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Санкт-Петербургский
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Berlin



German-Russian
Interdisciplinary
Science Center

St. Petersburg – Peterhof
November, 12-16
2012

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Lectures

German-Russian Interdisciplinary Science Center (G-RISC)

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The German-Russian Interdisciplinary Science Center (G-RISC) was founded as a binational platform of scientific research and education with two main offices at Saint-Petersburg State University, Russia and Freie Universität Berlin, Germany.

The Center of Excellence was established in March 2010. It builds on a long-standing tradition of scientific cooperation between scientists of Russia and Germany. G-RISC relies on funding and regulations of the German Academic Exchange Service (DAAD) and the German Federal Foreign Office. The Center supports education and research in binational projects between both countries. Focus is interdisciplinary research in four fields of natural sciences: physics, geophysics, physical chemistry, and mathematics.

G-RISC is operated by two scientific coordinators: Prof. Alexander Shikin (Saint-Petersburg State University) and Prof. Eckart Rühl (Freie Universität Berlin), supported by administrative coordinators and binational Steering Committee.

G-RISC encourages the experienced and novel promising groups to submit their projects. Proposals can be submitted by all research institutions in Russia and Germany and are selected by Steering Committee on the basis of their scientific quality. This type of competition is organized every six months. In January 2013 starts the seventh funding period.

G-RISC funds primarily mobility of young researchers between Russia and Germany. This concerns first of all research stays in laboratories of the partner groups in the other country. For outstandingly bright Russian students who are involved in interdisciplinary research projects with German partner groups it is also possible to receive a sur-place stipend for up to six months. It is anticipated that research stays and stipends are strengthening stable long-term collaborations between Russian and German researchers. Each single project is important to tie researchers and research interests together and to develop novel, interdisciplinary projects between Russia and Germany.

In total, more than 50 institutions and more than 200 young and experienced researchers from Russia and Germany conduct research and teach at the Center. Since the opening of G-RISC seven interdisciplinary workshops/conferences with over 540 participants have been held:

- “Structure and Dynamics of Matter” (Berlin, Germany, 2010)
- “Science and Progress” (St. Petersburg, Russia, 2010 and 2011)
- “Nanoscale Atomic and Electronic Structure of Materials” (Rostov-on-Don, Russia, 2010)
- “Spatio-temporal dynamical systems” (Moscow, Russia, 2011)
- “Hydrogen Bonds between the Disciplines” (Göttingen, Germany, 2011)
- “Fundamentals and Applications of Nanoscience” (Berlin, Germany, 2012)

Detailed information about the funded projects and the Center of Excellence can be found at the G-RISC website: <http://www.g-risc.org>.

Fullerenes Interaction with Si Reconstructed Surfaces

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Since the discovery of spherical C_{60} molecules, fullerenes, in 1985, the fullerene-based materials have attracted growing interest because of their very rich electronic properties. For this reason, nucleation, growth and structure of fullerene layers on various surfaces have drawn significant attention. It has been found that mechanisms involved in the formation of fullerene arrays on solids might be quite complex due to the interplay between intermolecular bonds and molecule-substrate interactions. In particular, there is a drastic difference in fullerene adsorption behavior on metal and semiconductor surfaces. The latter can even result in restructuring of the substrate surface structure.

In the present work we will discuss our recent results on the study of C_{60} interaction with adsorbate-induced reconstructions on silicon surface using STM and first-principal calculations.

Two-dimensional C_{60} island coarsening onto the $Si(111)\sqrt{3}\times\sqrt{3}-(Au,In)$ domain-wall-free $Si(111)$ surface demonstrates a giant island-size selectivity effect. As a result of the RT coarsening only 2D C_{60} closed-packed hexagonal islands which have 37 fullerenes are survived. Possible mechanism of such a behavior will be discussed.

We have found an unusual mutual interaction between adsorbing C_{60} and structural defects of the $Si(111)\sqrt{3}\times\sqrt{3}-In$ surface. It has been found that, on the one hand, substitutional Si-defects trap the adsorbed C_{60} molecules, which prefer to reside atop the In atoms neighboring the Si-defects. On the other hand, a group of a few fullerenes act as a trap for a „mobile“ vacancy.

C_{60} molecules form well-ordered closed-packed hexagonal arrays on the $Si(111)\sqrt{3}\times\sqrt{3}-Ag$ surface. These arrays contain a number of fullerenes which look dim with respect to the others. STM observation indicated that these dim fullerenes are mobile. They appear and disappear randomly at RT and this effect is frozen at about 100 K. One of the possible explanations of the C_{60} molecules dynamic could be related with the behavior of Ag atoms loosely linked in a trimer arrangement in the $Si(111)\sqrt{3}\times\sqrt{3}-Ag$ surface.

A bright view through a keyhole: NMR study of the structural and chemical properties of highly ordered nanoporous materials

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They are mechanically and chemically stable; they combine the traits of tunable pore size and shape with a large internal surface area; their surfaces are suitable for a selective anchoring of catalytically active functional groups. Mesoporous silica materials constitute a two-dimensionally ordered array of pores of uniform size disposed parallel to each other and separated by thin walls, as depicted schematically in the cartoon. The pore diameter is adjustable between 2 and 20 nm and the inner surface area of the pores is of the order of 1000 m²/g. These periodic materials open up intriguing new application possibilities in catalysis, drug delivery, size selective molecular separation, and are interesting as models for understanding self-organizing systems.

This presentation describes the application of NMR spectroscopy for the study of the structure and chemical properties of these materials at the molecular level. Special attention has been paid to the effect of surface functionalization. Besides a detailed characterization of different mesoporous silica materials, the one of the main results of these studies is the elaboration of a research strategy that is based on a set of simple and robust NMR measurements. This strategy is designed to deliver a general approach that will enable the study at the molecular level the structural and chemical properties of other application relevant, surface-rich amorphous materials.

We gratefully thank the German-Russian Interdisciplinary Science Center (G-RISC) funded by the German Federal Foreign Office via the German Academic Exchange Service (DAAD) and the Russian Foundation of Basic Research (11-03-00346) for the financial support of this studies.

Details of the used experimental approach and the obtained results are reported in:

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A. Chemistry

Influence of salts of biologically active metals on the gelation of aqueous cysteine-silver solution

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Was recently opened ability of L-cysteine and silver nitrate to form a dilute thixotropic hydrogels. Found that the gel in the L-cysteine-system can be triggered by various electrolytes (salts). Interesting to study the properties of the resulting new system – “cysteine-silver solution” (CSS). And the purpose of the work was to study the effect of metal salts on the process of gelation. In this regard, it was interesting solution of particular problems: 1. Finding the minimum concentration limit at which the possible process of gelation, 2. Establishment types of electrolytes, which can be formed with the most durable hydrogel, 3. Definition of influence of diluting and temperature on the maturation process of the solution.

Process of maturation is connected with formation of CSS oligomeric chains. After that into CSS was introduced a certain quantity of electrolytes (chlorides, sulfates and nitrates Na^+ , K^+ , NH_4^+ , Co^{+2} , Ni^{+2} , Al^{+3} , Mg^{+2} , Mn^{+2} , Zn^{+2} , Cu^{+2}), which led to formation spatial gel network of various kinds. A clear proof of this is the data obtained by transmission electron microscopy. By consideration of microphotographs of gels it is clearly visible, as from each other spatial grids of gels strongly differ. This is also confirmed by the data obtained from the study of particle size by dynamic light scattering.

CSS was prepared by mixing aqueous solutions of a given concentration of the initial components at a certain ratio. For this research the initial solution was subjected to diluting of many times for definition of the bottom concentration limit of the process of maturations. By UV spectroscopy studies were carried out: 1. maturation process CSS (establishment of concentration and temperature dependence); 2. the process of gelation CSS with metal salts.

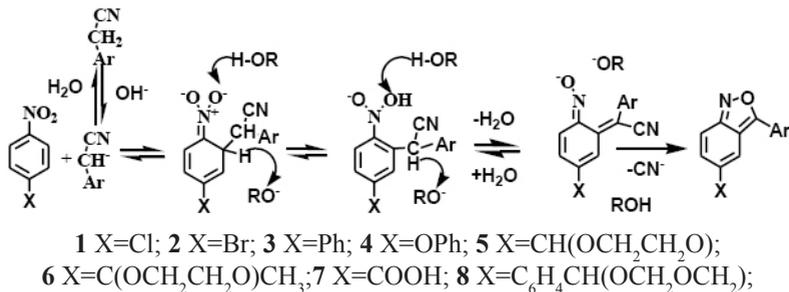
Thus, as a result of work install that CSS can be diluted in several times. Further it can form a basis for receiving medicines of new generation. Maturation process dependent on the temperature at its increase from 15 to 40°C speed of maturation of CSS considerably increases. Established that at introduction as electrolytes of sulfates and chlorides of various metals, it is possible to obtain a hydrogel, unlike nitrate, where the gel at any concentration could not be obtained. As a result, it is proved that the hydrogel can not be obtained with an excess of NO_3^- - anion, therefore for a gelation additional introduction of a cation and anion is necessary for other salt. By adjusting the concentration of the electrolyte, we can get a more durable gel with preset properties.

The 2,1-benzisoxasoles formation process modeling with consideration of various solvents, and substitutes in substratum structure

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Reactions of aromatic nucleophilic hydrogen substitution (S_NAr^H) is one of perspective methods for nitroaromatic compounds functionalization. The arylacetonitriles with nitroarenes interaction processes is one of the examples of nucleophilic hydrogen substitution reaction. The final product of such type reactions is 2,1-benzisoxazole.



In this work, the quantum-chemical modeling was carried out, for cyclization stage (2,1-benzisoxazolic cycle formation process) of arylacetonitriles with nitroarenes interaction. The modeling was performed for various *para*-substituted nitrobenzenes **1-8**, and for various solvents with *para*-substituted nitrochlorinebenzene **1**. Such solvents as methanol, ethanol, propanol, *iso*-propanol, butanol was used during calculation.

As the modeling result, the linear correlation dependence between calculated quantum-chemical parameters –activation energies of cyclization stage E_{act} , and experimental values of effective process rate constants k_{ef} , was obtained. It was shown, that correlation coefficient is 0,992 for various *para*-substituted nitrobenzenes modeling, and correlation coefficient is 0,735 for various solvents calculation.

The analysis of obtained results allows to make a definition, that 2,1-benzisoxasolic cycle formation stage for arylacetonitriles with nitroarenes interaction process is limiting stage, and this stage defines the specific characteristics of investigated process. Also, it is established, that solvents as *iso*-propanol and butanol are more effective, than the solvents with smaller molecular mass (ethanol or methanol).

Study on the effect of sampling and sample preparation on results of trace element content in saliva

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During last years saliva has become a promising subject for biological research because biochemical parameters of saliva reflect the state of the organism as a whole. Oral fluid has many advantages over traditional objects - blood and urine. For example, sampling is non-invasive and safe for a patient and an operator, it's also easy to implement. Moreover saliva can be taken in large amount for the analysis, so it makes possibility to perform continuous monitoring [1].

Determination of trace elements in the saliva has been used in various branches of science including medicine and ecology. In particular it was found [2] that the concentrations of manganese and copper were significantly higher in the saliva of welders than in the control group, also a correlation between the content of these elements in the saliva and one in serum was detected.

Besides several diseases and environmental pollution the composition of saliva depends on circadian rhythm, diet, oral hygiene, hormonal status [3]. Moreover sampling and preparation of samples have significant impact on the results of the analysis when determining the various organic components [1]. But there is no information in scientific papers about influence of these factors on the content of trace elements in the saliva.

The aim of this study was to identify and evaluate the influence of various parameters of sampling (stimulation of salivation, circadian rhythm, duration of period after eating, the rate and frequency of sampling) which can change the content of trace elements in samples of saliva. Method of atomic emission digital spectrographic analysis of biological fluids which previously had been developed in our laboratory was used to determine the concentrations of trace elements [4]. Also the report presents recommendations for the saliva sampling procedure based on our results.

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Nuclear and electronic fluxes during vibrations of single, double and triple bonds of H_nXYH_n ($X = C, Si, Ge; Y = C, Si, n = 1, 2, 3$) molecules

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All chemical reactions involve rearrangements of the nuclei and electrons as the molecular system changes from reactants to products. Our theoretical investigations concern the correlated dynamics of nuclei and electrons during chemical reactions and vibrations with sub femto second resolution, as the dynamics of such processes happen on the time scale of several femto seconds. We are motivated by the recent development of experimental ultra short pulse techniques to observe electron dynamics up to the atto second time scale.

Albeit not a chemical reaction but the most basic example of nuclear rearrangements are vibrations. Here we focus on quantum dynamic simulations of coherent model vibrations of single, double and triple bonds of type H_nXYH_n ($X = C, Si, Ge; Y = C, Si, n = 1, 2, 3$) model systems in the non-degenerate electronic ground state. A combination of the time dependent nuclear wave packets with time independent electronic densities gives an approximation to the time-dependent electronic density of the molecule. To evaluate the dynamics of the electronic and nuclear densities, the corresponding fluxes through hypothetical observer planes within the molecule are calculated. The time integration of the fluxes gives yields, i. e. the number of particles that have flown through the observer planes.

A recent study [1] of ethane, ethene and ethine, showed that more electrons participate in the concerted nuclear-electron vibrations in the case of ethane compared to ethene and ethine. The reason for this was found within the similarity of the reduced electronic densities between the carbon atoms at equal C-C distances in spite of the type of bonding.

Our current research is focused on the case of asymmetric vibrations and electronic densities by exchanging C for Si, and Ge atoms. I will present time dependent nuclear and electronic densities, fluxes and yields for different scenarios of the initial nuclear wave packets, and placements of the observer planes.

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Structural Transformations in Aqueous Solutions of Calcium Perchlorate

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The aim of the study is to determine the structural transformations of the aqueous solution in the concentration range (0.45-4.55 M) and the structure of calcium perchlorate crystalline hydrate, crystallized from the saturated solution.

The structure of the crystalline hydrate of calcium perchlorate, crystallized from the saturated solution, was established by the X-ray single crystal diffraction.

Spectra of solutions in the near and mid-IR regions as well as the ATR-FTIR spectra of solutions, liquid melt and crystalline hydrate were measured. Assignment of bands in the spectra was performed. The shapes of the contours of the observed bands were found to change as the concentration of calcium perchlorate solution grows.

Experimental spectral data matrix $A_{\text{exp}}(N_p, N_w)$, where N_p is the number of experimental points, N_w is the number of spectral channels, was processed by methods of chemometric analysis (principal components and soft modeling). The spectral forms and their abstract diagrams of distribution vs. concentration were obtained.

To attribute the spectral forms, a generalized phenomenological model of aqueous electrolyte solutions structure, data of solubility polyterm, ATR - FTIR spectra of crystalline hydrate, liquid melt and solutions were used.

The first form is pure water, the second form is calcium perchlorate hydrate $\text{Ca}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$. The existence of a third form in solution is explained by the interconversion of the two forms of calcium hydrates, which is due to a change in the neighbours of the calcium cation. That is, the third form is calcium perchlorate hydrate $\text{Ca}(\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$.

Thus, as the salt concentration increases, a change of dominant structures in calcium perchlorate solution takes place according to the branches of crystallization on salt solubility polyterm.

Determination's problem of tryptophane and sulfur-containing amino acids in complex matrices by HPLC

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Analysis of amino acid composition is important in assessing the quality of food, pharmaceuticals drug and biological fluids. There are different methods for determining these analytes, but needed HPLC with spectrophotometric detection.

There are a number of problems at analysis of amino acids: the lack of chromophore groups in the majority molecules, minor concentration of analytes, because additional purification and concentration are required, a particular problem is determination of tryptophan and readily oxidizable sulfur-containing amino acids. There are various ways of solution: a derivatization, using different variants of liquid and solid phase extraction, hydrolysis of the object in different conditions.

In this research the strategy of sample preparation was offered with using liqued extraction by ethyl alcohol for determination of free amino acids and hydrolysis sample by 6 M solution HCl for determination of total analytes.

Phenylisothiocyanate (PITC) was chosen as derivatization reagent.

Conditions of separation for phenylthiocarbamyl (PTC) derivatives were optimized on a model mixture of amino acids by RP-HPLC (gradient mode, $\lambda=254$ nm, $T=55^{\circ}\text{C}$). Calibration independency was built for all amino acids, quantitative analysis in viel was performed, limit of detection was determinate (0,12–1,04 mkg/ml). Determination of tryptophane and sulfur-containing amino acid in this condition was impossible.

Method of HPLC-determination of tryptophane in meat was provided after acid hydrolysis of sample with the addition glycolic acid (gradient mode, $\lambda=278$ nm, $T=35^{\circ}\text{C}$, detection limit - 0,079±0,004 mkg/ml).

Method of determination of total sulfur-containing amino acids in complex matrices on the example of veal was proposed. It includes preliminary oxydation of sample by performic acid, hydrolysis by 6 M solution HCl and derivatization by PITC (gradient mode, $\lambda=254$ nm, $T=35^{\circ}\text{C}$, limits of detection: cysteic acid - (0,18±0,02) mkg/ml, methionine - (0,16±0,02) mkg/ml).

