account the properties of central and peripheral collisions, has been done. According to obtained plots one can appraise the influence of the set on the value of measured dispersion and also can determine how much the requirements of devices ideality can be reduce. Finally the author obtained the results of background fluctuations, which one can compare with experimental data in the future.

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Dynamics of the car movement during braking

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To provide the stability of the car on the slippery roads is the main problem in designing systems of car stabilization [1]. Emergency braking – is the most difficult and dangerous case. More detailed study of these processes allows developing new versions of systems which improve the stability of vehicle - ESP and ABS every year [2]. In the case of an emergency, when the driver can not drive correctly, these systems intervene in the control over the car, and allow one to reduce the probability of an emergency.

The aim of the work was to develop physical model of the car and study its behavior under different variants of braking. It was necessary to determine the basic dynamic parameters of movement, which lead to instability and to develop the most rational action of the driver to reduce the effects of an emergency.

In our computer model of the car wheels are oriented straight. We neglect any dynamic movement of the car frame in the vertical plane. These simplifications are important for the normal operation of the car, but not essential for sudden braking situations considered in the experiment.

This work analyses changes of the forces and moments acting on the model of the car during braking with an arbitrary ratio of braking forces of front and rear wheels. The center of mass is located above the road. The conditions in which instability occurs were determined by modeling cases of sequential blocking of the wheels. Numerical solution of systems of equations and modeling were carried out in the program Matlab.

Based on the analysis, the car has less stability when its back wheels block in the first place. The angles of drifts, in which the car simply oriented in a new direction, were calculated. The critical angle when the vehicle turns around was found. Simplicity of the model clearly demonstrates the diversity of the dynamic aspects of the car movement during braking.

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Numerical simulation of dynamical chaos regime for Rydberg atoms based on the Split Propagation Technique

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A highly excited hydrogen-like atom in an electric microwave field of frequency ω and intensity F^2 exhibits an example of a physical system with distinct properties of its electron trajectory instability [1]. The extensive studies of time evolution of Rydberg electron (RE) moving in a Coulomb potential in presence of a microwave field have demonstrated that onset of the global dynamic chaos in semi-classical trajectories exhibits a threshold, which depends on the intensity F^2. For the given value of n_0, this threshold value $(F_c)^2$ satisfies the relation

$$(\sqrt{2}\,\overline{F}_c n_0^4 = 1/49 n_0 \omega^{1/3})$$

provided $s=\omega(n_0)^3>>1$. If $F^2 > (F_c)^2$, the evolution of RE acquires the character of strongly locally unstable Hamiltonian system (K-systems) with intense trajectory mixing in phase space [2]. The Hamiltonian of the problem studied here is $H=p^2/2+U_s(r)+\mathbf{F}\cdot\mathbf{r}\cos(\omega t)$ with the model atomic potential $U_s(r)=-1/r+\alpha/(2r^2)$. This problem has no analytical solution, so one needs to use numerical methods. The time we are interested in while considering the electron dynamic is usually the time before the atom is ionized. With intensities not strongly exceeding the threshold intensity, that time may reach very large values. Traditional methods of numerical solution of Hamiltonian equations, based on numerical differentiation and integration, give exponential error grows related to the lapse of time and therefore hardly may be applicable to our case.

In order to have reliable results of simulations, a special task was set to develop and realize a specific algorithm which makes it possible to limit essentially the errors.

A special numerical code based on Split Propagation Technique [3, 4] was adopted to provide reliable stable results for calculations involving a large number of RE evolutions along the atomic orbits.

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Calculation of the anomalous exponents in the Kraichnan's model of magnetofluid dynamics: two-loop approximation

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Today body of mathematics of quantum field theory, which was created for description of elementary particles interaction, frequently used in theory of phase transitions (critical behavior), where it helped to define existence of critical scaling and calculate critical exponents in form of ε-expansion.

The technique of renormalization group can be applied also for description of turbulence, where we are confronted with some new difficulties due to the existence of anomalous scaling in these problems. Therefore while investigating turbulence we have to apply both renormalization group technique and operator product expansion. In particular, last time Obukhov-Kraichnan's model of passive scalar turbulence advection is very interesting: for the first time the infinity set of anomalous exponents was calculated within the regular perturbation theory (similarly to ε-expansion). Three-loop approximation results are obtained (ε^3).

In this work we investigate more complex problem of passive vector advected by the Gaussian velocity field with zero mean and correlation function

$$\sim\delta(t-t')/k^{d+\varepsilon}.$$

This problem may be obtained by linearization of magnetofluid dynamics equations. Anomalous exponents, which are identified with the critical dimensions of composite operators, are calculated within the ε-expansion to order ε^2 (two-loop approximation). Also the existence of anomalous scaling is ascertained, what is closely related with presence of composite operators with negative dimensions in this model.

Effects of turbulent mixing on critical behaviour in the presence of compressibility

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We study the effects of turbulent mixing on the critical behaviour of a nonequilibrium system near its second-order phase transition between the absorbing and fluctuating states. The model describes the spreading of an agent (e.g., infectious disease) in a reaction-diffusion system and belongs to the universality class of the directed bond percolation process, also known as the simple epidemic process, and is equivalent to the Reggeon field theory. The turbulent advecting velocity field is modelled by the Obukhov-Kraichnan's rapid-change ensemble: Gaussian statistics with the correlation function <v,v> = f(k^(d+ ξ)), where k is the wave number, and $0 < \xi < 2$ is a free parameter. Using the field theoretic renormalization group we show that, depending on the relation between the exponent ξ and the spatial dimension d, the system reveals different types of large-scale, long-time asymptotic behaviour, associated with four possible fixed points of the renormalization group equations. In addition to known regimes (ordinary diffusion, ordinary directed percolation process and passively advected scalar field), the existence of a new nonequilibrium universality class is established, and the corresponding critical dimensions are calculated to the first order of the double expansion in ξ and $\varepsilon = 4 - d$ (one-loop approximation). It turns out, however, that the most realistic values $\xi = 4/3$ (Kolmogorov's fully developed turbulence) and d = 2 or 3 for the incompressible fluid correspond to the case of a passive scalar field, when the nonlinearity of the Reggeon model is irrelevant, and the spreading of the agent is completely determined by the turbulent transfer. If the compressibility becomes strong enough, the crossover in the critical behaviour occurs, and these values of d and ξ fall into the region of stability of the new regime, where both advection and the nonlinearity are important.