A special series of experiments was devoted to developing a method for determination absorbing in the UV-area of the amino acids (Tyr and Phe) without derivatization. Unfortunately, determination of tyrosine in complex matrices without modifying complicated overlapping chromatographic signal of tryptophan, and concentration of phenylalanine was lower than its limit of detection (detection limit = (19 ± 2) mkg/ml).

Synthesis of B-homo analogues of steroid estrogens

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Estrogens play an important role in many biological processes. Because of the regulatory function estrogens play an important role in cancer development. Up to 95% of human breast cancers, at the origin, are hormone-dependent. By combination of different modifications it is possible to alter biological activity of the estrogen analogue to use it as drug [1]. Most important modifications are to reduce hormonal activity of the analogue, to reduce toxicity of its metabolites and to introduce some new biological activity, e.g. ability to inhibit estrone sulfatase [2].

B-homo analogues of steroid estrogens (Fig. 1) are representing interesting class of estrogens. Conformational mobility of 7-member B ring reduces hormonal activity of these analogues and may prevent formation of cancerogenic metabolites. Further modifications may make them potential anticancer agents.

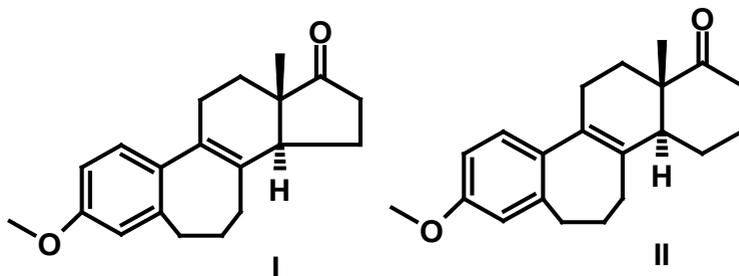


Fig. 1 B-homo analogues of steroid estrogens.

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Dendritic polymers like a modifier of chromatographic systems in the determination of vitamin and amino acids

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Dendrimers and hyperbranched (hb) polymers possess a number of properties, which make them promising candidates for various chromatographic applications: thermal stability, micelle like structure independent on external terms, the formation of inclusion complexes, high density of terminal functional groups and lability to further modification, controlled solubility and polarity.

The purpose of our study was to identify the possibility of using new polymers such as “core-shell”, which consist of functionalized dendritic core (polyethyleneimine) surrounded by maltose shell and rhodamine B [1], like a components of chromatographic systems by examples of separation of hydrophilic and hydrophobic analytes (water-soluble vitamins and amino acids).

The choice of high-performance thin-layer chromatography (HPTLC) method was caused by its advantages: easy replacement of the eluent, rapidity, high efficiency, analysis of both substances at once, etc.

To determine the dependences for “polymer-analyte” interactions we modified mobile (water) and stationary (silica gel) phases by different polymers, such as PEI-Mal 5 and 25 kDa (A, B, C), PEI-Mal Rh 5 and 25 kDa (A, B, C). Also we investigated the influence of pH on the parameters of retention and separation efficiency.

Dendrimers influence to separation of vitamin and amino acid, dependence from pH of medium, structure of polymers and method of modification were established.

The most important results: i) the increasing of retention parameters and efficiency of B12 (alkaline medium), R_f changed from 0,21 (without modified) to 0,68 (with dendrimer structure); ii) the increasing of R_f and efficiency of B2 (efficiency changed from 150 theoretical plates in acidic and alkaline mediums to 25000 ones for distilled water); iii) the increasing of retention parameters for lysine (in acidic medium till $R_f = 0,56$).

Thus, we established, that polymer has significant influence on chromatographic characteristics for water-soluble vitamins and amino acids.

This work was supported financially by grant of Russian foundation for basic research no. 11-03-91331-a.

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Reaction and mass transfer processes and their application in production of biodiesel

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Now the number of cars is almost equal to the number of people in the world. But this is the only one industry, which uses natural resources such as oil and gas. The amount of pollutants which are released into the atmosphere can be called critical. Moreover these sources of energy will run out in the nearest future. Searching for renewable energy sources that do not impact on the environment is one of the biggest challenges for scientists around the world.

Biodiesel is produced with the help of the transesterification reaction of fatty acid and methyl alcohol. Fatty acids contain various vegetable oils. This paper discusses the technology of using rapeseed oil. In the classical processing oil into biodiesel receive a number of additional products (glycerol and potassium sulphate). Such a process can lead to the overproduction of glycerol, and the result is a new type of waste.

There is another method for the synthesis of esters of rapeseed oil. High yield of the final product are obtained by adding of supercritical liquids (ether: ethyl acetate, methyl acetate, etc.) at the temperature of 623.15 K and pressures up to 17.8 MPa, without using of catalysts [1].

This study examines the features of multi-component systems and their application in the production of biodiesel. There are data on the solubility in three-component systems : acetic acid - water - ethyl acetate (313.15 K), ethyl alcohol - water - ethyl acetate (303.15 K and 313.15 K) and liquid-liquid equilibrium of a binary system ethyl acetate - water (313.15 K) is obtained. Literature data of the system ethanol - acetic acid - water - ethyl acetate are presented [2].

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Investigation of copper halides solvation in water – organic mixtures by IR spectroscopy

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The study of solvation processes is one of the main directions in Solution Chemistry for many decades. Despite the long story of its study ion solvation in mixed water - organic solvents still remains unexplored fields of science. At the same time, it is well known that the formation of different solvates influences on rates and mechanisms of reactions, phase equilibrium and so on.

So far the studies in this field were mainly focused on the investigation of the systems without competition between solvent molecules and anions in first coordination sphere – perchlorate, tetraphenylborate, hexafluorophosphate salts etc. However at the Lab. of solution chemistry of SPbSU vast data on solution – solid equilibrium in the systems metal halides – water – organic solvent were accumulated.

To understand the regularities of the processes that lead to solid phase formation at the systems studied investigation of ion solvation in corresponding solutions was now undertaken. As the objects of study the systems $\text{CuX}_2 - \text{H}_2\text{O} - \text{S}$ ($\text{X} - \text{Cl}, \text{Br}; \text{S} - \text{acetonitrile}, \text{N,N-dimethylformamide}$) were chosen. The salt concentration was kept constant and equal to 0.5 mol/100 solvent moles. Solvent composition varies at whole range.

Composition of first solvation sphere was determined with IR spectroscopy by method of differential spectroscopy. Substraction of mixed solvent spectrum from ternary solution spectrum with some coefficient enables us to get the differential spectrum where bands intensities are proportional to the concentration of coordinated molecules. The numbers of solvent molecules in coordination sphere of copper ions were determined from the intensities of OH_2 deformational band (1640 cm^{-1}), for acetonitrile – from the band of valence vibrations CN (2290 cm^{-1}), dimethylformamide – from the band of NCO deformations at 1240 cm^{-1} . (M.б., The numbers of solvent molecules in coordination sphere of copper ions were determined from the intensities of OH_2 deformational band (1640 cm^{-1}), CN valence vibrational band of acetonitrile (2290 cm^{-1}), NCO deformational band of dimethylformamide (1240 cm^{-1})) Processing of water valence vibrations gives the total hydration number of cation and anions. Therefore the hydration numbers of halide anions in ternary solutions were also obtained.

Detailed results will be presented at the poster session.

Study of pressure-induced structural transformations in bis(glycinium)oxalate

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Bis(glycinium) oxalate ($C_2H_6NO_2 \cdot 0.5C_2O_4$) is a complex of glycine, the simplest amino acid, and oxalic acid in 2:1 stoichiometric ratio. High-pressure structural investigation of these crystals may provide a significant insight into the nature of weak intermolecular interactions and their dependence on molecular packing that can be helpful in crystal engineering of molecular crystals with desired properties. In this project we have carried out single crystal structure refinement of bis(glycinium) oxalate ($a=4.917(1)$, $b=9.957(1)$, $c=10.873(1)$ Å, $\beta=97.57(0)^\circ$, $P2_1/n$, $R=0.04$) and high-pressure investigation of this crystals by means of Raman spectroscopy. It was found that at pressure above 2GPa the structure transforms to a new phase which quite possible has a non-centrosymmetric space group that was confirmed by appearance of new Raman modes. Some of marked changes were not observed earlier in published powder investigations [1]. This transformation is realized by breaking weak N-H...O hydrogen bonds and formation new ones between amino group of glycine molecules and oxalate ions. Above 7 GPa the structure becomes more disorder; some additional changes are observed at 19 GPa, then single-crystal sample breaks.

This work was partially supported by G-RISC project G-2011b-1 and by the Council on Grants of the President of the Russian Federation for the Support of Leading Scientific Schools (project no. NSh-2883.2012.5).

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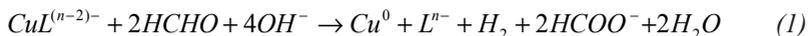
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Investigation of nonionic surfactants influence on topology of copper structures, obtained by laser-induced deposition method

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The interest in LCLD is due to the prospects of application of this method in microelectronics and technology, as it allows maskless manufacture of metallic structures on the surface of dielectrics. Focused laser beam scanning of the surface of a dielectric placed into a special solution results in local initiation of chemical reduction to give metallic copper according to equation (1)



where L is an organic complexing agent (usually sodium potassium tartrate or ethylenediaminetetraacetate (EDTA) salts); formaldehyde or sorbitol act as the reducing agent. The copper salt used is most often sulfate or chloride.

But under the action of laser radiation can take place adverse reactions of decomposition of organic components of the solution, leading to the release of carbon oxides. The formation gaseous products of reaction are the main reason for the appearance of defects in the deposited structures.

One of the possible ways to reduce negative effect of gas bubbles at laser deposition of copper is facilitate their separation from the surface of the dielectric. This can be achieved by using additives of surfactant.

In a prospective non-ionic surfactants in this study were considered Empilan and Tween in two versions, OP-10 and Noramox. As e results of the work was obtained by the qualitative dependence of the topology of the deposited structures on the HLB value of surfactants: improving topology structures with decreasing HLB value of surfactant.

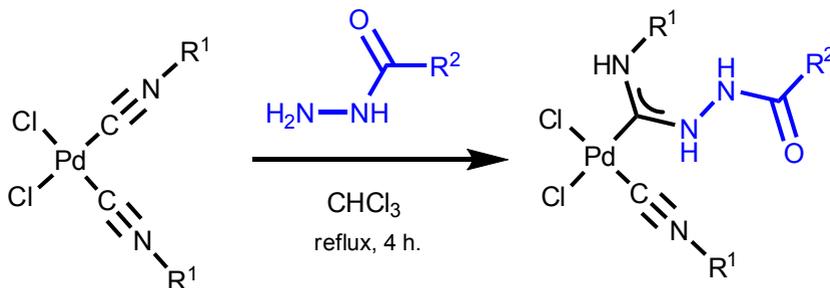
The resistivity of the copper structure was also estimated. Minimal resistance of deposited structure is only 3 times greater than the resistivity of pure copper.

New type palladium(II)-hydrazidoaminocarbene complexes

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The coupling of equimolar amounts of the palladium(II)-isonitrile complexes *cis*-[PdCl₂(CNR¹)₂] (R¹ = alkyl) with the various aromatic and aliphatic carbohydrazides R²CONHNH₂ (R² = alkyl, aryl, 12 species) proceeds for ca. 4 h in refluxing CHCl₃. The subsequent workup provides palladium-hydrazidoaminocarbenes *cis*-[PdCl₂{C(NHNHC(O)R²)=N(H)R¹}(C≡NR¹)] in 80–95% isolated yields.



Isolated species were characterized by elemental analyses (C, H, N), ESI⁺-MS, IR, ¹H and ¹³C{¹H} spectroscopies, and one complex by a single crystal X-ray diffraction.

Prepared carbene complexes exhibit high catalytic activity (TONs up to 9.4×10⁴) in Suzuki–Miyaura cross-coupling of aryl bromides with organoboronic acids (EtOH as environmentally benign solvent, K₂CO₃ as base, 80 °C). There results are comparable to those previously reported by some of use for the related palladium-diaminocarbenes [1].

This work has been supported by the FTP “Scientific and Scientific-Pedagogical Personnel of the Innovative Russia in 2009–2013” (contract P676 from 20/05/2010), RFBR (grant 11-03-00048-a), and the Fundação para a Ciência e a Tecnologia (FCT), Portugal (including FCT projects PTDC/QUI-QUI/098760/2008 and PTDC/QUI-QUI/109846/2009).

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Development of different *on-line* concentration techniques for electrophoretic determination of proteins by capillary electrochromatography

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Capillary electrochromatography (CEC) is microcolumn electrokinetic method of separation with that combines the desirable features of both high performance liquid chromatography (HPLC) and capillary electrophoresis (CE). New technology of the manufacture allows to define as high molecular weight compounds, and their low molecular weight metabolites. However the detection limits of analytes remain quite high, which makes active use of the CEC in the practice of clinical medicine difficult. A promising solution is the respective options *on-line* concentration, including a combination of different mechanisms of concentration, which give comparable high-performance liquid chromatography (HPLC) of the signal/noise ratio. The main techniques of the *on-line* preconcentration are stacking, sweeping, dynamic pH-junction, self-induced isotachopheresis.

In recent years science interest involves using as components in the mobile and stationary phase in chromatography and capillary electrophoresis new dendritic polymers. They have a stable structure like micelles, a large number of terminal functional groups, the intramolecular cavity, providing the ability to form inclusion complexes of the “guest-host” with the analytes of different nature. In this work we have investigated the possibility of different techniques of *on-line* preconcentration of analytes (LVSS, LVSS with “water plug”, electrostacking (FESI)) using derivatives hyperbranched polyethyleneimine to reduce the detection limits of proteins (albumin, myoglobin, lysozyme, insulin) by the electrophoretic methods such as electrokinetic chromatography and CEC.

It is shown that in an acidic sphere with the addition of the polymer electrolyte buffer stacking conditions with a large sample injection are realized. We investigated this fact (or used to concentrate the protein) in CEC. For this purpose, we synthesized columns coated with a thin layer of hyperbranched polymers (PLOT-column). The use of stacking on OT-columns allowed to lower detection limits of proteins (albumin, myoglobin, insulin, lysozyme) to 100-500 ng/ml and it gives possibility to determine proteins in biological materials. The factors of the *on-line* concentration efficiency (degree of functionalization of the dendritic polymer molecule, nature, concentration and pH of the working buffer, and so on) were established. The comparative characteristics as detection limits, efficiency, selectivity of separation are established. These laws were tested on real objects (human urea, serum).

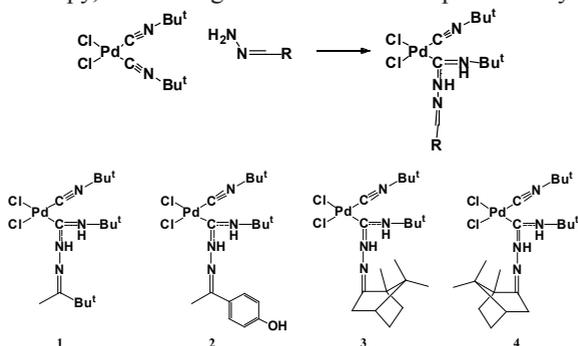
Novel ADC Pd(II) complexes: Synthesis and Catalytic Activity

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The palladium-catalyzed cross-coupling reactions is one of the most important methodology in synthetic organic chemistry for preparing precursors for natural products, pharmaceuticals, and materials with specialized optical and electronic properties. However, searching for new catalytic systems is still opened. Within the last few years the design of acyclic diaminocarbene (ADC) palladium(II) complexes have attracted increasing attention. These ADC Pd species are extensively studied as catalysts in various types of C-C coupling reactions with a large turnover number (TON) [1]. Several recent publications and reviews describe the interesting features of Pd-complexes bearing ADCs ligands in details. The strong sigma electron-donating and negligible pi electron-accepting (π -back bonding) ability of ADCs increasing electron density at the Pd center, thus ADCs are generally regarded as an alternative to the widely used phosphine ligands [2, 3].

Recently, we obtained several new ADC palladium(II) complexes through the metal-mediated addition of N-unsubstituted hydrazones to coordinated tert-butylisonitrile ligand. All new substances were fully characterized by ^1H , $^{13}\text{C}\{^1\text{H}\}$ NMR spectroscopy, IR and High-Resolution Mass spectrometry.



Catalytic activity of obtained compounds in Sonogashira coupling was investigated, and TONs (up to 9.5×10^3) for all complexes were estimated.

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Synthesis of diaryl ethers in the presence of CNT as the promoting agent

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Synthesis of diaryl ethers is usually performed by nitrochlorinebenzenes with phenoxide anions reaction. This reaction proceeds by nucleophilic aromatic substitution mechanism (S_NAr). In this case, alkali metals are the deprotonated agents [1-3].

As a model for the aromatic nucleophilic substitution investigation, the reaction of brombenzene with phenolate, which obtained *in situ* by interaction of phenol with potassium carbonate, was chosen. A copper-containing nanocomposites were used as solid-promoting additives. They were obtained by copper reduction on the surface of carbon nanotubes (CNTs). However, experimental data have shown that resulting structure does not produce a significant effect on investigated process. Therefore, further experiments were performed using copper salts and various modifications of CNTs as solid additives.

The following samples, containing CNTs, was used in investigation:

- “weakly activated” CNT, treated with nitric acid, which led to carboxylic groups formation on CNT surface (from 3 to 13 mmol per 100g);
- “highly activated” CNT, treated with nitric acid, which led to carboxylic groups formation on CNT surface (more than 30 mmol per 100 g);
- CNTs with a high specific surface area, known as the “feathery” fibers.

Experiments with this samples showed that the greatest effect is obtained for system, which contains “feathery” CNT and CuCl.

These results can be explained by high area of “feathery” CNT specific surface, which promotes the formation of a large number of the reaction centers and of the process of active aromatic nucleophilic substitution.

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Development and optimization of working parameters of the chip-analyzer for determination of neurotransmitters by capillary electrophoresis with electrochemical detection

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One of the fastest growing trends in modern analytical chemistry is the development of micro total analysis system (μ -TAS), in which all the stages of chemical analysis (injection, reaction, separation, detection) are performed on the same device.

Capillary electrophoresis (CE) in chip format with electrochemical detection was quite widespread overseas, but in our country is studied very little.

This study focuses on the development and optimization of working parameters of the specific μ -TAS for CE with electrochemical detection.

Chip Analyzer for capillary electrophoresis consist of a glass substrate with microelectrodes and a “cover” of a polydimethylsiloxane with a system of canals and reservoirs. It uses a fully integrated electrochemical detector.

The conditions of manufacturing of the polymer part of the chip are optimized, the configuration of an electrochemical detector is “off-channel” with platinum decoupler, the material of electrodes is gold due to the high inertness of this metal and ease of use on the glass part of the chip. It is shown that the optimal distance between working and counter electrodes is 50 microns, between working and decoupler - 150 microns. Optimal separation voltage is 800 V and borate buffer (pH 10.8) was used.

The reproducibility of EOF (electroosmotic flow) in the optimized conditions was 3-5%. A 3% solution of DMSO was used as a marker.

System performance was carried out on standard solutions (1 mg / l) of compounds containing electroactive groups: diatomic phenols and polyphenol antioxidants such as catecholamines (epinephrine, norepinephrine, dopamine) - diagnostic markers for many diseases of the central nervous system.

A Study into Thermodynamics and Structure of Smeared Charges Fluids: The Hypernetted-Chain Closure of the Fluid State Theory

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Over recent years increasing attention has been drawn to the properties of fluid systems which could be qualified as big charged particles immersed in a neutralizing “sea” of substantially smaller particles of a solvent. Examples include, *i.a.*, colloidal suspensions, water solutions of polymers and polyelectrolytes, mixtures of ionized isotopes in the stars and so-called dusty plasmas. Theory and computer simulations predict, that un-damped periodic oscillations of density may evolve in a macro-phase of such systems, the phenomenon heralding an appearance of the so-called “cluster” phases; one may speak about the micro-phase separation in the system. Theoretical analysis of fluid structure is based on investigation into the behavior of the pair correlation functions. As soon as periodic changes of density develop the asymptotic decay of the pair correlation functions crosses over from monotonous decay to the exponentially damped oscillations. There are criteria allowing to link the nature of such transition, termed a crossover, with the features of phase behavior of a system. Theoretically established phase behavior of such systems casts in favor of a perspective possibility to use them for the development of self-organizing matrices.

In this project the fluid is that of identically or oppositely charged particles of the same size. The interactions between these particles are described by a modified Coulomb potential with a term corresponding to their soft quadratic repulsion within the cut-off radius. This fluid can model the solution of a polyelectrolyte, of two oppositely charged poly-electrolytes or of poly-electrolytes and a polymer in the “sea” of solvent smaller particles, presented as a medium of no structure, whose individuality may be accounted for by potential parameters.

We determined the asymptotic behavior of the pair correlation functions in a wide range of thermodynamic conditions in such systems employing the hypernetted chain closure of the Ornstein-Zernike equation.

We have confirmed the presence of the crossover in asymptotic behavior of the pair correlation functions in one- two- and three-component fluids. The calculations of the law constraining the state parameters for the established crossover have shown that it is well presented by the Kirkwood line. The latter is an evidence of the formation of micro-inhomogeneities in the systems.

The study of the gas-chromatographic method for determination of singlet oxygen in gas flows by reaction with α -terpinene

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Research is devoted to the development of method for determination of singlet oxygen in the air based on the reaction with α -terpinene using gas chromatography.

Singlet oxygen is excited state of molecular oxygen. It is used in many areas of human life: in medicine, for sterilization of blood and in photodynamic therapy of cancer, chemical synthesis, waste water treatment, production of chemical lasers, etc. However, singlet oxygen has a number of negative properties: contributes to degradation of polymers, causes programmed cell aging – apoptosis and it is a component of photochemical smog.

In [1] Japanese researchers offered a gas chromatographic method for the determination of singlet oxygen in the atmosphere using α -terpinene: air containing singlet oxygen is pumped through the absorption tube filled with adsorbent XAD-2 coated with a layer of α -terpinene. The result of their interaction is formation of endoperoxide - ascaridole, the number of which is calculated content of singlet oxygen.

Previously, we studied this reaction to the possibility of its application for gas chromatographic determination of singlet oxygen with flame ionization detection. Revealed the presence of underlying processes: the decomposition of ascaridole to isoaskaridole, the ozonolysis of α -terpinene.

On standard solutions of ascaridole and α -terpinene chromatographic conditions for separation of the components were optimized (HP 6890 gas chromatograph with FID, silica capillary column DB-5MS, stationary phase 5% phenyl-aryl-metilpolisiloksan 95%). For a quantitative analysis performed by ascaridole calibration using a mixture of C10-C13 hydrocarbons as internal standard.

We used the generator of singlet oxygen produced by CJSC “OPTEC”. It allows to obtain singlet oxygen by selective excitation of oxygen in the ground triplet state.

The developed technique allows to determine the content of singlet oxygen in the gas flows and the ambient air. The detection limit is 160 ng/m³ at sampling rate of 3 L/min during 60 minutes.

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Direct determination of cobalt in human whole blood by GFAAS with Zeeman background correction

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Nowadays life science development requires a large number of trace elements to be monitored in biological matrices. Cobalt is an essential element in human body. It acts as a component of vitamin B₁₂, however, the excess of cobalt may pose a health threat. Thus a control of cobalt background and toxic concentrations in human biological media is quite important.

Whole blood trace element analysis is a complicated task due to severe matrix effects. In case of cobalt both organic matter and chloride ion influences should be taken into account. The performance of 7 different modifiers for cobalt determination in blood by atomic absorption spectroscopy with Zeeman background correction was investigated. Namely: NH₃, NH₄NO₃, Mg(NO₃)₂, Tl(NO₃)₃, LiNO₃, Pd(NO₃)₂, H₃PO₄. Sodium chloride water solutions were used for chloride interferences modeling. Pd(NO₃)₂ showed the best efficiency due to its oxidizing properties and, presumably, due to the formation of intermetallic compounds with cobalt that increased analyte – surface bonding energy.

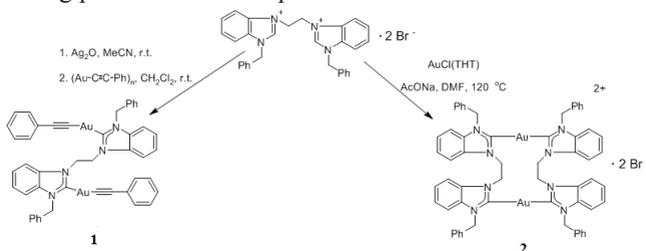
Conditions of cobalt direct determination in human whole blood by GFAAS with Zeeman background correction were optimized. New technique was validated using real human and white rat blood samples. Best performance were found for 10-fold blood dilution with adding of Pd(NO₃)₂ as matrix modifier. Detection limit achieved was 0.01 µg/L. Relative standard deviations varied in the range 1–15% depending on blood cobalt concentration. Developed technique was used for pre-clinical studies of cobalt containing pharmaceuticals.

Synthesis, photophysical properties, and characterisation of dinuclear Au(I) complexes with a bridging bidentate N-heterocyclic carbene ligand

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Luminescent coinage metal complexes with N-heterocyclic carbene (NHC) ligands are attracting increasing attention due to their remarkable characteristics, such as stability, desirable luminescence wavelengths, high quantum yields, and the promising phenomenon of vapochromism.



Two related Au(I)-NHC complexes were prepared by facile synthetic procedures with the objective of studying their photophysical properties. Dinuclear complex **1** featuring a relatively uncommon structural motif consisting of two linearly coordinated alkynyl units and a bridging bidentate NHC ligand was obtained by a two-step reaction sequence outlined above. Its cationic congener **2** lacking alkynyl moieties, but instead bearing an additional bridging NHC ligand was synthesized in one step. Such a modification unexpectedly imparts intriguing peculiarities of extremely scarcely observed solid state white colour luminescence, as well as vapour sensitivity towards hazardous volatile organic compound (VOC) methanol. To the best of our knowledge, **2** is the first example of a white-emitting phosphor based on the Au(I)-NHC framework, whereas **1** shows luminescence pattern typical of such species. The novel compounds were characterised by NMR spectroscopy and ESI mass spectrometry. Preliminary insights into the nature of the emitting states were drawn on the basis of previous investigations.

The work was carried out using scientific equipment of the Center of Shared Usage "The analytical center of nano- and biotechnologies of SPbSPU" with financial support of the Ministry of Education and Science of the Russian Federation. XRD study is carried out in the X-ray Diffraction Centre of St.Petersburg State University. Financial support from Saint-Petersburg State University research grant 12.37.132.2011 and Russian Foundation for Basic Research (grants 11-03-00974-a and 11-03-92010) is gratefully acknowledged.

Clustering of adsorbed acridine molecules on amorphous silica surfaces

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The specific current aim of this work is to inspect the effect of adsorbate-adsorbent interactions on the luminescence of acridine adsorbed on silica surfaces. The goal is to study the feasibility of spectral methods to characterize adsorbate-adsorbent interactions and the dynamics of complex heterocycles loaded into silica pores of 4 to 20 nm in diameter. The temperature at which the silica was trained was insufficient to complete water desorption.

Obtained results afford ground for assumption that acridine forms strong ionic hydrogen bonds with the hydroxyl part of silanol groups [1, 2]. This conclusion was made from smaller long-wave shift of luminescence spectrum of adsorbed acridine as compared to its protonated form. By comparing the luminescence spectra of acridine in water and acridine adsorbed on silica from vacuum it was concluded that silica surface, dried in high vacuum at 420 K, contained a variety of adsorption centers, including adsorbed water. The proton transfer to the nitrogen of acridine happens in the dark process, without the promoting photo excitation.

Previous investigations of acridine adsorbed from chloroform solution showed that acridine formed excimers on the surface. This conclusion was made based on lifetime's data and the position and the shape of the luminescence band [3]. Excimers can be formed in the case of island-type of adsorption, when acridine aggregates can be organized on the silica surface. Therefore acridine polycrystals were investigated particularly. Considerable long-wave (crystalline) shift was observed. It can be supposed that being adsorbed from solution acridine aggregates on the surface as islands, but individual molecules present on the surface when adsorption occurs from vacuum. Difference in the maxima positions in the luminescence spectra of acridine adsorbed from vacuum obtained at different excitation wavelengths can mean that there are present different hydrogen-bonded complexes with acridine.

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Rheological properties of cysteine – silver solutions and hydrogels

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The process of gelation in the system based on L-cysteine and silver nitrate is of particular interest because it occurs at very low contents of dispersed phase. Since the initial components are biologically active and play a special role in the human body, hydrogels obtained may be a promising matrix for the creation of pharmaceutical formulations of various actions.

The aim of this work is to study rheological properties in L-cysteine based systems by Physica MCR 301 instrument produced by Anton Paar GmbH in the following modes of deformation:

- dynamic low-amplitude regime corresponding to the linear domain of viscoelastic behavior in the range of frequencies from 0.5 till 250 s⁻¹; relative error in the modulus values did not exceed 0.5%;
- amplitude dependence of elastic modulus by the means of amplitude deformation sweep at constant frequency equal to 6.28 s⁻¹;
- flow curve measurements – by measuring the apparent viscosity as a function of shear stress in the regime of stress sweep in the range of stresses from 0.01 till 40 Pa.

Their viscous properties (flow curves) of the investigated subjects are very typical for “weak” gels. Maximum of dynamic modulus passes through a maximum at the certain content of electrolyte and this maximum surely correlate with the minimum of solvent pH values.

Rheological properties of gels with additives of medicines or polymer additives which can play the role of covers in the medicine transportation do not change with addition of polymeric substances though absolute values of the rheological parameters (the yield stress and modulus) increase.

In the results, gels formed in the aqueous solutions of L-cysteine/Ag systems in the presence of different electrolyte are visco-plastic media with dualistic properties. They behave as solid-like materials (elastic modulus does not depends on frequency) but can flow at very low stresses. Their apparent viscosity drops down by several decimal orders in a narrow stress range (that is typical for visco-plastic materials). However this effect is most likely obliged to shear banding and the flow taking place inside a low-viscous layer. Quantitative parameters of the systems under study depend on the details of their content but in all cases gelation is possible at concentrations not exceeding 0.036 wt%. Moreover the existance of the gel structure can be observed at extremely low concentrations of the order of $6 \cdot 10^{-4}$ wt%.

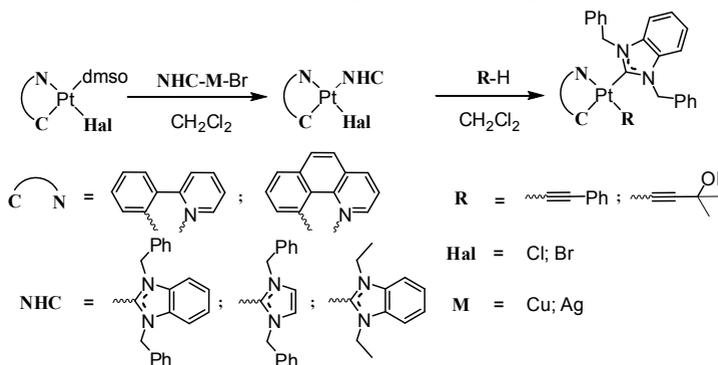
Synthesis and luminescence properties of cyclometallated platinum(II) complexes with N-heterocyclic carbenes

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There has been an increasing interest in the photophysical properties of luminescent square planar platinum complexes. These complexes have been investigated as emissive probes for DNA, singlet oxygen sensitizers, liquid crystal optical storage materials, and as luminescent centers in organic light-emitting diodes (OLEDs) [1].

Synthesis and investigation of photophysical properties of cyclometallated platinum(II) complexes with N-heterocyclic carbenes are presented in the work. Goal substances were obtained according to the following scheme:



The compounds obtained were characterized using NMR spectroscopy and ESI mass spectrometry. Absorption and emission spectra in degassed and aerate solutions were measured for these complexes. Excited state's lifetimes and quantum yields in solutions were determined. Solid state structures of key compounds were established using X-ray crystallography.

The work was carried out using scientific equipment of the Center of Shared Usage "The analytical center of nano- and biotechnologies of SPbSPU" with financial support of the Ministry of Education and Science of the Russian Federation. XRD study is carried out in the X-ray Diffraction Centre of SPSU. Financial support from SPSU research grant 12.37.132.2011 and Russian Foundation for Basic Research (grants 11-03-00974-a and 11-03-92010) is gratefully acknowledged.

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Developing of sample preparation for atomic emission digital spectrographic determination of heavy metals in lipstick

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In recent decades decorative cosmetics especially used regularly became more and more popular. One of the general products of this group is lipstick. According to statistics, a woman eats for a day on the average 13 mg of lipstick [1], by which a heavy metals hit in the body, that have a negative effect on health.

Determinations of microelements in cosmetic products are already included in the area of interest of medicine. When studied lipsticks of different companies presented in the market of Saudi Arabia, it was found that 26 samples contain lead, and in four samples the lead content was higher than one in United States Food and Drug Authorities standards [2]. The relevance of these studies is determined by devastating effect of lead on the human body that can lead to hypertension, casting, bone loss during menopauses, kidney damage and anemia [3].

Besides lead lipstick can contain other metals – xenobiotics. Although lipstick due to low contents is a minor source of metals in comparison with water, food, and air, heavy metals have a tendency to accumulate in the body during a long time.

The aims of this work were optimization of technique of lipstick sample wet mineralization, qualitative identification of the aggregate of heavy metals presented in lipstick, and assessment of these metals content. Method of atomic emission digital spectrographic analysis of liquid subjects which previously had been developed in our laboratory was used to determine the concentrations of metals [4].