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Numerical simulation of the nucleation equations. Growth stage and Ostvald ripening regime

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Nucleation theory is based on the discrete set or continuum Fokker-Plank type kinetic equations (in partial derivatives) for the distribution of embryos over sizes coupled with the integral equation of material balance. It is used extensively for analysis of a variety of physical, chemical and biological systems undergoing first order phase transition such as crystallization of liquids, kinetics of colloidal systems, growth of thin films, semiconductor quantum dots and many other growth-related phenomena. The aim of the present work is to understand the role of the diffusion (related to second-derivative term in the Fokker-Plank equation) in kinetics of the first order.

Numerical modeling has been performed for two-dimensional (2D) and three-dimensional (3D) condensing systems with different growth laws, under a constant and zero material influxes. This modeling has been carried out with several approximations: with including and excluding second derivative, and with including and excluding ripening process (in the growth stage). The Crank-Nicolson method has been used for the modeling second-order partial equation, since this method is considered to be stable for the "diffusion type" equations. However, for the first-order partial equation (in case of neglecting the diffusion part of the equation) another computational method has been used, which describes changing in time of the concentration of embryos of a given size. This method is quite acceptable for solving the first-order in space variable equation, however it requires a large amount of initial embryos being included in the model.

Calculations of the distribution function of the sizes of embryos have been carried out in both stages: embryo growth and Ostwald ripening. It was shown that the accounting of the second derivative part and the ripening part of the kinetic equation can cause sufficient effects on the evolution of the distribution on the embryo growth stage. However, in the Ostwald ripening regime the influence of the diffusion provokes some, although insuffiecent, slowdown of convergence of the evolution density to the limited function in the Lifshitz-Slezov variables.

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Numerical simulation of micellization kinetics

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The process of forming micellae (that is known as micellization) has been staying very important problem not only because of multiple physicochemical and technological applications, but also because of the fundamental interest to this process itself.

In equilibrium state, the micelles (the aggregates of surfactant molecules dispersed in a liquid colloid) form two metastable phases: micellas of spherical type and cylindrical type. The goal of this work is to present the computational model of the dynamical process of formation of these two types of micellae and to describe the ways the micellae can form.

The micellization process conventionally is described with the essentially non-linear integral-differential Becker-Doring kinetics equation. In the present work this equation has been solved numerically with a well-convergent iterative procedure.

It has been shown that the process of micellization can be divided into two main steps that determined by different characteristic times. First step is the formation of maxima in the distribution functions that correspond to the spherical and cylindrical micellas. The second step is the relaxation of the distribution function to the equilibrium function. It is shown that this relaxation can be described analytically as an exponential convergence to the equilibrium with the characteristic time which equals to the minimal non-zero eigenvalue of the matrix of the linearized coalescence equation.

An analysis of empirical data and modeling of processes on a financial market

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The term «economics» is usually associated with the notion of complex systems. Speaking of complex systems, we should consider systems with a large number of interacting units. Nowadays an intensive integration of applied mathematical methods in economic theory and finance takes place, associated with the desire to produce more accurate forecasts of market behavior. Due to long-term observations, a large amount of financial data is available, which can be analyzed in various aspects. Rapidly developing understanding of the behavior of self-organizing systems allows suggesting that in the economic sphere stable patterns in the formation of statistical data should be observed.

One of the most interesting and promising trends of research in this area is an attempt to describe the formation mechanism of the asset market price, as well as identification of common stable characteristics of such systems, which do not depend on specific conditions.

In this paper an analysis of financial mechanisms that control the market was carried out. In particular, the formation of market prices of foreign currencies was considered.

The aim of the present work is to study peculiarities and regularities of such system, to reveal some stable independent characteristics and to create a mathematical model that could accurately describe the development of the financial market.

Based on the task, the statistical properties of historical time series of relative EUR/USD rate and their behavior were explored. Also, this work describes the market prices formation model for foreign currencies, as well as the mechanism of market trading between players. Based on this model, a software implementation, which generates the time series, was developed. Then their properties were compared with those of historical data. Also there are considered certain mechanisms of internal market regulation, which influence the trade mechanics and the outcome results.

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Quantum-electrodynamic corrections: Z-boson loop

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The measurements of parity-nonconservation (PNC) effects in atoms is one of the most efficient tools to provide sensitive tests of the standard model now. Particularly, the nuclear spin-independent part of PNC matrix elements could be proportional to a conserved weak charge, which is sensitive to physics beyond the standard model. It has been shown in [1] that experimental value of the weak charge of Cesium-133 differs from the standard model value by 2,3σ.

The Breit operator in PNC has decreased the difference to 1,6σ [2]. Then it was pointed out that QED-corrections could be of value comparable with Breit ones'. The numerical evaluation of the vacuum-polarization corrections increases weak charge difference from the standard model prediction [3]. This has caused a great interest to calculations of the comprehensive QED corrections to the PNC amplitude. Using the whole gauge-invariant set of the one-loop QED corrections (self-energy) to the 6s-7s PNC transition amplitude in Cesium-133 it was shown that the experimental value of the weak charge of Cesium-133 differs from the standard model value by 1,1σ [4].

The aim of present work was to evaluate the electron self-energy in weak interaction, using Z-boson propagator instead of photon's one. It can be easily shown, that in the above case the Feynman diagrams are of lower order in fine-structure constant (α) expansion, thus such a calculation should be performed in order to get more precise value of the weak charge of the Cesium-133.