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Hydrated forms of lithium salts in aqueous solutions

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Basic research of the structure of LiCl , LiNO_3 and LiClO_4 aqueous solutions has an enormous practical supplement. Lithium chloride is exploited in dryers because of its huge water affinity. Also it is used in aircraft engineering as a aeroplanes defroster. LiClO_4 aqueous solutions are frequently needed in creation of chemical current.

A chemical feature of lithium salts is high hydration of lithium ions in aqueous solution. Because of this property of the lithium salts they are crystallize from the solution as crystallohydrates. It is not typically for salts of other metals from the first group of the Periodic Table of the elements as evidenced by the solubility polyterm. In its turn the polyterm indicates changes in the determinate structure in aqueous solutions as far as salts concentration grows.

The aim of the study is determination of these solutions structure with different salts concentrations.

During the research the near IR spectra were recorded on Spectrum BX spectrometer in steps of 2 cm^{-1} . Received spectra data was treated by multiple chemometric analysis. For these were used soft modeling methods and principal component analysis (PCA). As a result were obtained spectra of forms of water and their abstract distribution diagrams in dependence of molar concentration.

The data matrix analysis by PCA showed that there are two components for LiClO_4 , LiNO_3 and three components for LiCl . Data were interpreted in accord with phenomenological model of the structure of aqueous electrolyte solutions. The conclusions were based on the correlation between spectra of forms of water and branches of crystallization on salt solubility polyterm.

In all the investigated systems one of the spectral forms is related with the spectra of free water. For lithium perchlorate the second spectra form is best of all akin to the spectra of the most concentrated solution in the series. It was found that this form is corresponds to the structure of three-water hydrate. In like manner for lithium nitrate one of the forms is correlated with free water and other is correlated with crystallohydrate $\text{LiNO}_3 \cdot 3\text{H}_2\text{O}$. It is interesting that as far as salts concentration grows new spectral form generates. For system $\text{LiCl} - \text{H}_2\text{O}$ was established that the second form refers to hydrates $\text{LiCl} \cdot 5\text{H}_2\text{O}$ and $\text{LiCl} \cdot 3\text{H}_2\text{O}$. The third form is assigned to two-water hydrate. In this system the process of new form creation is more intensive that in previous one and because of this were obtained three components by PCA.

Gelation in low concentrated aqueous solutions based on N-acetyl-L-cysteine and silver nitrate

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Low molecular weight supramolecular hydrogelators attract increased attention due to variety of potential application including tissue engineering, vehicles for controlled drug release, pharmaceutical formulations and others. Amino acids are interesting candidates for hydrogelation as they can be self-assembled using various non-covalent interactions in water including H-bonding, electrostatic, π - π and hydrophobic interactions. These interactions can give rise to the formation of organized supramolecular assemblies that can capture and immobilize a large number of water molecules under appropriate conditions.

A recent study of L-cysteine based hydrogels [1-3] shows that gelation in the system occurs at remarkable low minimum gelation concentration of 0.015 % w/v and can be induced by addition of the electrolytes with definite anions, alkali or certain non-electrolytes, for example, alcohols. L-cysteine is a unique amino acid, it has three functional groups – thiol, carboxyl and amino – not far separated from each other. Mechanism of gelation and role of each group in the process are not understood completely. To clarify these points it is of great importance to reveal conditions of gelation in various systems based on cysteine derivatives. It is found out that N-acetyl-L-cysteine (NAC) and silver nitrate also form supramolecular hydrogel at low concentrations.

In NAC molecule in contrast to L-cysteine a hydrogen atom of the amino group is substituted on the acetyl group that changes acid-base properties of the molecule, charge distribution in the functional groups and as a result conditions of gelation. Gelation in the novel system is a one stage process occurring in a narrow ranges of pH (2.4-2.6) and concentrations of the initial components (0.90-1.75 mM) at molar ration 1:1. The NAC based gel is non-thixotropic, less stable over time and weaker in comparison to the gels based on L-cysteine. TEM data showed that three-dimensional network of NAC gel consists of nanofibers with high aspect ratio. Investigations of the NAC-AgNO₃ based gels by means of different techniques (UV-vis and FTIR spectroscopy, dynamic light scattering, TEM) allowed to suggest mechanism of gelation in this supramolecular system.

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B. Geo- and Astrophysics

Advanced cross-well time-lapse velocity analysis

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Over the past decade, time-lapse 4D seismic imaging has been developed into an important tool for hydrocarbon reservoir monitoring and the subsurface velocity changes characterization is an important part of time-lapse analysis. Conventional time-lapse cross-well tomography utilizes direct arrivals to recover velocity changes in the subsurface due to oil and gas production, steam or CO₂ injection, steam assisted gravity drainage, etc. First-arrival traveltimes are picked in baseline and monitor data, and then the resulting time-lapse time delay is inverted into velocity change. The result of tomography significantly depends on the first-arrival signal quality and picks reliability.

The first-arrival time delays may be also estimated by a cross-correlation approach. The cross-correlation of baseline and monitor data waveforms is maximal when their relative time shift is zero. However, this is only valid if the source spectra of the baseline and monitor data are identical. This is not always the case and it may impact tomography results [1]. Following van Leeuwen and Mulder [2] we measure the traveltime difference via a weighted norm of the cross-correlation of baseline and monitor waveforms. Cross-well traveltime tomography usually has limited lateral resolution due to specific acquisition geometry. The use of reflections in the cross-well data improve the resolution and provide additional information to constrain velocity model.

We propose to optimize the functional based on the weighted norm of correlation of first arrivals and reflection images. This functional is not sensitive to waveform differences and may handle uncertainties of determination of lateral extent and magnitude of an anomaly. The numerical experiment proves the theoretical concept of time-lapse anomaly characterization by joint analysis of direct arrivals and reflection images. The proposed functional has sharp maximum corresponding to the true velocity anomaly and it depends monotonously on the anomaly parameters. Therefore, this type of functional may be very useful for accurate determination of velocity changes from a time-lapse cross-well data.

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Double-square root traveltime approximation for converted waves – field data example

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Shear waves play an important role in seismic imaging because they lead to knowledge of subsurface properties that cannot be obtained from PP-reflection surveys alone [1]. However, corresponding SS-reflection experiments are rarely carried out, mainly due to the acquisition problems associated with SS-surveys. As an alternative to SS-surveys, PS-converted waves can be investigated. Although several traveltime approximations for PS-converted waves may be found in literature, all of them are designed for the common-mid-point geometry and are not applicable to an arbitrary distribution of source-receiver pairs.

Recently introduced double-square root traveltime t^{sq} approximation for converted waves [2] is valid for arbitrary observation geometries and curved reflectors. It was demonstrated that for converted waves this approximation is applicable to large offsets. Also the pragmatic search strategy for t^{sq} approximation was introduced [3]. The key step of the strategy is the simulation of a zero-offset section by the stack of so-called γ -CMP gathers. These gathers can be considered as the first approximation of common conversion point gathers.

In this work, we demonstrate results of application of the method to three component synthetic data and field data from Blackfoot Field, Strathmore, Canada. For both datasets stacked sections were constructed using PP and PS waves. It was shown that effective wavefield attributes of converted and monotypic waves display comparable values and may be used in a joint interpretation. The difference in subsurface illumination and reflection coefficients of PP and PS events allows to obtain a better image in some parts of the PS stacked section compared to the PP section.

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Estimation of accuracy of dielectric constant determination by the method of hyperbolas in GPR

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Applying of ground penetrating radar (GPR) method to research the structure of the Earth is possible due to the difference on the electrical properties of rocks. Permittivity is one of the basic electrical properties. Almost all substances, except pure metal, can be attributed to the dielectric with finite conductivity. Thus, the knowledge of the dielectric constant is essential for the correct interpretation of GPR data. If we know the velocity of propagation of electromagnetic pulse in the medium then the propagation time of the reflected pulse can determine the depth of the search item, and this is the main task of GPR.

Sensing method, based on the approximation of geometric optics, is commonly used to determine the dielectric constant. The approximation of geometrical optics - the assumption, that the propagation of electromagnetic waves in the medium is the same, as the spread of the beam, and is described by the laws ray. But this approximation is highly conditional - it works, if heterogeneity are smooth and large compared to the wavelength. The another method is evaluation by hodograph of wave diffracted from a point reflector (method of hyperbolas). However the practice of radar work has shown that the dielectric constant in this method of determination is always understated. This problem is particularly acute in connection with radar studies of the lake "Vostok" in Antarctica, where estimates of the rate of propagation of electromagnetic pulse in the ice on hyperbolic travel-time curves of the diffracted wave is significantly different from the estimates obtained with allowance for the depth of the drilling data and seismic data.

The main objective of this work is to study the difference between the experimental values of the dielectric constant with the theoretical in the formal application of the method of hyperbolas, asking these differences depending on the size of the inhomogeneity, separating unit (the size of the base of GPR), the distance to the discontinuity.

To solve this problem the mathematical modeling of the cylindrical inhomogeneity, placed in a homogeneous environment, in the software package MEEP, and physical modeling of this problem on the laboratory bench (with water as the host medium with known dielectric constant) have been performed. The simulation results have established the basic laws of distortion values of the dielectric constant, suggest a methodology to assess the size heterogeneity of these distortions. At present, works on the application of this technique to the results of radar research in Antarctica is carried out. This work will not only improve the accuracy of interpretation of the data, but in some cases can be expected to evaluate the dimensions of the irregularities in the glacier bed.

Head waves and diving waves from a transition zone

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A. Wolf [1] was the first geophysicist to derive and analyze the reflection coefficient for a model of two homogeneous acoustic halfspaces with a transition layer between them in which the velocity varies linearly with depth, but only for plane waves at normal incidence. For plane waves at oblique incidence, R. Gupta [2] solved the problem analytically. Unfortunately, the analytical expressions for the reflection coefficients are so complicated that the analysis, still continuing today [3], is often restricted to normal incidence.

To simplify the expression for reflection coefficient we consider point source in a model of two acoustic halfspaces one with constant velocity and the other with constant gradient of velocity (infinite transition zone). This is one of the most simple models where both head and diving waves appear. We derive and analyze the reflection coefficient of plane waves from the halfspace with constant gradient of velocity and then build integral representation for a point source solution in the upper homogeneous halfspace. We try to extract head, diving, and “multiple diving” waves from this exact representation.

Seismograms by finite differences modeling, analytically obtained traveltimes for head, diving and “multiple diving” waves and the exact solution given by the integral representation show that at low frequencies very big offsets are needed to distinguish these wave types in a land seismic experiment.

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Ionosphere Profile Reconstruction With Oblique Sounding Ionogram

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Investigation and analysis of the ionosphere state are very complicated problems that can not have any absolute solution because of various ionospheric perturbations. Nowadays the most popular tool for receiving ionosphere profile is IRI (International Reference Ionosphere). IRI is the system that had been developed in respect to Radio propagation via the ionosphere. This system is based on a plenty of stations of vertical sounding all over the world.

There has developed a three-dimensional high frequency ray tracing program for numerical modeling in approximation of geometrical optics. This code has several ionospheric models for electron density, perturbations of electronic density, the Earth's magnetic field and electron collision frequency. Refractive index is represented by Appleton-Hartree formula.

The program implements the solution of the direct problem of oblique sounding and using algorithm of finding raytrace between two stations (for given ionospheric profile and frequency of transmitter) can solve the problem of reconstructing the ionosphere profile for either one or many hops ray trace. In contrast to IRI this approach helps to determine ionosphere perturbations in radio traces.

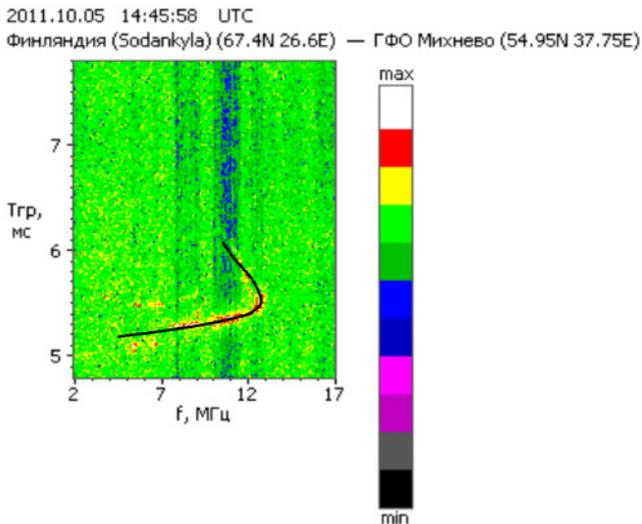


Fig. 1. Example of ionogram in reconstructed ionosphere with experimental ionogram.

Scattering of the elastic waves on the nonlinear elastic sphere

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

One of the main problems of the seismic studies is the search of the hydrocarbons reservoirs. These reservoirs are usually two-and three-phased media. Some studies show they should have nonlinear properties, which can be detected in the observed fields [1].

Interaction of the elastic waves with the nonlinear-elastic medium causes the appearance of the scattered nonlinear field [2-3]. In 1993 Beresnev [4] studied the interaction of the two spherical waves from different sources in the nonlinear-elastic region. He stated that the amplitude of the scattered field for the quite big objects have the value which can be detected in seismic experiment.

In the current study interaction of the elastic waves from the point source of the directed force with the nonlinear-elastic sphere is considered. The main goal is to define the highest possible amplitude value of scattered nonlinear field for the

size of the scattering object typical for the real seismic survey.

The conditions to obtain the maximum possible amplitude of the nonlinear scattered field were derived. The scattering diagrams of the maximum module of the scattering field were obtained for the set of the models. Unfortunately, even the maximum obtained value of the scattered field module can not be detected in the seismic experiment with the model parameters as were considered

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C. Mathematics and Mechanics

Consensus in Stochastic Systems with Uncertainties in Measurements

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Distributed coordination in networks of dynamic agents has attracted an interest numerous researchers in recent years. In [1] the stochastic approximation algorithm for solving consensus problem was proposed and justified for the group of cooperating agents that communicate with imperfect information in discrete time, under condition of switching topology and delay. Stochastic gradient algorithms were used for such problems before. Stochastic approximation with decreasing step-sizes allows each agent both to extract state information from its neighbors and to reduce the noise influence.

Under dynamic changes of the external conditions (getting new task, etc.), stochastic approximation algorithms with decreasing step-size are not efficient. In [2, 3] the efficiency of stochastic approximation algorithms with constant step-size was studied. Their applicability to the problem of load balancing in centralized network system where noisy information about load and productivity of nodes was analyzed in [4, 5]. Analyzing of discrete stochastic systems may be complicated in practical applications.

These problems show the relevance of study in the properties of stochastic approximation type algorithms with small constant or not decreasing to zero step size in the nonlinear formulation of the problem with switched topology and noise.

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Bifurcation in 4-dimensional piecewise linear dynamical systems

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Nowadays, piecewise smooth linear systems (PWLS) are extensively used to model many physical phenomena such as some problems of mechanic devices and electronic circuits [1]. Further, PWLS exhibit a rich variety of dynamics due to a sudden change of vector fields on a switching manifold.

In this talk I will briefly present the concept of the existence of invariant cones for PWLS depending on the existence of a generalized Poincaré map and their properties.

Further I will deal with a rather surprising phenomenon that we have discovered in a simple PWLS. It concerns the existence of multiple periodic orbits for homogenous 4D-PWLS which is quite different from smooth systems and is not known for 3D-PWLS with one discontinuity surface [2].

Additionally I will show, how to generalize the notion of an invariant cone when sliding motion takes place on the switching manifold.

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The Image of Mathematics in Germany and the World

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“Arithmetic and higher mathematics seem to be universally accepted as a difficult subject which will bring tears and frustration to all who learn it”. This quotation from a student’s training book reflects the global view on mathematics. Today, society sees no need to learn higher level mathematics. Moreover it is a widespread opinion, that deficits in math are nonrelevant. In contrast to this, math still has a privileged place in school curriculum. This leads to a disequilibrium, which should somehow be lifted.

This talk deals with the question if and to what degree math – especially in school – is necessary today. In addition to that, a short comparison of the situation in different countries all over the world will be given, referring to a recent international study on mathematics and sciences (TIMSS). Finally, the Cologne KinderUni, which is a month of university for 8 to 12 year-old children, will be introduced. This is one possibility to support the image of math and natural sciences, as well as to increase children’s interest in these subjects.

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The periodic orbits in canard-like functions

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In slow-fast dynamical systems the canard solutions are solutions that evolve along the attracting and repelling critical manifold. Generally the canard phenomenon describes the transition between stable and instable cycle.

The interesting property is that first we investigate the *Filippov-systems* and then use the method of the pinching to create piecewise-smooth dynamical systems. At the *Filippov-systems* we have the behavior of the sliding and crossing motion. They are the typically phenomenon of this model. At this point we use the method of the pinching to create a pinch-zone and then create a non-smooth system.

The pinched system has the characteristic, that we compress the cascade of the cycle. For this case we consider the Van-der-Pol system. First we investigate the normal stability of this model and then with the pinching method we choose a function and the pinch-zone.