All the theoretical researches were done. Integration over virtual Z-boson momentum is performed analytically, therefore the remaining integration can easily be done numerical. Now the work is in the stage of performing numerical calculations and comparing them to calculations of ordinary electron self-energy part with photon propagator. This is to check all the theoretical results achieved for the case concerning Z-boson propagator. As Z-boson mass equals zero, result should be similar to the ordinary electron self-energy part.

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Modelling of exclusive parton distributions and pp interaction features in the approach with the colour strings formation

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The present work is devoted to the investigation of soft pp interaction at high energy. Perturbative QCD methods are inapplicable in this kinematics and phenomenological models are being used. The model with the colour strings formation [1] is used at the work.

The aim of the present work is to construct the exclusive parton distributions [2] form inclusive structure functions and to develop the methods for generating and applying them for studing of pp interaction features. For this purpose with the special attention the opportunity of modelling the exclusive parton distributions was examined taking into account the energy conservation and holding the centre of mass. Monte-Carlo methods for generating this distributions was developed for arbitrary number of patrons in the hadron. Proton-proton cross sections are estimated with the assumption that the elementary collision is realized as the interaction of two colour dipoles [3] from projectile and target protons. The influence of confinement on that elementary cross section was studied.

Multiplicities are calculated in the framework of independent strings with the assumption that mean multiplicity from one string is fixed. The parameters of the model are determined form experimental data for pp cross section or for multiplicity [4-5]. It **was found** that agreement in results can be achieved only with the assumption that see quarks do exist in protons even at low energy. Usual supposition that there is no sea quarks at low energy in this model does not give the agreement with the experimental data.

In is possible to amplify presented model by taking into account the string fusion effects and to extend the set of quantities being calculated. The algorithms used in this work can be applied for the description of the heavy ion interactions.

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Effects of turbulent mixing on critical behaviour

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Consistent quantitative description of the critical behaviour of various systems, subjected to strong turbulent mixing, can be achieved within the framework of the renormalization group (RG) method. In this work the model describing the second-order phase transition between the so-called absorbing and fluctuating states is investigated. Specifically, the Gribov process is studied, which is named so, because the corresponding field-theoretic model is similar to the well-known Reggeon field theory [1]. This model describes the spreading of an agent in a reaction-diffusion system and belongs to the universality class of the directed bond percolation process. Turbulent mixing is modelled by the stochastic Navier-Stokes equation with random stirring force with the correlator $\propto \delta(t-t')k^{-d-y}$, where k is the wave number, d is the space dimensionality and y – the arbitrary exponent.

In the work it is shown that, depending on the relation between y and d, the system exhibits various types of large-scale asymptotic behaviour, associated with possible infrared attractive fixed points of the RG equation. In addition to known asymptotic regimes (ordinary diffusion – Gaussian free theory, ordinary directed percolation process and passively advected scalar field without self-interaction) existence of a new strongly non-equilibrium universality class is established, and the corresponding domains of stability in the $y–d$ plane and the critical dimensions are calculated to the first order of the double expansion in y and $\varepsilon=4-d$ (one-loop approximation). It turns out, however, that the most realistic values $y=4$ (Kolmogorov's fully developed turbulence) and $d=2$ or 3 correspond to the case of a passive scalar field, when the non-linearity of the Gribov process is irrelevant in the sense of Wilson and the spreading of the agent is completely determined by the turbulent transfer.

It is also found out that our one-loop results for the critical exponents and the domains of stability of the scaling regimes coincide with the ones, derived earlier in [2] for a simpler model. That model involves the same Reggeon field, while the turbulent mixing is modeled by the Obukhov-Kraichnan (OK) rapid-change ensemble: Gaussian statistics with zero mean and the correlation function $\propto \delta(t-t')k^{-d-y/3}$. Such coincidence of the results allows us to conclude that the OK ensemble, in spite of its relative simplicity, may serve as an acceptable model of turbulent mixing.

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Direct photon production in hadronic collisions beyond the leading order

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Direct photons are the photons produced in particle collisions which are not decay products of any known resonances. The cross section of the production of high-transverse-momentum (high-p_T) direct photons can in principle be calculated within the parton model framework using perturbative QCD which is guaranteed by the factorization theorems [1].

There are only two leading order (LO) subprocesses: "$q\ g \to \gamma\ q$" and "$q\ qbar \to \gamma\ g$", where q means any quark or antiquark, *qbar* means the antiquark of q, g is a gluon and γ is a direct photon. The next-to-leading order (NLO) also contains another subprocess, "$g\ g \to \gamma\ q\ qbar$", which is significant for low-p_T direct photon cross section due to dominating gluon distribution functions in the low-x region.

NLO radiative corrections to the LO processes include loop diagrams and tree 2 $\to$ 3 diagrams: "$q\ g \to \gamma\ q\ g$" and "$q\ qbar \to \gamma\ g\ g$". The loops, apart from the usual ultraviolet divergences treated by renormalization, contain infrared and collinear divergences because of the massless virtual gluon coupling to the massless real gluon. When the hard scattering cross section is calculated, infrared divergences are to be canceled with the corresponding infrared divergences of tree diagrams. Collinear divergences must be eliminated in view of the factorization framework of the parton model within the same subtraction scheme which is used to define parton distribution and fragmentation functions.

Therefore, careful treatment of the aforementioned divergences is needed to produce a complete NLO calculation. The main topic of this paper is the treatment of infrared and collinear divergences using the regularization scheme in which both real and virtual gluons are provided with nonzero masses. Numerical results of the tree-level calculations for two LO processes ("$q\ g \to \gamma\ q$" and "$q\ qbar \to \gamma\ g$") and one NLO process ("$g\ g \to \gamma\ q\ qbar$") and comparison with the Fermilab D0 experimental data [2] are also presented.

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About asymptotical behavior of Yang-Mills field

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In our work we study solution of the Dyson equation $D^{-1} = D_0^{-1} - \Sigma$ for Yang-Mills field B_μ with the action:

$$S=-1/4\, F_{\mu\nu}F^{\mu\nu},\ F_{\mu\nu}=\partial_\mu B_\nu-\partial_\nu B_\mu+ie[B_\mu, B_\nu].$$

For investigation of the asymptotical behavior of Yang-Mills field Green functions we introduce auxiliary antisymmetric tensor field $T_{\mu\nu}$ and ghosts ψ^+,ψ for gauge fixing. This results in the action

$$S= \psi^+\partial^\mu[B_\mu\ ,\ \psi]+1/2\ T_{\mu\nu}[B^\mu\ ,B^\nu]\ [3].$$

We analyze the asymptotic of propagators by means of self-consistent Dyson equation $D^{-1} = -\Sigma$. We look for a solution in the form of power (scaling):

$$G(x) = A/x^{2a}\ [1].$$

Calculations show that in space dimensions D=2, 4, 6, … scaling form is broken and asymptotic of propagator has the form:

$$G(x) = \frac{A}{x^{2a}(\ln x^2)^\alpha}$$

(considered in [2]).

We have shown that the scaling in a critical point can be broken, this results in arising of the logarithmic factors in asymptotic of Green functions.

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Influence of Quantum Noise on an Ensemble of Trapped Interacting Bose Particles

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The problem of quantum-limited control of single particles as well as trapped gases is currently one of the most attractive for both experimentalists and theoreticians. The influence of the quantum measurement on a state of an ensemble of ultra-cold atoms is of our private interest. Continuous center-of-mass position measurements performed on an interacting harmonically trapped Bose-gas are considered. The evolution of the quantum state of this gas is governed by the master equation that can be analytically solved in the absence of interaction. However, in the case of interacting particles we reformulate the dynamics in terms of stochastic differential equations to treat the problem numerically. Such equations are solved with Monte-Carlo algorithm [1].

Using both semi-analytical mean-field approach and completely quantum numerical technique, it is demonstrated that the atomic delocalization due to the measurement back action is smaller for a strongly interacting gas. The numerically calculated second-order correlation functions demonstrate appearance of atomic bunching as a result of the center-of-mass measurement. Though being rather small the bunching is present also for strongly interacting gas which is contrast with the case of unperturbed gas. The performed analysis allows to speculate that for relatively strong interactions the size of atomic bunches can become smaller than the initial cloud size resulting in a sort of squeezing effect.

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Two-center nature of H_2: electron interference in (e, 2e) ionization process

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There has been considerable interest recently in the possibility of observing quantum mechanical interference effects in the case of ionization of diatomic molecules. This interference is similar to a Young's double slit experiment and can be considered as a "Young-type" interference where the two slits are the two atomic centers in the molecular target. These two scattering centers act as localized sources of coherent electron emission during ionizing collision. These interference effects can be seen in the oscillatory structure of the ionization differential cross section that is a function of the emitted electron angle.

It was theoretically predicted [1] that the triple differential cross section (TDCS) for molecular hydrogen can be directly compared with the TDCS of two separate hydrogen atoms multiplied by interference factor. Most of the work has concentrated on comparison between the cross sections for diatomic molecules and comparable atoms (see, for example, [2, 4-7]). Evidence of two-center effects has already been observed in (e, 2e) ionization measurements [3-7]. There are contrasted conclusions about this type of interference.

H_2 is the simplest neutral molecule and it is an advantage of studying it. Theoretical description of H_2 ionization requires minimum approximations and the resulting cross section can be derived even in analytical form. Analytical approximation considering the two-center structure of the molecule is used to investigate these interference effects.

One of the aims of this work was to explore such a fundamental phenomenon.

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Mechanical unfolding of homopolymer globule by applied force

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In the past decade, experimental techniques allowing mechanical manipulation on single macromolecules, such as atomic force microscope (AFM) or optical and magnetic tweezers has appeared. In particular, these approaches allow one to study mechanical properties of single macromolecules. Proper interpretation of numerous experimental data requires a development of the corresponding theory of deformation of single macromolecules.

In present work, the theory of unfolding of a homopolymer globule by applied force is developed. Assuming that a deformed globule may exist in one of three states [1, 2] namely (i) weakly deformed prolate globule, (ii) stretched "open" chain and (iii) microphase-segregated "tadpole", Gibbs free energies were calculated for the each of the three possible states. The comparison of the free energies demonstrates that the "tadpole" state is unstable. It means that in the framework of the mean-field theory, the globule unfolding occurs in the following way: at small applied force the globule acquires a weakly prolate shape, then, when the force reaches some critical value the globule abruptly unfolds as a whole. The value of the critical force as well as the end-to-end distance of in transition point increase with the deterioration of solvent quality and/or with an increase in the chain length [3].

On other hand, it is possible to take into account the effect of the fluctuations if the intermediate "tadpole" states are considered with the corresponding statistical weights. It is demonstrated that fluctuations wash out the (jumpwise) transition from globular to "open chain" state.

Force dependences of the Gibbs free energy and average distance between chain ends can also be extracted from the data on globule unfolding by applied deformation (in the conjugate *D*-ensemble) obtained earlier using self-consistent field method [1]. Comparison of deformation curves for three different approaches shows very good quantitative agreement.

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The perturbation theory for the set of self-similar asymptotics in diffusion-controlled Ostwald ripening

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Since the set of self-similar asymptotics in addition to Lifshitz-Slyozov's [1] and Wagner's [2] ones were found computationally and analytically [3] in the theory of Ostwald ripening, the problem of time corrections to these asymptotics raised and to this day it wasn't resolved properly and completely.

Considering the perturbation theory for the complete system of equations for the diffusion-controlled Ostwald ripening, we got first-order power corrections to the concentration of metastable phase, to the critical radius of drops and we found explicit form of self-similar correcting distribution functions that have power decay to their asymptotics. Their normalization and scaling, which depends on experimental parameters, were obtained computationally. Limiting Lifshitz-Slyozov's case was represented individually and it got formal similarities with the work [4].