With this method it is shown, that we can characterize very precisely the canard behavior by considering the vector field on the switching manifold.

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A priori estimates of solutions for second-order ordinary differential equations with integral boundary conditions

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Consider the problem

$$Au + \lambda^2 u = f_0(x), \quad (x \in (0,1)) \quad (1)$$

$$B_\rho^{k,m} u = f_\rho, \quad (\rho = 1, 2)$$

Here $Au := -a_0(x)u''(x) + a_1(x)u'(x) + a_2(x)u(x)$. (2)

Boundary conditions are given by the Riemann integrals

$$B_\rho^{(k,m)} u := \int_0^1 (g_\rho(x)u^{(k_\rho)}(x) + h_\rho(x)u^{(m_\rho)}(x))dx, \quad (\rho = 1, 2), \quad (3)$$

where $k_\rho < m_\rho$ can take on values from the set $\{0, 1, 2\}$.

Here $\lambda \in \mathbb{C}$ is a spectral parameter, $f_0 \in L_2(0,1)$ is a complex-valued function, and f_ρ ($\rho = 1, 2$) are complex constants.

Let $\mathcal{W}(0,1) := L_2(0,1) \times \mathbb{C} \times \mathbb{C}$. We introduce the equivalent norms $\|u\|'_{W_2^2(0,1)}$ and $\|f\|_{\mathcal{W}(0,1)}$ depending on the parameter λ , $|\lambda| \geq 1$.

Consider a linear operator $L(\lambda): W_2^2(0,1) \rightarrow \mathcal{W}(0,1)$ of the form

$$L(\lambda)u := \left((A + \lambda^2 I)u, B_1^{k_1, m_1} u, B_2^{k_2, m_2} u \right). \quad (4)$$

Our aim is to obtain (for sufficiently large values of the spectral parameter) the following inequality

$$\|u\|'_{W_2^2(0,1)} \leq C |\lambda|^{1/2} \|L(\lambda)u\|_{\mathcal{W}(0,1)}, \quad (5)$$

where the constant $C > 0$ does not depend on λ , u .

From the a priori estimate (5) it immediately follows that the operator is of $L(\lambda): W_2^2(0,1) \rightarrow \mathcal{W}(0,1)$. Fredholm type and $\text{ind} L(\lambda) = 0$ for all $\lambda \in \mathbb{C}$.

In the present work, constructive sufficient conditions under which estimate (5) holds will be discussed as well as the minimal restrictions on the weight functions g_ρ and h_ρ ($\rho = 1, 2$).

This work was supported by the Russian Foundation for Basic Research, project No. 12-01-31454.

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Analytical researches on the parametric pendulum

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A parametrically forced planar pendulum is excited by vertical harmonic oscillations. The equation of motion is described by the following nondimensional equation, $\ddot{\theta} + \gamma\dot{\theta} + (1 + \cos(\omega\tau)) \sin \theta = 0$.

Because of the time-consuming numerical simulation for this equation, robust analytical and approximate solutions are provided for investigating the systems dynamics. The aim of the work is to develop an automatic control system maintaining the desired motion.

The fundamental resonance structure is determined for the undamped model. The so-called resonance tongues are plotted into the parameter space for the generator frequency and amplitude. Based on these curves the instability, focusing on rotational motion, and stability, based on oscillation regions are determined.

For the damped model the parameter space is extended by a third dimension, the damping. This implies that a resonance surface appears. Moreover the rotational and oscillatory motions are studied by the perturbation method of multiple scales. In addition the approximate analytical solutions of the differential equation are calculated for the two typical responses, oscillation and rotation.

To conclude, a good correspondence between approximate analytical and numerical results could be achieved.

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CPGs) as oscillators for locomotion and synchronization of two coupled CPGs

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Repetitive and rhythmic activity like locomotion, respiration and scratching in invertebrates and vertebrates can be described by central pattern generators (CPGs) [1]. CPGs can be seen as special neuron groups which generate rhythmic behavior. A usual half-center CPG is composed of two inhibitory coupled neurons.

The half-center CPG I use here is based on persistent sodium current and it is a model to simulate walk-behavior of stick insects.

First of all this is a three dimensional system of ordinary differential equations and due to its neuron characteristics the system is based on the commonly known Hodgkin-Huxley model. Nevertheless it can be reduced to a two dimensional system which simplifies the analysis by dynamical systems theory. This will be helpful later on for synchronization study.

Furthermore, the system can be divided in slow and fast subsystems because of the very different timescales. This feature leads to considering the synchronization of slow and fast dynamics, similar to the paper of Omelchenko, Rosenblum, and Pikovsky [2]. So I consider two coupled CPGs via synaptic excitatory coupling (inhibitory coupling is reasonable as well) and I vary the coupling-parameter in order to determine in which parameter states slow dynamics are synchronized while fast are desynchronized or when both are completely synchronized.

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Central pattern generators (Stability of travelling waves in Ginzburg-Landau equation with weak diffusion)

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Ginzburg-Landau equation is well known and it has a lot of physical applications. Consider this equation with weak diffusion:

$$u_t = (1 - (1 + ib)|u|^2)u + \varepsilon^2(1 + id)u_{xx}$$

and periodic boundary conditions

$$u(t, x + 2\pi) \equiv u(t, x).$$

Here b and d are some real constants and ε is a small enough positive parameter. This equation has family of solutions $\rho_k \exp(i\omega_k t + ikx)$ where k belongs to set of integer numbers. Stability of each k -th wave in dependence of parameters b and d (in the case of small enough positive values of parameter ε) is studied. Sufficient conditions of stability and instability are found. Multistability and even hypermultistability is proved. (Hypermultistability means that for any natural number n we can find parameters of our problem, such that we have greater or equal than n stable coexisting solutions).

MINToring – an attempt of schooling tomorrow’s researchers and inventors

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MINT – these four letters stand for Maths, Informatics (i.e. computational science), Natural science and Technology. “MINToring” is a programm of the Stiftung der Deutschen Wirtschaft (sdw, foundation of German economy). Its aim is to show pupils how fascinating and important subjects like physics or biological informatics can be.

In school, for most of the young people the MINT-subjects are still just theoretical thoughts and abstract formulars. They do not always see the exciting link between school and their future work and life. Nevertheless, most of inventions and innovations that make life easier are ideas of alumni of MINT-subjects. Regarding that the number of first-year-students enrolling in MINT-courses is very low and the number of drop-outs very high, it is extremely necessary to support pupils and encourage them to study such subjects and participate in scientific research and progress.

Can we change something in school or in the education of the young people so that their interest for those subjects is raised? How can we especially support those pupils, who are generally interested in science, but do not really know what exactly they could study and what kind of scientific work fits to their abilities and passion?

Therefore, the MINToring program was established. It is a three year-program, starting with the pupils two years before they take their final exams in school. The mentors or tutors are students of MINT-subjects who can provide their insight view and are able to give good advice concerning the subjects. In the first year, the pupils have some excursions, visit universities, get insight views in laboratories etc. The pupils also participate in workshops about learning-methods and so on to improve their scientific manner of work.

In the second year, the pupils work together in small groups to engineer or invent something. The aim is to evoke their inventive genius and their fascination for science. If they start to study a MINT-subject afterwards, they have their former tutors as contact person for all problems that occur in University and as an adviser.

This program has a huge impact on the occupational path of the young people and especially encourages those, who are interested in science, but not aware of what exactly they should do in their near future. MINToring supports the individual potential of the young pupils and gives the opportunity to find the subjects which are corresponding to their talents.

Homogenization of the two-dimensional periodic Dirac operator

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We discuss homogenization problem for the two-dimensional periodic Dirac operator with the help of operator-theoretic approach to homogenization for matrix elliptic second order differential operators suggested by M.Sh. Birman and T.A. Suslina.

We consider the Dirac operators with a non-singular magnetic potential,

$$D_\varepsilon = (D_1 - A_1(x/\varepsilon))\sigma_1 + (D_2 - A_2(x/\varepsilon))\sigma_2 + m\sigma_3;$$

and with a singular magnetic potential,

$$D_{\varepsilon, sing} = \left(D_1 - \frac{1}{\varepsilon} A_1(x/\varepsilon)\right)\sigma_1 + \left(D_2 - \frac{1}{\varepsilon} A_2(x/\varepsilon)\right)\sigma_2 + m\sigma_3.$$

Here $\sigma_{1,2,3}$ are the Pauli matrices, m is a real positive.

Sharp-order approximations of the resolvent of the Dirac operators in the L_2 -operator norm are obtained, with error terms being $O(\varepsilon)$.

Periodic Orbits in Anti-Lock Braking Systems

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In dynamical systems asymptotic stable, periodic orbits are of great interest. They correspond to a certain behavior of the system, which can be desired or unwanted. Thus, finding and analyzing periodic orbits is one major area of application. Normally dynamical systems are non-integrable and can only be solved numerically.

The talk introduces a model of anti-lock braking systems (ABS), which is by now a standard component in every modern car. An ABS prevents the wheels from going into a lock situation, where the wheel is fixed by the brake and the stopping distances is greatly prolonged. Instead the system holds the wheel's slip within certain limits by creating a stable limit cycle.

The talk presents two different ways to prove the existence and stability of limit cycles: On the one side via geometrical arguments, on the other via a perturbation-theory approach.

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Rotation number of a class of periodically pulsed forced mechanical systems

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In our talk a class of periodically pulsed forced mechanical systems with angular coordinates is considered. This class can be treated as non-autonomous differential equations on the cylinder. The theory of cocycles is used for the mathematical description of such non-autonomous differential equations. The existence of the cocycle and its global B -attractor in the form of an invariant curve is shown. That allows us to introduce the notion of the rotation number for cocycles on an invariant curve. The method of Poincare maps is also used to investigate periodically pulsed forced mechanical systems. Time-discrete dynamical systems are obtained as the result of the application of the Poincare map's method. Similar to the cocycle approach in this case the existence of a global B -attractor in the form of an invariant curve is shown. This allows us to introduce the notion of the rotation number for time-discrete dynamical systems.

On the existence of homoclinic orbits to invariant KAM-curves

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We study a C^r -smooth symplectic diffeomorphism f on a C^∞ -smooth 4-dim symplectic manifold $(M; \Omega)$, Ω is C^∞ -smooth 2-form. We assume f to have an 1-elliptic fixed point p , that is differential $L = Df_p$ has one pair of multipliers $\exp[\pm i\alpha]$ on the unit circle and a pair of real multipliers μ and μ^{-1} , $0 < \mu < 1$.

Near an 1-elliptic fixed point there is a C^{r-1} -smooth 2-dim invariant symplectic center submanifold W^c corresponding to multipliers $\exp[\pm i\alpha]$. The restriction of f on W^c is a C^{r-1} -smooth 2-dim symplectic diffeomorphism and p is its elliptic fixed point. We assume p to be of the generic elliptic type, that is, the first coefficient in the Birkhoff normal form for $f|_{W^c}$ does not vanish. Then the Moser's invariant curve theorem holds for f near p that gives a positive measure Cantor set of closed invariant KAM-curves on W^c which enclose p and accumulate at it.

The center manifold W^c is a normally hyperbolic with smooth 3-dim stable manifold W^s and unstable manifold W^{cu} , since two other multipliers μ , μ^{-1} are respectively lesser and greater than 1 in modulus. This implies that each invariant KAM-curve on W^c is saddle one, since it has 2-dim strong stable and strong unstable manifolds. Topologically such stable/unstable manifold is a local cylinder being Lagrangian submanifold in M . The existence proof of these manifolds follows from expanding family theorems [2].

The fixed point p has also two C^r -smooth local invariant curves through p being its local strong stable $W^s(p)$ and strong unstable $W^u(p)$ manifolds. Our main assumption here is the following:

Assumption 1. When extending by f local curve $W^u(p)$ it returns to a neighborhood of p and intersects $W^s(p)$ at some its point q generating thus a homoclinic orbit Γ to p , moreover, we assume the intersection at q of $W^s(p)$ and the extension of $W^{cu}(p)$ to be transverse.

Our main result is the following theorem:

Theorem 1. If some additional genericity condition for the homoclinic orbit Γ holds, there is a neighborhood U of Γ such that each closed invariant KAM-curve on W^c possesses in U four transverse homoclinic orbits.

We formulate genericity condition in terms of a so-called scattering linear operator that acts from $T_p W^c$ to itself.

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Generalized and classical solutions of boundary value problem for differential-difference equation

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In this paper we consider the following boundary value problem

$$-\frac{d}{dt}(R_0 u'(t)) + R_2 u(t) = f(t) \quad (t \in (0, d)) \quad (1)$$

with homogeneous boundary conditions $u(t) = 0$ ($t \in (0, d)$) (2)

Where R_i are difference operators, that are defined by the formula

$$R_i u(t) = \sum_{j=-m}^m b_{ij}(t) u(t+j) \quad (i = 0, 1, 2). \quad (3)$$

Here m is an integer number, $b_{ij}(t)$ is a function belonging to the $C^\infty(\mathbb{R})$. Let $d = N + \theta$, where $0 < \theta \leq 1$, N is an integer number.

The question is under what conditions on the coefficients of the difference operators boundary value problem (1), (2) will have a classical solution for any continuous right-hand side.

Smoothness of generalized solutions of boundary value problem for differential-difference equations with a shift in the argument of high terms can be broken even for infinitely differentiable right-hand sides equations [1-3]. In [3], sufficient conditions of existence of classical solutions in terms of the orthogonality of the right-hand side to a finite number of functions.

In the case of constant of coefficients difference operators [4], necessary and sufficient condition of existence of classical is the lack of shifts of arguments in the derivatives of unknown function. In contrast, in the case of variable coefficients we obtain the following.

Theorem. Let $f \in C[0, d]$ and $\theta < 1$. Let $\det R_{0s}(1) \neq 0$ and $\det R_{0s}(\theta) \neq 0$, where elements of the matrices R_{0s} are given by the following relation

$$r_{jk}^0(t) = b_{0,k-j}(t+j-1) \quad (s = 1, 2; j, k = 1, \dots, N+1).$$

In this case every generalized solution of the problem (1), (2) is classical solution of the problem if and only if $b_{0,-l}(l) = 0$ и $b_{0,N+1,-l}(l-1+\theta) = 0$ ($l = 1, \dots, N$).

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Homogenization for periodic elliptic second order differential operators in a strip

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The talk concerns homogenization for the elliptic operator in $L_2(\Pi)$, $\Pi=\mathbf{R}\times(0,a)$, defined by the differential expression

$$B_\lambda^\varepsilon = \sum_{j=1}^2 D_j g_j(x_1/\varepsilon, x_2) D_j + \sum_{j=1}^2 (h_j(x_1/\varepsilon, x_2) D_j + D_j h_j^*(x_1/\varepsilon, x_2)) + Q(x_1/\varepsilon, x_2) + \lambda Q_*(x_1/\varepsilon, x_2)$$

with periodic, Neumann or Dirichlet boundary conditions. All the coefficients are assumed to be periodic of period 1 with respect to the first variable. Sharp-order approximations for the inverse of B_λ^ε in the norms of $\mathbf{B}(L_2(\Pi))$ and $\mathbf{B}(L_2(\Pi), H^1(\Pi))$ are obtained, with error terms being $O(\varepsilon)$.

Mathematical modeling of water flow in open channels

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The paper presents a one-dimensional differential model of Saint-Venant, which describes the free movement of water in open channel [1, 2]. For the kinematic approximation of the model, which is a quasi-linear first-order equation in the stationary case, we obtained a general analytical solution. For the non-stationary case an original numerical algorithm was obtained. The paper presents numerical results for some test tasks and also practical task. These results were compared with the solution of the same tasks in the Ansys CFX system and it showed good equivalence .

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Numerical Methods in Stem Cell Research

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Considering stem cell research as a relatively new field of medicine, we observe increasing importance by means of the variety of applications it could be used for. Therefore, physical observations and mathematical methods including modeling and simulation are inevitable for further improvements.

To describe the integrability of pluripotent stem cells in heart tissues, we record multiple HCG-signals arranged in a grid.

On one hand, we apply discrete Fourier transform on each HCG-signal to receive the intrinsic dimension of the cells' beating frequency.

On the other hand, we observe their function in the tissue by comparing the HCG-signals to each other while using several numerical mapping methods as well as beat detection and interpolation algorithms. Hence we can validate the primary cells' influence on stem cells i.e. are the stem cells beating and if so, are they at regular intervals.

As we accomplish these results, we could figure out which cells took the role of the impulse generator and whether they stay in time with the original beat. Due to these techniques we can accelerate investigations in stem cell research.

Coerciveness conditions for the functional-differential equations with orthotropic contractions

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Let B_r – a two-dimensional ball of radius r . We consider the following functional differential equation in B_r :

$$A_R u(x) = - \left(\frac{\partial}{\partial x_1} \left(R_1 \frac{\partial u}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(R_2 \frac{\partial u}{\partial x_2} \right) \right) = f(x), \quad (1)$$
$$R_i u(x_1, x_2) = a_{i0} u(x_1, x_2) + a_{i1} u \left(\frac{x_1}{q}, px_2 \right) + a_{i,-1} u \left(qx_1, \frac{x_2}{p} \right).$$

Here $p, q > 1$; the coefficients are complex numbers; the function f is square-summable in B_r . The functions are supposed to be extended by zero outside the ball before applying operators R_i , $i=1,2$, to them.