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H. Biophysics

Dielectric birefringence of PBIC in different solutions

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Electric birefringence (EBF) is a subject of both experimental, and theoretical researches. The phenomenon of EBF lies in the base of the method of studying conformational, electrooptical and kinetic properties of polymeric molecules in solutions. Essential progress in the development of high-sensitivity methods of measurement of small anisotropies in a combination to the variation of the form of external electric field (constant, rectangle-pulse, sinusoidal-pulse, etc.) has allowed to investigate a wide range of synthetic and natural polymers. The development of science also let to receive the extensive information on mobility, the sizes, the form, and parameters of electric structure and times of a relaxation of macromolecules.

The purpose of the work was in studying of influence of dielectric permeability of solvent on EBF of rigidly-chain polymer in a solution. The solution of no fractioned *poly*(n-*butyl isocyanate*)**,** shortly PBIC, was object of studying. This sample of PBIC was stored 32 years in benzene. EBF and dynamic double refraction of the fractions received from this sample have been investigated earlier in solutions in carbon tetrachloride[1].

The whole spectrum of various researches has been made in the given work. The value of specific Kerr constant of investigated sample of PBIC was defined; it matched the results obtained earlier by the order of value in the solutions of PBIC in carbon tetrachloride. It was necessary to check up, as PBIC for 32 years could deteriorate, but fears have not proved to be true. Specific EBF of polymer has found out the tendency to saturation at increase in intensity of a field. An establishment of the equilibrium EBF has been defined from the received data time. Experimental dependences of the specific EBF of PBIC in benzene have been approximated theoretical by the dependence of Langevine-Born for polar molecules. The received results have allowed to define the average value of the dipole macromolecule moment. Specific EBF of PBIC has appeared less in 2 times in the mixed solvent, than in benzene. It is possible to assume that the given effect can be connected with increase in dielectric permeability of solvent, but only further researches can put a definitive point.

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Investigation of Radiation-Induced Damages in DNA Structure in Different Ionic Surroundings by Spectral Methods

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It is well known that ionizing radiation causes destruction and modification of nitrogenous bases in DNA molecule. It also causes partial denaturation of DNA molecule (local breakages of hydrogen bonds) [1]. To evaluate the amount of these damages we applied UV absorption spectroscopy and circular dichroism (CD). Radiation-induced changes in DNA structure influence its UV absorption spectrum in different ways: partial denaturation causes hyperchromic effect while destruction of the bases causes decreasing of absorption. At the same time both of them result in the same changes in DNA CD spectra: the decrease in its intensity.

We studied the influence of DNA ionic surroundings on the radiation effect. We attempted to segregate the described damages in DNA structure making hydrolysis and thereby destroying DNA secondary structure. So we can exclude influence of partial denaturation on UV adsorption spectra and try to evaluate the amount of damaged nitrogenous bases in DNA molecule.

We investigated spectral parameters of DNA molecule gamma-irradiated by the dose of 0 –1000 Gy in solutions with different cations: Na^+, K^+, Mg^{2+}.

High doses (300 – 1000 Gy) cause changes in DNA absorption spectra: decrease of intensity in maximum (260 nm), increase of intensity in minimum (230 nm) and little shift to long-wave region. Intensity of CD spectra decreases with increasing of radiation dose. Also with increasing of radiation dose concentration of nitrogenous bases in DNA molecule decreases and molar extinction coefficient $\varepsilon_{260}(P)$ increases. These changes occur in presence of monovalent and divalent ions in solution.

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The primary component analysis of the reactions of dichlordiammineplatinum(II)

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Platinum based coordination compounds are considered some of the most effective anti-tumor drugs. One of the most effective compounds in this group is cisplatin (*cis*-diamminedichloroplatinum(II) or CDDP). It is used in treatment of several types of tumors, yet its detailed mechanism of action remains unknown [1].

In vivo, CDDP forms DNA crosslinks, causing apoptosis (cell death). It is probable that the mechanism of interaction between CDDP and DNA is depended to some extend on the interactions with nuclear proteins. HMGB-domain proteins possess the ability to bind to distorted DNA structures, including cisplatin-DNA crosslinks. HMGB1 is a protein found in the cell nucleolus, it plays an important role in DNA packaging. It has been shown that HMGB1 has an affinity for cisplatin-DNA adducts [2]. Also, this protein possesses an ability to interact with the DDP molecule itself.

The goal of present research is to find out how HMGB protein affects DDP - DNA interactions *in vitro*. Using electrophoresis, UV-spectroscopy and kinetic studies, DNA-DDP and HMGB-DDP systems were investigated. Principle component analysis was applied to the spectroscopic data obtained in kinetic experiments. The kinetic parameters for the reactions with DDP were obtained at 37˚C in presence of 15 mM NaCl.

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Temperature behavior polarized and depolarized components of light scattering in liquid water

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We investigate temperature dependence of Rayleigh scattering in pure water cleared by vacuum distillation.

In the experiment standard scheme of scattering by 90 degrees is realized. We used 40 mW He-Ne laser with λ=633 nm. Chosen temperature range (17-44°C) was gone towards raising the temperature and back. Every temperature point was held not less than 24 hours.

Water has many unusual properties such as compressibility, density variation and heat capacity. The origin of these anomalies is the presence of hydrogen bonds. It determines the internal structure of the liquid. Hydrogen bond strength depends on both temperature and pressure. Ralph C. Dougherty and Louis N. Howard offer the "equilibrium structural model [1] of liquid water".

We discuss our result using "equilibrium structure model". This model describes liquid water as a random structural network that is held together by hydrogen bonds. Water is represented as an equilibrium mixture of four different competing components: tetrahedral, "planar"-hexagonal, pentagonal and square. At temperature near 307,6 K (minimum in the heat capacity at constant pressure) expected "weak continuous transition" [2].

The dominant geometry in the hydrogen bonded arrays in the liquid undergoes equilibrium shifts with increasing temperature.

Temperature dependences having complex nonmonotonic character were obtained in experiment. Nonlinear dependence polarized and depolarized components – reflect the evidence of cooperative process of rebuilding in the internal structure. The most marked feature manifests in depolarized component of scattering at 39°C. R. C. Dougherty and S. R. Dillon obtained similar result near this temperature. They explained this result as "weak continuous phase transition". There are another features in the graphics. These features wasn't explained in framework model.

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Molecular properties of the polybetaines in water solutions

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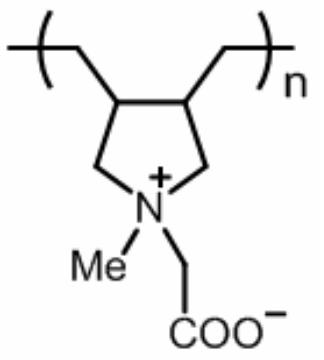

Polyampholytes attract considerable interest therefore they can serve a simplified and synthetically less expensive model of proteins.

Hydrodynamic and conformational properties of poly(diallylmethylammonioacetate) (polyDAMA) in aqueous media were investigated in this work. This polymer consists of pyrrolidinium rings linked by ethylene groups and bearing positive and negative charges. The opposite charges are precisely balanced so that each monomer unit comprises a zwitter-ion.

A raw of samples with different MW was prepared by free radical polymerization in water at 70°C with 4,4'-azobis(4-cyanovaleric acid) as an initiator. The polymers were characterized by NMR, viscosimetry, SLS and DLS.

Intrinsic viscosities [η] and translational diffusion coefficients D_t of polyDAMA samples have been measured. MWs and degrees of polymerization (DP) were calculated from these values. Estimation of persistence length (Kuhn length) was done. Hydrodynamic radii of molecules were calculated using Stocks-Einstein equation in solutions with different pH and ionic strength.

Mark-Kuhn's equation $D=KM^{-\alpha}$ for polybetaines in different solutions were received. It was found that hydrodynamic and conformational characteristics of polybetaines depend on pH and ionic strength of the solvent. The observation was attributed to anti-polyelectrolyte effect that caused by the screening of electrostatic interaction between zwitterionic groups in macromolecules.

Molecular properties of conjugates formed by Poly(ethylene glycol) and sterically hindered phenols in solutions

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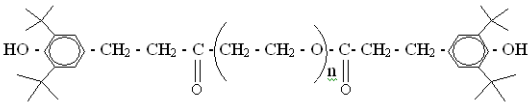
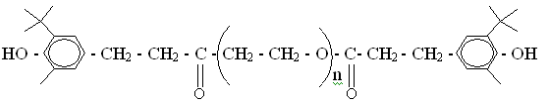
An important direction in the design of modern drugs with programmable properties is the incorporation of biologically active compounds (BACs) into macromolecules of various chemical structures and characteristics. High solubility and prolonged action of preparations, an increased stability of BACs, and their low toxicity level determine prospects of their practical application. At present, this fruitful approach has found wide use in medicine for obtaining implants, suture materials, and new drugs based on polymers.

Water_soluble conjugates are prepared via the chemical modification of poly(ethylene glycol) by antioxidants taken from the family of sterically hindered phenols. The chemical structures of PEG-based conjugates are presented in the following scheme:

PEG-KF1
MM: 3400, 3900, 6800, 21600



PEG-KF2
MM: 6800, 21600



Poly(ethylene glycol) molecules carrying end groups of sterically hindered phenols form micellar aggregates that are absent in the solution of the initial polymer. The dimensions of molecules and their aggregates are studied by viscometry and light scattering in dilute solutions. The mean number of molecules involved in such an aggregate is 83. It is found that the presence of hydrophobic end groups in poly(ethylene glycol) molecules causes a sharp reduction in the lower critical solution temperature of a solution relative to that of the initial polymer [1].

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DNA complexes with light-sensitive surfactants

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For performing gene therapy it is of crucial importance to compact DNA molecules to sizes necessary for entering into cells. Different vectors such as viral and non-viral have been developed for the cellular uptake. In case of viral vector approach immunological risks is the main trouble, that strongly motivates to use non-viral agents for DNA compaction. Many compounds such as multivalent ions, cationic polymers, some lipids and surfactants can induce DNA packing in a solution. One of the perspective way is to use the compacting agents for the formation of gene vectors. The previous scientific work was dedicated to the formation and investigation of gene vectors based on DNA-polycationic complexes. The involving of light-sensitive surfactants into the rank of potential agents for the creation of different DNA nanostructures can open new possibilities for their utilization not only for medical and pharmaceutical aims, but also for other nanotechnological applications. The distinguishing feature of light-sensitive surfactants is their reversible conformational changes. For example, more hydrophilic *cis*- isomer of azobenzene group in surfactant appears during the irradiation of solution with UV light. The visible light induces its transformation into more hydrophobic *trans*- conformation. The same transition is observed as a result of the relaxation in darkness [1]. The reversible transition of DNA in solution between compact and swollen coil states can be induced by surfactant binding and switching the azobenzene group between *cis*- and *trans*- forms. The treatment with light seems to be promising and the development of photo-reversible DNA complexes could greatly modify the gene vector properties.

Experimental data were partly obtained during the internship at the University of Potsdam.

DNA size, state and stability of its secondary structure during interaction with compounds under the study were characterized by the methods of spectrophotometry and low gradient viscometry.

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Molecular properties of water soluble derivative of chitosan

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Chitosan is cationic polysaccharide widely spread in the nature. The spectrum of biological activity of chitosan, its biocompatibility and biodegradation ability causes application of this biopolymer in medicine and pharmacology. However, the practical usage of chitosan is strongly limited due to its poor solubility in aqueous media at physiological pH values and ionic forces range. Additionally, chitosan is insoluble in the majority of organic solvents. That is why the development of chemical modification methods leading to derivatization of chitosan and improving its solubility, is an actual task.