The equation is called strongly elliptic in the closure of B_r , if there exist the constants $c_1 > 0$ and $c_2 \geq 0$ such that for all u from $C_0^\infty(B_r)$ the Gårding type inequality holds:

$$\operatorname{Re} (A_R u, u)_{L_2(B_r)} \geq c_1 \|u\|_{H^m(B_r)}^2 - c_2 \|u\|_{L_2(B_r)}^2. \quad (2)$$

For a broader class of operator this inequality guarantees the Fredholm solvability as well as discreteness and sectorial structure of the spectrum of the Dirichlet problem for (1) in $L_2(B_r)$. positive solutions for well-known problem of T. Kato about square root of m -accretive operators

We obtain the necessary and sufficient conditions in algebraic form (coerciveness problem) for the operator A_R to satisfy the Gårding type inequality. This problem was solved for difference-differential operators by A.L. Skubachevskii [1]; for functional differential equations with isotropic contractions – by L.E. Rossovskii [2, 3].

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Analysis of hit-sticking phenomena in a drillstring model

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In conventional oilwell drillstrings nondesired oscillations, as stick-slip and other bit-sticking phenomena, due to the presence of different types of friction can arise.

Because of the complexity of dynamical phenomena in these mechanical systems and for the sake of simplicity in the presentation of results a simplified torsional lumped-parameter piecewise-smooth model of three degrees of freedom, describing a conventional vertical oilwell drillstring, is considered. In this model a characterization of bit-sticking phenomena and resulting different dynamical behavior, by investigations of system equilibria in different surfaces, different parameter regions and the existing sliding motion (when the bit velocity is zero) is performed.

It is shown, that the existence of a sliding motion and the position of the equilibrium of the switching surface can dominate the dynamic behavior and therefore plays an important role for nondesired vibrations at the bit. Safe drilling parameters can be detected and can help the driller to design the well drilling profile before starting the operation.

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D. Solid State Physics

Investigation of system Ge/LC by field-effect in electrolyte methods

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Liquid crystals(LC) have been widely investigated over the last few decades and have been adopted in numerous fields of technology. But with all of interest to LC, electrophysical properties of system “LC-solid surfaces”, Ge/LC in particular, was poorly understudied [1]. Our work can help with filling of this gap. In terms of applied physics abilities to control of charge properties of Ge surface by switching polarized state of LC, formation of passivating thin films on the Ge surfaces, and possibility of another technological applications of Ge/LC system are quite interesting too.

Present research was based on capacity-voltage and current-voltage characteristics. These characteristics were carried by using field-effect in electrolyte methods, which strongly differs from field effect in MIS (see [2]).

Ge surface was cleaning by etching in concentrated H_2O_2 . We used nematic type of LC. LC films were deposited on Ge from solution LC in toluol. Film's thickness was about 40 nm. We used p-Ge with doping level $\sim 10^{14} \text{ sm}^{-3}$ and surface orientation (111). Capacity-voltage and current-voltage measuring was carried on variable signal, frequencies differed from 1kHz to 70kHz. Electrode potential values was varying from -1 V to 0,5 V.

Our results shows possibilities of formation of LC films on the Ge surfaces without substantial increasing of surface states density and built-in charge and possibility of modification of LC films by prolonged polarization.

Authors would like to thank DPhil professor Kovshik A.P. (department of physics of polymers) for LC film's formation and his consultations.

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Optical properties of GaN epitaxial layers doped with Si

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Gallium nitride (GaN) and various related nanostructures are among the wideband semiconductor systems in demand for the most important applications and scientific purposes. The energy structure and dynamics of charge carriers in GaN were studied intensively by the optical methods during last two decades [1]. Optical properties of wurtzite type GaN crystals are governed by the transitions from valence subbands Γ_9 , Γ_7 and Γ_7 to the conduction band Γ_6 , which manifest the strong exciton resonances (A, B and C excitons respectively).

The aim of this work is to study the exciton spectra, Raman spectra and electrical conductivity in GaN epitaxial layers with donor concentrations $4.1 \cdot 10^{16}$, $3.1 \cdot 10^{17}$, $1.4 \cdot 10^{18}$, $3.4 \cdot 10^{18}$ and $4.8 \cdot 10^{19}$ cm^{-3} (samples № 1 – 5, respectively).

Exciton resonances in the absorption (reflection) spectra of GaN layers grown on sapphire substrate are shifted toward the low energy side relative to their positions in the freestanding crystal. As the donor concentration N_d increases exciton reflection spectrum broadens and shifts to lower energies. For $N_d > 3 \cdot 10^{18}$ cm^{-3} exciton bands $A_{n=1}$ и $B_{n=1}$ are no longer observed. The shift and broadening are caused by the lattice strains and degradation, as well as by the band gap renormalization under the screening of Coulomb interaction.

The emission spectrum of the sample № 1 at $T = 5$ K contains $A_{n=1}$, $A_{n=2}$, $B_{n=1}$ free exciton bands, and D^0x , A^0x bands originated from the excitons bound to neutral donors and acceptors, as well as the phonon replicas of free and bound excitons (LO-phonons emission with the energy 91 meV).

Peak intensity of the luminescence spectrum decreases considerably at the high doping level. In the range of silicon concentrations from 10^{18} to $5 \cdot 10^{19}$ cm^{-3} , the formation of the impurity band and its overlapping with the conduction band are clearly manifested in the luminescence spectra and conductivity of GaN epitaxial layers.

Raman spectra of the system sapphire substrate-gallium nitride epilayer were studied, the phonon components active in the light scattering are identified and analyzed.

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Factor analysis of Raman spectra of nanowhisker GaAlAs with wurtzite-blende structure

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Bulk crystalline semiconductor gallium arsenide GaAs at normal pressure grows in a stable phase with a sphalerite structure (ZB). In microscopic crystals of GaAs, which are characteristic for quantum dots and nanowires, structure of wurtzite (WZ) can be stable. In such structures, new electronic and optical properties appear that are not known in the bulk semiconductor material, and are of interest of researchers. Growth of nanowhiskers are often accompanied by either a random contribution of defective wurtzite layers in the structure of ZB, or the continuous growth of wurtzite nanowhiskers. Sphalerite (cubic) and hexagonal polytype structures (wurtzite-2H polytype and 4H) are very similar in the short-range order, but differ in the relative arrangement of the atoms in the neighbor layers.

This paper deals with the use of factor analysis for identification of the set of linear-independent contributions from spectra in order to study sphalerite and wurtzite phase spectra of nanowhiskers.

In the spectrum of mixed crystal $\text{Al}_x\text{Ga}_{1-x}\text{As}$, which is characterized by two-mode behavior of fundamental frequencies, there are two areas with the bands relating to the longitudinal LO and transverse TO fluctuations of gallium arsenide and aluminum arsenide with the frequencies about $250\text{--}300\text{ cm}^{-1}$ and $360\text{--}400\text{ cm}^{-1}$, respectively.

With the method of factor analysis, 55 spectra of the nanowhisker sample in the 55×300 matrix form were analyzed in frequency range of $130\text{--}400\text{ cm}^{-1}$. It was found, that there are two pairs of lines in the studied spectrum region with frequencies of $360, 380$ and $266, 276\text{ cm}^{-1}$, corresponding to LO and TO frequencies of the solid solution $\text{Al}_x\text{Ga}_{1-x}\text{As}$, and a group of bands $194, 254$, relating to the wurtzite phase of nanowhisker, and also two separately located lines at 270 and 287 cm^{-1} , the origination of whose is the GaAs substrate.

In the scattering spectrum six lines can be observed, whose origination is associated with the addition of the Brillouin zone of ZB crystal phase. Factor analysis showed that the number of detected lines can be interpreted as an occurrence of the wurtzite structure in nanowhiskers. The coexistence of sphalerite and wurtzite crystal structures in nanowhisker samples GaAs was experimentally confirmed by electron microscopic studies data, obtained from the literature.

Investigation of SiC-heterostructures by X-ray reflection spectroscopy

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In recent years new types of semiconductor heterostructures consisting of only one material in different crystal structures, such as heteropolytypic structures are under discussion. In this field, silicon carbide (SiC) is the most promising candidate because SiC crystallizes in numerous different stable structures. Among them there are one cubic (C or α -SiC) and several hexagonal (H) and rhombohedral (R) structures. The most common non-cubic polytypes (β -SiC) are 4H, 6H, 15R, and 21R. Some physical properties of SiC depend strongly on the crystal structure. For an example, the band gap varies from 2.4 eV in 3C-SiC to 3.4 eV in 2H-SiC. Using a combination of different polytypes opens new possibilities for application of SiC: creating of new types of hetero- and low-dimensional high-power, high frequency, high-temperature and radiation-resistant devices.

The preparation of heterostructures by only changing of the crystal structure during the growth is a great challenge. In this connection the main goal of this work is to study heterostructures on basis of different polytypes of SiC synthesized by vapor phase epitaxy on Si wafers in different technological conditions with purpose to establish the polytypes (and its thickness) of SiC constituted the heterostructure. It should be emphasized that special requirements for the control methods for such structures are nominated. Soft X-ray reflection spectroscopy, which is a non-destructive in-depth characterization tool of the local atomic structure, is a most suitable technique in this case. It is recalled that different polytypes SiC have a distinctive shape of the absorption spectrum in the vicinity of Si $L_{2,3}$ -absorption edge.

The measurements were performed on X-ray spectrometer-monochromator RSM-500. Spectral dependences of the reflection coefficient $R(E)$ of the samples in the vicinity of Si $L_{2,3}$ -absorption edge were obtained at different grazing incidence angles that means at different depths of the formation of reflected beam. On the basis of the measured reflection spectra the absorption spectra were calculated using the Kramers-Kronig relation.

It was established that all studied samples are heterostructures constituted from two polytypes (3C and 6H polytypes of SiC) of different thickness. In each heterostructure the surface layer of the film is formed by cubic SiC (3C) polytype. The thickness of this layer varies in different samples and depends strongly on the growth conditions.

Spectroscopic Characterization of Sr-rich SrTi_{1-x}O_y films synthesized by Atomic Layer Deposition method. Influence of Interfacial Layer Material on Structure of Film

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Further scaling of dynamic random access memories with 1 Gbit density or higher requires an equivalent oxide thickness (EOT) in the 0.5–0.7 nm range for metal-insulator-metal capacitors in the memory cell, maintaining low leakage current densities. To achieving these conditions the dielectrics with high-k values (>50) are required. The perovskite Sr-rich SrTiO₃ (STO) is one of the potential candidates for this application. The dielectric properties of STO are critically dependent on the film thickness and stoichiometric composition of the film. In Sr-rich STO a significant decrease of leakage current compared to stoichiometric STO for the same values of the EOT can be achieved. Including an interfacial layer can reduce the leakage current and the thickness dependence of the dielectric constant.

In the current work the results of study of the internal structure of Sr_{0.62}Ti_{0.38}O_x / interfacial layer (SiO₂ or HfO₂ or Si₃N₄)/Si – ALD stacks are discussed. The Sr-rich STO films of 7nm and 15nm thick were analyzed by X-ray photoelectron spectroscopes (XPS and HXPS) and external X-ray photoeffect quantum yield in current mode (NEXAFS spectra). A joint spectroscopic analysis indicates the following regularities:

1. Only in films grown onto Si₃N₄ interfacial layer there is a tendency to enrich the film with strontium.
2. The analysis of TiL_{2,3} - and OK - NEXAFS spectra clearly demonstrates that the enrichment of the structure of Sr atoms accompanied by a violation of the cubic symmetry of the STO connection.
3. The surfaces of the all investigated STO films are carbonate-rich surfaces in the form of SrCO₃.

Ultrathin Co₂FeSi Heusler alloy films formed on silicon surface covered with a barrier layer

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The half-metallic Heusler alloys are of great theoretical and technological interest due to their high degree of spin polarization of electrons at the Fermi level. Among these compounds much attention was paid to the formation of Co₂FeSi due to its highest Curie temperature (1100 K) and the large magnetic moment (6 μ B) of all known Heusler alloys. Further development of the spintronic devices requires the decrease of the Heusler alloy film thickness and the minimal thickness of the grown Co₂FeSi layer is reported to be about 100 nm [1]. The aim of this study was to produce the ultrathin Co₂FeSi Heusler alloy films of a few nm thickness on the silicon substrates and to study their electron and magnetic properties.

The ultrathin films of the synthesized Co₂FeSi Heusler alloy were formed in ultrahigh vacuum by solid phase epitaxy. To prevent the interdiffusion between deposited layers and silicon substrate we used the barrier layers. The elemental content of the synthesized films was controlled by x-ray photoelectron spectroscopy with the Mg K α line ($h\nu = 1253.6$ eV). The electronic structure of the films was studied by spin-resolved photoelectron spectroscopy with a Helium lamp ($h\nu = 21.2$ eV). The measurements were performed in magnetic remanence after applying a magnetic field pulse of about 1000 Oe along the in-plane direction of the samples.

At the first stage of the experiment silicon (2 nm), cobalt (2.4 nm) and iron (1.1 nm) films were sequentially deposited on the samples covered with one of two types of the barrier layers – SiO₂ or CaF₂. To form the Co₂FeSi Heusler alloy the sample was subjected to 5 min annealing at fixed temperatures. The diffusion of deposited Si, Fe and Co into the Si substrate was blocked by the barrier layer at temperatures below 450 °C. The sample annealing at 400 °C produces a compound, whose elemental composition is identical to that of the Co₂FeSi Heusler alloy. We studied the electron structure of this compound and obtained the values for spin polarization of 20% at room temperature.

This work is supported by the German-Russian Interdisciplinary Science Center (G-RISC) funded by the German Federal Foreign Office via the German Academic Exchange Service (DAAD).

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Study of electron spin-polarization relaxation in LiF

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The thin non-magnetic films of lithium fluoride were deposited on the surface of ferromagnetic FeNi₃(110). Secondary electron polarization coming from such systems 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].

Before every measurement the FeNi₃(110) sample's surface was cleaned by consecutive cycles of ion etching and annealing.

Deposition of LiF was made from heated ceramic capillary in ultra high vacuum in the same chamber where electron spectroscopy was then carried.

The main idea of this work was to measure secondary electron spin polarization for different LiF-FeNi₃(110) systems. Because the secondary electron polarization is due to ferromagnetic properties of substrate deposition of LiF film leads to its decay. And rate of this decay in studied structures is several times less than rate of substrate's auger-peak decrease. So spin-relaxation mean-free path in lithium fluoride is several times bigger than inelastic mean-free path. Measurements were made for different electron energies (50-550 eV) and different film thicknesses (up to 50 Å).

Such behavior of thin LiF film can be explained by its simple electronic structure and absence of d-electrons. Which reduces the probability of spin-flip process while secondary electron is moving from substrate through film to vacuum.

This work was supported by RFBR grant number 11-02-01092-a.

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Monte Carlo Simulation of Photostimulated Processes in Heterogeneous Systems

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Photostimulated processes in heterogeneous systems are very complex and involves such steps as photogeneration of free charge carriers, their migration and trapping by either bulk or surface defects resulting in formation of the color centers (in the bulk) and surface active centers respectively, which are able to interact chemically with the molecules at the interface.

Although by definition all these steps of photostimulated processes are stochastic the typical approach to analyze such processes is based of formal “chemical” kinetics. The major disadvantage of formal kinetics is that in general, it cannot distinguish between the surface and bulk processes. Besides, the elementary entity in heterogeneous systems is a nanosize particle for which the term “concentration” of charge carriers used in formal kinetics makes no sense.

Previously, we reported the results of stochastic simulation by Monte Carlo method of photostimulated processes such as photocoloration and photoadsorption of molecules [1]. Unlike formal kinetics the stochastic approach easily distinguishes between bulk and surface steps and provides the possibility to analyze the dependence of the efficiency of different photoprocesses on the size and shape of the solid particles. Particularly it was shown that this approach results in good accordance with experimentally observed effect of photoadsorption on photocoloration of solids.

In present study we aimed to understand at what conditions the stochastic approach would significantly differ from classic formal kinetics. To achieve this goal we analyze the dependence of the time evolutions of color center and surface active center formation with respect to the defect distribution in the bulk and at the surface of the particle. We infer that each photoprocesses in each individual particle following the stochastic approach are rather different from the average behavior of the particle ensemble. At the same time the time evolution of photoprocesses in the particle ensemble is similar to what can be obtained using formal kinetics tools.

The detailed discussion of the results obtained by stochastic simulations and formal kinetics solutions will be given during presentation.