A present contribution is devoted to study of molecular properties of a novel chemically modified chitosan (*mCH*). Homologues series of *mCH* composed of the samples with the different degree of polymerization, have been investigated in 0.33 CH_3COOH+0.2M $NaCOCH_3$ and in H_2O+0.2M NaCl as the solvents. These conditions correspond to full suppression of polyelectrolyte properties of chitosan. Viscometry, static and dynamic light scattering have been used as the main experimental methods of the study. The absolute values of molecular mass, intrinsic viscosities [η], translation diffusion coefficients D_0, and the average hydrodynamic radii R_h of macromolecules have been determined. The scaling Mark-Kuhn-Hauvink-Sacurada relations between the hydrodynamic characteristics and molecular mass for the homologues series of chitosan samples have been received. A comparative analysis of molecular and conformational properties of *mCH* and non-modified chitosan, investigated earlier [1], have been done.

The obtained data has a great importance for the development of the based on *mCH* systems for drag and genetic material delivery to the cells of vivid organisms.

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Interaction of DNA with the benzoimidaftalozin derivatives

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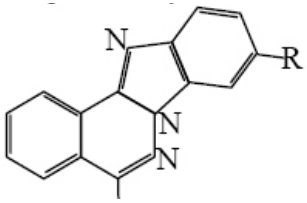
In this work we have studied the DNA interaction with benzoimidaftalozin derivatives having different substitutes in 10th position: piperazine (I), morpholine (II), pyrrolidine (III), piperidine (IV) by the methods of spectrophotometry, circular dichroism (CD) and viscometry.



I R= – N⬡NH
II R= – N⬡O
III R= –N⬡
IV R= –N⬡

These compounds can be classified as alkaloids. A large number of alkaloids reveal different kinds of biological activity, including the anti-tumor one, explaining thus the interest to the ability of these compounds to get bound to the DNA molecule.

During the spectrophotometric titration of I-III compounds it was found that a strong bathochromic shift is observed with the increase of DNA concentration, while the compound (IV) causes a hypsochromic effect. The compounds I-III possess the induced CD at the DNA presence. The changes in electron absorption spectra and the appearance of induced circular dichroism in the presence of DNA are the evidence of formation of complexes of these compounds with DNA.

According to the results of spectrophotometric titration of the compounds were determined the thermodynamic binding parameters (binding constant, the number of binding sites).

Induced CD of I-III compounds have a small intensity and a negative sign, which can indicate the intercalation of planar chromophore of the compounds in the DNA double helix. To determine the way the compounds bind with DNA, was carried out determining of the characteristic viscosity of the complexes. According to the results of viscometric studies the models of binding was proposed.

The results of research have shown that the nature of substitutes in the 10th position influences the way of binding benzoimidaphtalosine derivatives with DNA.

Hydrodynamic properties of interpolyelectrolyte complexes in chloroform

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The aim of this work is to investigate the process of interpolyelectrolyte complexes (IPEC) formation in the result of reaction between two polyelectrolyte complexes (PEC) in the low-polarity organic solvent chloroform. There have been spent measurements of dynamic and static light scattering in solutions of initial components and their mixes of various composition to find the decision of the problems put in work. In this work have been investigated samples of polyelectrolyte complexes formed by poly(N-ethyl-4-vinylpyridinium) cations with dodecyl sulfate anions (PEVP-DDS) and polyacrylate anions with cetyl **-3-**methylammonium cations (PA-CTMA).

It was found that in PEVP-DDS and PA-CTMA mixes in chloroform there is a phase separation. The phase, containing both polymeric components is formed. It was established that the order of component mixture influences on phase behavior of a mix. At addition to a solution of the PA-CTMA solution of PEVP-DDS sharp increase of intensity of light scattering is observed up to value of the charging relation m +/n - = 0.6. It was established that for other order of component mixing the intensity of light scattering monotonously increases right up charging relation = 1. The mechanism of IPEC formation can be connected with ion-exchanging process. It was established that the sizes of IPEC particles depend on the charging relation. Analysis of the hydrodynamic sizes of the particles shows that individual IPEC form micelles. The hydrodynamic radius R_h of micelles containing about 100 individual IPEC was calculated in the frame work of spherical micelles model. It was established that theoretical experimental values of R_h coincide in the limit of experimental error.

Light scattering in solutions of the complexes formed by water soluble dendrimer and polyanion

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Now the significant attention is given studying of structure and properties of interpolyelectrolyte complexes (IPEC) formed by ionogenic dendimers and oppositely charged linear polyelectrolytes, and biopolymers. There are a number of studies in which linear polyelectrolytes or DNA interacts with dendrimers containing charged ending groups. It was found that stoichiometric and nonstoichiometric IPEC in solution of oppositely charged polyelectrolytes and dendrimers are formed. At the same time, the influence of the chemical structure of polyelectrolytes and dendrimers on morphology and sizes of IPEC particles is one of the important problems of the polymer physics.

In present work static and dynamic light scattering were used as methods to study the interaction between dendrimer containing charged groups on the surface and in the volume of the molecules with low – molecular surfactant as well as with oppositely charged sulfonated polystyrene (PSS) in water solution. Hydrodynamic radii of dendrimer and PSS molecules were determined in water solutions also.

It was found that interaction of 4 number of generation dendrimer with oppositely charged surfactant anion leads to formation of polyelectrolyte complexes and phase separation in solution.

Interaction of dendrimer with PSS in water solution was studied for different charging relations X. It was established, that in a wide range of X values formation of IPEC complexes takes place. Hydrodynamic radii of these complexes were determined for different X.

The micelles formed by IPEC in water solution were found. It was shown that the core of these micelles is formed by hydrophobic block of IPEC containing PSS tails combined with dendrimer. The shell of these particles, which stabilized micelles in water solutions, contain the part of PSS chains which does not interact with dendrimer molecules.

Electrooptical and conformation properties “cross-linked” polymerized micelles

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Polymerized surfactants now cause a great interest from the point of view of high potential of their practical application. In the given work as the sample used “cross-linked” comb-like polymer: poly(N-akriloil-11-aminoundekanovoj acids) (s-PAAU). S-PAAU received at polymerisation in micellar a condition of the surfactant bearing double communications in waterproof “tail” between which it was spent «cross-link». The particular interest was represented by comparison of the “cross-linked” and “embroidered” polymers, and also influence of alkali on given samples. «Embroidered» it was spent by hydrolysis (processing NaOH). As solvent the mix of cyclohexanol and dioxane with volumetric value 1:1 was used. Detailed researches of the received polymer by methods of viscometery, dynamic light scattering, flow birefringence, equilibrium and non-equilibrium electric birefringence are executed.

Processing NaOH has led to deterioration of thermodynamic quality of solvent (reduction of the hydrodynamic sizes of balls and great values of a constant of Hagginsa K_η), but has not caused “degradation” of a polymeric chain.

The negative sign on a constant of Kerra of the studied polymers is caused by negative optical anisotropy of their macromolecules (the sign of Maksvell effect of the studied polymers is negative).

By results of dynamic light scattering it is revealed that in s-PAAU there are particles of two sizes. Big – are caused «cross-link» between several macromolecules that is reflected in values of characteristic viscosity. Particles of the smaller sizes correspond «cross-link» in one polymeric chain, and their size has appeared in 1,5 times less, than at the “embroidered” sample.

The mass fraction of the big particles makes an order of 10-20 % (according to dynamic light scattering) and they corresponding “intermolecular cross-link” between 5-10 macromolecules.

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Hydrodynamic properties of lithium-containing sulfonated polystyrenes

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By viscometry, isothermal diffusion and dynamic light scattering study sample of two lithium sulfonated polystyrenes (PSLi) with molecular weight 5200 and 11,600 (Mw / Mn = 1.04) in low-polarity solvents. According to the isothermal diffusion, the size of molecules PSLi in benzene in the low concentrations behave as aggregates, whose sizes are close to the size of PS with a molecular weight of an order of magnitude greater. In more polar cyclohexanone molecule dimensions PSLi in low concentrations close to the size of a single molecule, and in high concentrations (1-2%) according to dynamic light scattering observed in single molecules and their aggregates, whose sizes two orders of magnitude greater.

Relaxation of electric birefringence in solution of polybutilisocyanate in a strong field

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Electric birefringence (EB) in dilute solution of polybutilisocyanate (PBIC) with molecular weight $M = 770.10^3$ was studied. EB was measured in pulsed electric field, which was applied to the Kerr cell with gap between electrodes 0,017 cm and 3 cm in length along the beam path.

A He-Ne laser was used as light source ($\lambda = 632.8$ nm). The voltages fed to the electrodes did not exceed 3000 V.

The linear dependence of EB Δn on the square of electric field voltage U was obtained only for a low $U < 200$ V. The increasing of electric field voltage U leaded to a strong nonlinear field dependence of Δn.

The EB relaxation time was determined.

The study of biological disperse ambiences with the help of backscattering light

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The investigation of light scattering by particles is the most efficient way for extraction information about different dispersant media (atmosphere, ocean different biological solutions and media). There are different theoretical speculations and approximations determined by the problem`s specific demanding.

Our approach is based on registration of the backscattering light radiation with the use of CCD-matrix and last numerical calculations sequences electromagnetic fields created by disperse media. The special facility for study of natural (biological disperse media) water was build and Mi theory of the scattering of light by "soft" particles was used to explain experimental data.

Our method showed high efficiency in the measurement of scattering and absorbing properties of particles, which provides the possibility of obtaining estimates of integral characteristics of the medium, not a "point" estimates with the size of about 10^{-5} to 10^{-3} cm. Such method of natural disperse media studies is convenient because of its non destruction character and possibility to control simultaneously large amount of disperse media as well.

This method of measurement can be used for rapid optical method for monitoring of natural ecosystems, bulky technical water systems, ets.

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Polystyrene melts: electric birefringence and short order

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Investigation of electric birefringence in isotropic melts of mesogenic substances showed orientational order reduction at temperature increasing in comb-like LC polymers. This leads to formation of phase change isotropic liquid – LC. Free spatial organization of polymer molecules or side-chain groups is the main reason supporting short orientation order. In comb-like LC polymers aliphatic spacer provides moving freedom of side-chain groups. Situation may differ in case of direct connection of side anisometric groups as they are a chain part. For check this out we investigated temperature dependence of electric birefringence in three narrow fractions of polystyrene. Samples with molecular masses MM equal to 500, 2630 and 9100 have been studied in wide temperature range from glass transition up to 200 C^o.

Polystyrene have been studied earlier and its electro-optical properties are well known. It has been showed [1] the Kerr constant does not depend on molecular weight of polymer in a diluted solution but we established another dependence for the Kerr constant in polystyrene melts. For oligomer MM = 500 the Kerr constant does not depend on temperature and is close to constant Kerr value in solution, so that indicates lack of correlation in orientation of benzene rings. The Kerr constant severely increases in polymer melts of samples MM=2630 and MM=9100. As for sample with MM=9100 the Kerr value grows on all temperature range from 110 C^o to 190 C^o. The possible cause of anomalous change of electrooptic properties is creation of polymer coil at transferring from oligomer with small MM to polymer with larger MM and subsequent conformational change of polymer coil at a temperature variation.

Dynamic light scattering method was used to study the behavior of polystyrene (M_η=820000) molecules in cyclohexane at different temperatures. Translation diffusion coefficients of polystyrene molecules for a number of temperatures were determined by linear extrapolation of corresponding concentration dependences to infinite dilution. Hydrodynamic radii of the molecules were calculated for different temperatures in according to the Stokes-Einstein relation.

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