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Spin polarization of surface states of Bi and Bi/Ag on W(110)

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Effects of spin polarization of electronic states attract increasing attention in recent years, as they have important significance in rapidly developing spintronics. Spin-orbit splitting, firstly founded in semiconductor heterostructure, had already been investigated in many systems [1], and the simplest way to describe this effect is Rashba-Bychkov model [2]. For more complicated situations one can include some factors into RB Hamiltonian, such as in-plane gradient of potential, asymmetry of wavefunctions and influence of interatomic gradient of substrate. In papers [3, 4] spin splitting of surface states of Bi and Bi/Ag surfaces had been shown.

Another way to obtain spin-dependent electronic structure is polarization of initial states at the surface due to the reflection of bulk Bloch states from the surface barrier. Model presented by Krassovki et. al. was successfully confirmed at Bi(111) surface [4]. Then Rybkin et. al. applied this model to W(110) and 1ML Al/W(110) and showed that there is non-Rashba and non-TI (Topological insulator) topology of surface states and surface d-resonances [5]. It is interesting as new type of material and as possible application in spin devices.

This paper is dedicated to analysis of electronic states of system consisting of 1 monolayers of Ag and monolayer of Bi on W(110). System was investigated by angle- and spin- resolved photoelectron spectroscopy with the application of synchrotron radiation. Experimental electronic structure and spin resolved spectra show that quantum and interface states are spin-polarized. In present work we will analyze effects influenced at spin states of W, spin polarization of Bi-surface and quantum well states, and its modification with presence of Ag.

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Study of Al_2O_3 nanolayers synthesized onto porous SiO_2 using X-ray reflection spectroscopy

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The size scaling trend in Complementary-Metal-Oxide-Semiconductor (CMOS) technology implies dramatic decreasing of distance between metallic connections inside integrated circuit. RC signal delay caused by this connection's nearing challenges the further progress now. Thus permittivity of interlayer dielectric has to be strongly decreased e.g. by use of porous low-k SiO_2 .

In order to improve mechanical properties of por- SiO_2 and avoid pores contamination it's necessary to seal the porous surface by deposition of thin continuous film. But this one is nontrivial because there is probability of precursor penetration through the entire dielectric layer. Also the process of film growth can distinguish strongly for deposition on porous and nonporous substrates.

The most optimal method of deposition of continuous homogeneous film on por- SiO_2 is Atomic Layer Deposition (ALD). Al_2O_3 (alumina) is chemically stable and it's deposition on traditional substrates has been broadly investigated. Therefore alumina may be used as model material in investigation of process of film growth on porous substrate.

The structure of alumina films of various thicknesses grown by ALD method on porous silica substrates has been studied using soft X-ray reflection spectroscopy. Also some measurements have been carried out for films deposited on crystalline Si and nonporous SiO_2 .

Continuity of films deposited onto por- SiO_2 was established. It was found that all the synthesized films were amorphous and the ratio of Al atoms with tetrahedral and octahedral environments in the film depended on the film thickness. It turns out that in case of porous substrate the film growth starts from excess of tetrahedrons AlO_4 . On the contrary thin films deposited on crystalline Si consist generally of AlO_6 octahedrons [1]. It was established that thickening of the film led to increasing of AlO_6 octahedrons consistence in the structure and when the thickness reached 13 nm rate the film structure correlated well with the massive amorphous alumina. For thickness more than 13 nm the film structure doesn't depend on the substrate material.

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Influence of annealing treatment on structure of Al_2O_3 -films used as blocking layer for non-volatile memories

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Because of the rapid development of information technology for reliability and duration of storage of information, as well as power devices makes more and more stringent. Therefore it is relevant to develop of new type of media for non-volatile memory. In this work, the nanocomposite films $Al_2O_3(12nm)$ -Si (annealed in N_2 at 1000 °C), $Al_2O_3(10nm)$ -TiN(6nm)-Si (annealed at 1000 °C), $Al_2O_3(12nm)$ -TiN(10nm)-Si (Al_2O_3 annealed in O_2 at 1100°C, TiN annealed in N_2 at 850 °C), $Al_2O_3(12nm)$ -TaN(10nm)-Si (Al_2O_3 annealed in O_2 at 1100 °C, TaN annealed in N_2 at 850 °C), TaN(10nm)- $Al_2O_3(17nm)$ -TiN(10nm)-Si (unannealed) and $Al_2O_3(12nm)$ -Si (no anneal) are discussed. All the films were grown by atomic layer deposition method and subjected to rapid thermal annealing at various conditions. It is known that amorphous oxides (in particular am- Al_2O_3) are key technological oxide in application such as a gate dielectric in Complementary Metal-Oxide Semiconductor devices, in Silicon-Oxide-Nitride-Oxide-Silicon and TANOS (TaN- Al_2O_3 - SiN_4 - SiO_2 -Silicon) flash memories [1]. But defect states in such structures act as hole and electron traps and influence the information retention in electronic devices. Therefore need to reduce the role of defect states. Annealing leads to a decrease in the concentration of defects, and allows to achieve greater uniformity of the structure. In this connection the aim of the current work is to determine the influence of the annealing conditions on the structure of Al_2O_3 films in different systems. All the samples were studied using the X-ray reflection spectroscopy. From the measured reflection spectra the absorption spectra were derived with help of Kramers-Kronig refashion. Analysis of the Al $L_{2,3}$ - absorption spectra points to that the thermal annealing leads to the formation of the crystalline phase γ - Al_2O_3 in all the films. It is this phase provides the desired dielectric properties in terms of band gap and electron affinity [2]. The O K- absorption spectra shows that thermal annealing the system as a whole reduces the oxygen defects but not eliminated. On contrary the stepwise annealing the systems increases defects.

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Graphene on Ni (111) formed on SiO₂/Si substrate. Intercalation of Cu

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The investigation of the electronic structure of graphene, obtained by CVD method on the thin Ni film by Auger electron spectroscopy and X-ray photoelectron spectroscopy was held in this work. We succeeded in the synthesis of graphene by the cracking of propylene C₃H₆ on the surface of Ni (3000 Å) and Ni (1700 Å) on Si substrate. It was observed that on a polycrystalline nickel sample reaction of propylene cracking is not limited. By attempts to intercalate Cu, it was found that in this system several layers of graphene are formed instead of one.

Coulomb embedding in ionic crystals

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In crystal electronic structure calculations, especially for crystals containing point defects, the embedding approach is proved to be useful and convenient. In this approach a finite part of the crystal, referred to as cluster, is considered. The influence of the rest of the crystal onto cluster is simulated by a potential referred to as embedding potential. It consists of two parts - near part, which corresponds to the border atoms of the cluster and far part which corresponds to the atoms situated outside the cluster. The far part of embedding potential is described by the series which is divergent in the case of an infinite crystal. There are different methods of solving this problem and for the ideal lattice the commonly adopted is the Ewald method. However, another method was proposed to calculate the far part of embedding potential [1]. It is based on a new crystal unit cell constructing. In the present paper the far part of MgO crystal embedding potential was calculated with the help of the method described above. Several initial unit cells were used, namely, primitive unit cell with two atoms, cubic unit cell with twenty seven atoms, eight primitive unit cells and eight cubic unit cells. Two latter cases were considered in order to take account of the system full symmetry and, as a result, to obtain data with better precision.

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Study of heterogeneous materials hardness by atomic force microscopy methods

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Obtaining of materials with certain desired properties is of great importance for industry. That is why the various methods of investigation of the properties and structure of materials are essential. Understanding the processes of formation and change of their structure under different treatments will allow to predict the properties of the material.

Use of atomic force microscopy (AFM) and nanoindentation techniques in the study of construction materials provide detailed information on the hardness of single phase components and structural properties of materials up to nanometer scales that are inaccessible to optical metallography methods and thus allow the detection of changes in them at an early stage, which will be of great practical importance.

The aim of this work was to study the structural properties and hardness of the material in different conditions at the micro and nanoscale.

AFM and nanoindentation studies were conducted on widely used in modern industry, low-carbon-steel, taken in different conditions. Conducted AFM research allowed to obtain detailed information about grain and subgrain structure of examined steels and about its change depending on the condition. Obtained data on hardness showed that the hardness of the samples at the nanoscale is very different from the microscopic. Secondly, conducted research showed the possibility of using the nanoindentation to measure the hardness of single structure components of the material such as grains and subgrains. Also it was shown that both micro- and nanohardness significantly change depending on material condition. These changes in hardness were connected with structural and phase composition changes.

The results presented here can serve for the development of methods of non-destructive testing and detecting a change in the structure and hardness of the early stages.

Spin-Doublet Branching Ratio Anomaly in Mg and Al Metals $L_{2,3}$ X-Ray Emission Bands

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We have examined well known since 1930-th Mg and Al metals $L_{2,3}$ ultra soft X-Ray emission bands (USXEB) [1]. In 1960-th a discussion on origin of the sharp peaks near Fermi edges in metal $L_{2,3}$ absorption spectra and USXEB has started [2-4]. It led to a declaration that the dynamical screening of 2p holes by metal valence electrons is responsible for an appearance of the so called MND singularities both in absorption and emission edges. In [2] deviation of the intensity ratio of L_3/L_2 spin-doublet in absorption from the expected 2:1 value was treated by introducing electron-hole exchange scattering, or spin-flip scattering in MND model. In $L_{2,3}$ USXEB L_3/L_2 branching ratios were not discussed because of a large destroyed influence of the self-absorption effect on them. In our work we try to overcome this trouble. Electron beam excited Mg and Al metal $L_{2,3}$ USXEB were registered with resolution about 0.05 eV for the beam energy E_0 varied in the range 0.8...4.5 KeV. The dependencies of measured $L_{2,3}/L_2$ intensity ratios on E_0 were extrapolated to $E_0 = 0$ (absence of selfabsorption). With about 10% accuracy L_3/L_2 intensity ratios were found to be 3,8:1 for Mg and 2,8:1 for Al, much larger than in absorption spectra and in the simple $L_{2,3}$ spin-orbit splitting model. Since for Al metal absolute values of $L_{2,3}$ absorption are known [5], Borovsky-Rydnik model of X-ray emission generation in solids under electron bombardment [6] have been successfully used to check a validity of our extrapolation. Possible reasons of the so strong effect are discussed in the report.

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DFT Calculations of the X-Ray Spectra of Wide Band

Materials Including Dynamical Screening and Auger Effects

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It is well known emission band and absorption edges of simple metals contain features which can't be described by one-electron approximation. In emission bands two many-electron effects may significantly distort a shape of the emission spectra: so-called dynamical screening of core hole in the initial state of emission and auger decay of valence band hole in the final state. The first theoretical model for dynamical screening effects was proposed by Mahan [1] and generalized by Nozieres and De Dominicis (Mahan-Nozieres-De Dominicis (MND) theory [2]). Their theory describes correctly only narrow part of X-Ray spectra just before and just above Fermi level. In this work we propose significantly improved real multiband calculation scheme described the spectral distribution in whole energy scale including MND effect. This scheme may be consider as generalized and improved formalism proposed in [3,4] papers. Moreover we include auger correction procedure [5] to describe low-energy "tail" in the emission band and estimate lifetime of the hole in valence band of simple metals.

Described calculation schemes were applied to Mg and Al crystal metals K and $L_{2,3}$ emission bands. It was got an excellent agreement with experimental high resolution $L_{2,3}$ spectra by including both MND singularities and auger tail effects. In contrast, neither MND, nor the auger effects do not influence on the Mg and Al K emission bands shape. The reasons of this difference are discussed in the report.

Of considerable interest is a discovered effect of asymmetry in MND singularity manifestation in the carbon K X-Ray emission band and K absorption edge of graphene. In the range of K absorption edge MND contribution is very prominent [4], but in the emission band is rather weak. A reason of this effect may be high electron mobility at Fermi level (Dirac point) as discussed in the report. Effect discovered may be used for a study of electrons dynamics in graphene and other systems.

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The study of surface $(5 \times 5)\text{Cu}/\text{Si}(111)$ and $(\sqrt{3} \times \sqrt{3})\text{Au}/\text{Si}(111)$ phases for the interface blocking of the reaction of silicide formation in the system with thin films of Ni on Si(111)

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Investigations of graphene monolayer have attracted enormous interest in recent years due to its unusual electro-physical properties and possibility of using graphene as a basic element in future nanoelectronics and spintronics. The most well-known way of graphene synthesis nowadays is the cracking of propylene on a Ni substrate. However, using of this system for any practical applications is complicated due to metallic substrate. Therefore it is very important to find the technology allowing to transfer the idea of formation of graphene by cracking of carbon-contained gases on a silicon substrate with a thin layer of Ni on top.

Previous experiments showed that the thermal annealing of Ni/Si system up to temperature needed for formation of graphene leads to intense reaction of Ni-silicide formation. However it was suggested that the surface phases $(5 \times 5)\text{Cu}/\text{Si}(111)$ and $(\sqrt{3} \times \sqrt{3})\text{Au}/\text{Si}(111)$ formed at the Ni/Si interface by preliminary deposition of about one monolayer of Cu and Au on top of Si(111) would passivate the reaction of silicide formation. So, the main aim of the work was the study of passivating properties of the Cu/Si and Au/Si interface phases for the Ni-silicide formation. The experiment was devoted to the study of modifications in the structure of the core levels during the synthesis of Au(Cu) monolayers and following Ni deposition for analysis of the reactions of silicide formation. Investigations were carried out by photoelectron spectroscopy of core levels (for study of photoelectron intensity of C, Ni, Au(Cu) and Si peaks) and LEED (to analyze the crystalline structure of the formed systems). It was showed, that in spite of the Au(Cu) monolayers presence, silicide of Ni and of the noble metals were formed in the systems. It greatly influences the process of the surface graphitization, because despite of some passivation of the reaction of Ni-silicide forming thin Au(Cu)-silicide layers formed on top of the system stimulating formation of Ni-carbides instead of graphene. Possible ways of solving the problem will be discussed.

Research of capacity of the system “germanium-liquid crystals”

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A fundamental aspect of the research systems of liquid crystals-semiconductor is in understanding the nature of: the formation of the contact of the organic film and a semiconductor at the atomic level, as well as the mechanism of formation of «thin» and «thick» organic film on the surface of the semiconductor.

The aim of the work is to explore the capacity of the system germanium-liquid crystals-aqueous electrolyte depending on the electrode potential while varying the frequency of the measuring signal.

Significant progress in the current study has been made. The measurements were carried out by the method of field effect in electrolytes. Set the type of the curve capacity in the range from -0.4 to 0.8 V. After liquid crystals introduction capacity is reduced. With the growth of the measuring signal frequency capacitance value is reduced. This is due to the fact that the surface states do not have time to recharge at high frequencies (of about 80-100 kHz), so the system does not receive contribution of the capacity. In spite of the fact that the study is completed, not all of the regularities in the behavior of the capacity understood in the framework of the existing theory.

High-order diffraction of light from 3D Photonic Crystals

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Spatially periodic solid-state structures with the dielectric function, modulated with a period comparable to the wavelength of light, attract close attention of researchers. These structures, called the photonic crystals, have a number of unusual properties. The increased interest in photonic crystals is associated with the possibility of effective light distribution managing within these structures, as well as promising new applications in photonics, laser and optoelectronics.

According to the usual Bragg formulae, with increasing the angle of incidence θ a blue shift of the reflection peak occurs in reflection spectra. However, as we have observed in our experiments, the spectra of some samples apparently demonstrate the opposite, red, shift of the reflection peak when the incidence angle increases, which is in contrast with the standard Bragg law.

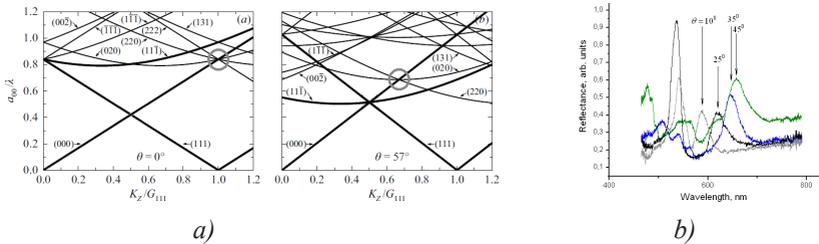


Fig. 1. a) The dispersion curves of electromagnetic field eigenmodes in the “empty lattice” approximation for the photonic structure with a face-centered cubic lattice at two angles of incidence of light, $\theta=0^\circ$, 57° , b) the measured reflection spectra at the angles $\theta=10^\circ$, 25° , 35° , 45° .

In the approximation of nearly free photons (“empty lattice” model), when the amplitude of modulation of the dielectric function of a photonic structure can be considered negligible, the complete system of dispersion curves of electromagnetic field eigenmodes in a photonic crystal was analyzed (results shown in Fig.1a). An explanation for the experimentally observed shift is given, which takes into account a high-order diffraction of light from the photonic crystal planes (222), (220), (020) and (200).

This work was supported by the Saint Petersburg State University Development Program under Scientific Research No. 11.37.23.2011.

Spin structure of W(110) and Au/W(110) surfaces

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The effects of spin splitting at surface have attracted much attention in recent years. It gives rise to the opportunity of manipulation of the electron spin without any magnetic field, which is crucial for the emerging field of spintronics, where it is not the electron charge but its spin that carries information.

In non-magnetic materials the spin splitting is caused by spin-orbit interaction. Especially interesting are crystals with inversion symmetry, where the bulk continuum states are doubly Kramers degenerate, whereas discrete surface states are energy split and spin polarized. This so called Rashba effect occurs due to the presence of surface which breaks the inversion invariance of the system [1]. The similar effect is observable in thin metallic film on the surface of noble metals. The size of spin splitting is depends on the atomic number of substrate material. This can be understood by the following suggestion that the wave functions of 2D QWS penetrate in the substrate surface atoms with high atomic number, where they are strongly influenced by the atomic potential gradient.

Not so long ago the specific spin polarization of bulk continuum states in the surface region has been found [2]. Still the Kramers degeneracy is not lifted for continuum states the surface spin polarization originates from the spin dependent beating between the incident and reflected Bloch waves. In contrast to the Rashba effect for surface states the spin polarization of 3D states is not a consequence of the energy splitting of pure spin states.

This paper is devoted to the investigation of spin effects in W(110) single crystal and thin gold layer on W(110). Since the Rashba-type splitting of sp -derived states of clean W(110) is well explored, the more interesting effects of spin polarization is revealed in the present work. In order to demonstrate the strongly spin-polarized surface resonance in these systems the spin- and angle- resolved energy distribution curves is represented. The analysis of the second derivative of intensity obtained from SARPES measurement provides an important information about origin and character of the surface states for both W(110) and Au/W(110).

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Manifestation of surface and interface modes in the Raman spectra of semiconductor nanostructures

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Semiconductor nanocrystal objects produced interest because of the presence in them quantum size effects in the exciton and vibrational states. Properties of excitons and phonons in them must be considered by finite crystals that, when considering the polar phonon leads to the existence of interface IF modes. The amplitude of these phonons is large near the boundary and decreases exponentially interior of the crystal. In finding the crystal in vacuum interface mode occurs at a frequency ω_{IF} for which the dielectric constant of the crystal is equal to the dielectric constant of the environment with the opposite sign $\epsilon(\omega_{\text{IF}}) = -1$. The excitation of these modes at normal incidence of light on the crystal does not occur. Manifestation of interface modes can occur especially clearly in the objects, in which the size of the surface region of the crystal is comparable with the size of the bulk structure. Important types of such objects are heterostructures, superlattices and quantum dots or nanocrystals. In nanocrystals and quantum wires (whiskers) interface modes due to the smallness volume of the crystal in fact be surface oscillations (SO-phonons), in which the amplitude of movements of the atoms are large near the boundary of nanocrystal and decreases with distance from the surface. In all these cases, the scattering spectra usually observed complex structure of the scattering line near the line of the polar LO modes. This report is devoted to the analysis of such excitement.

In this work we attempt to identify the thin structure of Raman scattering lines of quantum dot binary semiconductor CdSe, CdS and nanowhisker GaAs. Low-dimensional objects (quantum dots and whiskers) were investigated in a liquid medium with different dielectric constant.

In the Raman spectra of quantum dots and nanowhiskers shape of the line of the scattering has asymmetry in a low-frequency region. Found that in the contour of the experimental LO scattering line is always possible to have 2 contributions with frequencies near the maximum and 10-15 cm^{-1} lower in frequency, as it should be in theory. However, the behavior of the experimental spectrum is not consistent with the theoretical interpretation of the model of the mechanical or dielectric confinement. The reasons for such a significant difference at the moment are not entirely clear.

Induced spin-orbit splitting in graphene after Au and Bi intercalation

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Graphene monolayer is a promising material of the nanoelectronics and spintronics due to its unique physicochemical properties and distinctive electronic energy and spin structure.

The spin-dependent valence-band dispersion dependences of graphene synthesized on Ni(111) with the subsequent intercalation of Au, Cu and Bi monolayers are analyzed. We have previously shown that the graphene π band dispersion relations in the region of the K point of the Brillouin zone remain linear after Au intercalation even though the systems exhibit a noticeable hybridization of the graphene π states with the d states of Au [1]. We have also demonstrated a noticeable spin splitting of graphene π -states in systems with intercalated Au [2]. At that time we show that intercalation of Cu does not produce a noticeable spin-orbit splitting of the π states of graphene although both systems demonstrate a similar hybridization of the graphene π states with the d states of Au and Cu. To clarify the role of Au, a comparison with the electronic and spin structure of Au monolayers on Ni(111) without graphene on top was made, and the role played by the original spin polarization of the d states is revealed. This Au-d-band region was further studied in detail by spin- and angle-resolved photoemission for graphene/Au/Ni(111) with revealing the spin dependence of hybridization. On the other hand, intercalation of the sp metal Bi, despite its high atomic number as in Au, does not lead to a noticeable spin-orbit splitting of π states of graphene.

In conclusion it will be showed that for a substrate-induced spin-orbit splitting in graphene π states, that the presence of d states alone as in Cu and the high atomic number as in Bi are insufficient and their combination as in Au is required [2].

Investigations were carried out by the method of angle- and spin-resolved photoemission spectroscopy with application of synchrotron radiation at Helmholtz Zentrum Berlin, BESSY II. Atomic and crystalline structure of the formed systems were analyzed by low energy electron diffraction and scanning tunneling microscopy.

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Electron microscopy and high-pressure Mössbauer study of ringwoodite

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The uppermost part of the Earth's mantle is dominantly composed of (Mg,Fe)-silicates. High-pressure (HP) phase transformations of (Mg,Fe)₂SiO₄ and (Mg,Fe)SiO₃ (perovskite) phases play key role in the transition zone (410-660 km) and lower mantle (660-2900 km) respectively. Due to the steady development of HP techniques the changes in mantle mineralogy with depth can be investigated by laboratory experiments in diamond anvil cells (DAC) that duplicate high mantle pressures.

We studied the sample of Fe-bearing silicates, synthesized from the ⁵⁷Fe-enriched enstatite powder (Mg_{0.9}Fe_{0.1})SiO₃ under relevant pressure-temperature condition of the lower-mantle region ($P=23$ ГПа, $T=2100$ K). The phase composition and microstructure of the sample were characterized by scanning and transmission electron microscopy (SEM and TEM respectively) with energy-dispersive x-ray analysis (EDX). The high-pressure electronic state of iron ions in the sample have been studied by the synchrotron Mössbauer technique in DAC at 16-IDB beamline (Advanced Photon Source, USA).

We defined that the sample exhibit polycrystalline microstructure consisting of particles of 0.1 – 1.5 μm in size separated by amorphous intercalations of 0.01-0.7 μm in width. EDX elemental mapping made it possible to reveal local inhomogeneity of the Fe distribution in the sample. The electron diffraction pointed that Fe concentrated mostly in ringwoodite particles (HP olivine polymorph adopted spinel structure (sp.gr. $Fd\bar{3}m$, $a=8.06$ Å), while the predominate phase was found to be the perovskite (Mg,Fe)SiO₃ ($Pnma$, $a=4.933$ Å, $b=6.902$ Å, $c=4.784$ Å), which was notable for low Fe content.

Determination of Fe-rich ringwoodite phase enabled to interpret HP Mössbauer spectra that were untypical for perovskite structure. At ambient conditions, spectrum reveals two nonequivalent iron species (Fe²⁺)1 and (Fe²⁺)2 in octahedral and tetrahedral sites of the ringwoodite structure. The HP Mössbauer measurements revealed the transition of Fe²⁺ ions in both iron sites from high spin to low spin state in the region of 45-70 GPa.

This work was partially supported by Russian Foundation for Basic Research grants for young scientists (project no. 12-05-31342) and by the Council on Grants of the President of the Russian Federation for the Support of Leading Scientific Schools (project no. NSh-2883.2012.5).

NEXAFS study of various graphite fluorides

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Due to their numerous applications, such as electrodes of primary lithium batteries, solid lubricants, reservoirs for storage of strong oxidant and fluorinating agents (BF_3 , ClF_3 , etc), graphite fluorides (C_nF) are extensively studied since several decades. For all these uses, the chemical and electrochemical properties depend strongly of the C-F bonding into the fluorocarbon matrix [1]. The main aim of the present work is to study x-ray absorption spectra for a set of C_nF ($n=1, 2$, etc) samples synthesized in different ways with a different content of fluorine and a different character of chemical bonding between carbon and fluorine atoms. All measurements have been performed at the Russian-German beamline at the BESSY II [2] and at the D1011 beamline of the electron storage ring MAX-2 [3]. The C 1s and F 1s NEXAFS spectra of CF, C_2F , $\text{C}_{2.5}\text{F}$ as well as of reference samples (HOPG, nanodiamonds) were obtained in the total electron yield mode by detecting a sample current and in the partial electronic yield mode by detecting the electron yield using a multichannel plate with retarding potential of -150V. Based on the comparative analysis of the C 1s and F 1s absorption spectra of $\text{C}_{2.5}\text{F}$, C_2F , CF, HOPG, and nanodiamonds samples it was shown that valence 2s, 2p electron states of all carbon atoms in C_2F , CF are sp^3 -hybridized. A comparison of C 1s and F 1s absorption spectra of C_2F and CF points to the similar strength and the character of the C-F bond in both fluorides. In this case, the intensity of the lowest-energy absorption band in C 1s spectrum characterizes the number of $\sigma(\text{C-F})$ bonds between carbon and fluorine atoms in samples. On the other hand, the C1s spectrum of $\text{C}_{2.5}\text{F}$ reveals the existence of the C-atoms with sp^2 hybridized orbitals which correspond to non-fluorinated graphitic-like areas. The presence of two types of chemical bonding for carbon atoms in $\text{C}_{2.5}\text{F}$ is explained by the hyperconjugation of carbon $2p_z$ states. Thus NEXAFS spectroscopy is shown to be an efficient method for characterization of chemical bonding for different graphite fluorides.

This work was supported by the Russian Foundation for Basic Research (project no.12-02-00999 and no.12-02-31415) and the bilateral Program "Russian-German Laboratory at BESSY".

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E. Applied Physics

Increase conversion coefficient of X-ray emission from a femtosecond laser plasma using nanostructured targets

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Now advanced technologies provide the ability to build compact lasers with high repetition rate sufficiently short pulses. The pulses generated by these lasers, even at low energy, and by focusing the laser radiation make it possible to get a great intensity. During the interaction of ultra-short laser radiation of high intensity and a solid target at the target surface laser plasma is formed where there is a range of effects associated with the behavior of matter in states far from equilibrium conditions. In particular, these laser pulses can be used to implement the X-rays radiation of high power and short duration. With increasing laser intensity and the use of different methods of modifying the target can be expected to increase the efficient generation of X-rays up to 100 keV with pulse duration shorter than a few picoseconds.

These sources of characteristic radiation are mainly used for diagnostics of fast processes. Also their implementation is very important for medical applications, flaw detection, materials radiography, X-rays analysis, X-rays topography, X-rays microscopy, spectroscopy of solids and molecules, X-rays analysis of elemental composition of materials.

One of the main problems is to increase the coefficient of transformation of the laser pulse energy into the energy of the X-ray $K\alpha$ radiation. By varying the parameters of the laser target (geometric shape and size, chemical composition, density, relative position of the chemical elements), you can increase the absorption coefficient and to obtain greater value of the number of fast electrons of laser plasma. That causes an increase of yield of X-rays. It is also known that coating the surface of the laser target periodic micro relief with a height and a period comparable to the wavelength of laser radiation can increase the conversion of laser radiation into fast electrons up to 90% at relativistic intensities of laser pulse.

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Transmission Electron Microscopy of Polycrystalline Alloys $\text{Al}_{85}\text{-Ni}_9\text{-Fe}_2\text{-La}_4$ After Intense Plastic Deformation

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One possible way to obtain nanocrystalline multiphase composites is the intensive plastic deformation (IPD) of alloys under a high pressure. This method was applied to Al-RE-TM alloys, where RE- rare earth (La) metal and TR - transition metal (Ni, Fe). Two as received alloys, namely $\text{Al}_{85}\text{Ni}_9\text{Fe}_2\text{La}_4$ and $\text{Al}_{85}\text{Ni}_7\text{Fe}_4\text{La}_4$ and specimens after the IPD under the pressure of 8 GPa with simultaneous rotation (180° , 360° , $6 \times 360^\circ$ and $10 \times 360^\circ$) were studied by scanning/transmission electron microscopy (STEM), energy dispersive X-ray (EDX) microanalysis and X-ray diffraction (XRD). The microstructural analyses were performed in a aberration corrected TITAN 80-300 TEM/STEM (FEI, USA) attached with EDX spectrometer with ultrathin window (EDAX, USA) and Gatan image filter (Gatan, USA). The specimens for transmission electron microscopy (TEM) were prepared by an electrochemical or ion etching.

It was found that as received alloys exhibits a mixed polycrystalline microstructure containing three or four phases: face-centered cubic a-Al, binary phases Al_3Ni and $\text{Al}_{11}\text{La}_3$ and a phase contained Fe. The Al particles adopted equiaxed morphology and had diameters in the range of 0.5-2 μm , while intermetallic particles found to be elongated with aspect ratio in the range of 2-10 μm . The EDX mapping indicated that both Ni and La atoms could be substituted by Fe. The structure of Al_3Ni particles were orthorhombic (Fe_3C -type crystal structure, Pnma, $a=0.661$ nm, $b=0.736$ nm, $c=0.481$ nm) and $\text{Al}_{11}\text{La}_3$ also orthorhombic (Immm, $a=0.44$ nm, $b=1.31$ nm $c=1.01$ nm).

After the IPD the particle sizes in both alloys changed drastically: we observed equiaxed grains with the size distribution in the range of 5-40 nm. The peak of the distribution depends on IPD conditions and mostly on the rotation.

The phase analysis performed by the study of electron diffraction patterns and high resolution TEM (HREM) together with EDX microanalysis pointed to the presence of the same four phases in the samples: a-Al, binary phases Al_3Ni , $\text{Al}_{11}\text{La}_3$ and Al-Fe particles, presumably $\text{Al}_{13}\text{Fe}_4$. The particle size distribution of each phase also depends on IPD conditions. For example, the $\text{Al}_{11}\text{La}_3$ particles sizes found to be larger than average, however their sizes were too small for accurate analysis. The close interplanar distances in the Al_3Ni , $\text{Al}_{11}\text{La}_3$ and Fe contain phases makes it impossible to separate certain phase with dark-field technique.

The author acknowledges the help of Dr. N.D. Bakhteeva. This work was supported by RFBR grant 10-03-00622-a.

Monte Carlo simulation of electron beam scattering

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The scanning electron microscope (SEM) is one of the most commonly used instruments for observation features on nanometer to micrometer scale. The popularity of the SEM stems from its capability to obtain three-dimensional-like images of samples composed of a very wide range of materials. The SEM operation is based on electron beam - solid interaction which results in electron scattering, secondary electron and Auger electron emission, x-ray generation, etc. These signals can be used for sample characterization.

One of the main tasks of electron microscopy is to receive high lateral resolution. It requires further knowledge of the electron scattering process.

Due the complexity of electron beam –solid interaction processes there is no any precise theory which can describes the behavior of this system. So one of the most easy and accessible methods to study the electron scattering is a computer simulation. The most often used approach for this simulation is Monte Carlo method.

Monte Carlo simulation enables to receive the information about different useful electron scattering parameters such as electron elastic scattering angular distribution, the most probably electron energy losses, the electron backscattering coefficient and the secondary electron emission coefficient and others. Characteristics mentioned above mainly depend on electron beam energy and the sample composition so the electron beam seems to be a promising offer for the sample composition investigation.

Here we present some Monte Carlo simulation data regarding the lateral electron current distribution and material properties of the sample radiated by the focused accelerated electron beam. Electron backscattering coefficient values for Si, Al, Au are obtained and compared with known experimental data. Also the comparison is carried out between our results and well-known CASINO pack ones in number of characteristics such as backscattered electron energy distribution and backscattered electron lateral distribution. A sufficient agreement is achieved.

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Application of audible range acoustic waves for nondestructive testing

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In science and technology has long been used a non-destructive testing and a different defectoscopy methods. In particular, a ultrasonic testing is well-developed. This is due to good resolution of an ultrasound and a possibility of using a model of geometrical acoustics (wavelength $\lambda \leq$ size heterogeneity). Therefore, it is widely used to control a metal work and welding. However for complex periodic structures as masonry, the applicability of these methods is limited due to a strong attenuation of ultrasound and high ability of brick and cement cracking. Even to control a relatively homogeneous structure as concrete, the ultrasonic methods often give conflicting, poorly reproducible results.

This paper proposes a method of monitoring a state of the brickwork with an audible frequencies. Source of a sound pulse is a regular steel hammer weighing about one kilogram. The spectrum of a fall of the hammer on a brick contains a frequencies up to 15 kHz, i.e. a shortest wavelength is approximately 10 cm. Thus, one can examine the state of masonry in a broader sense, ignoring small local heterogeneity. Typically, these details (small cracks in the brick and cement, hammered nails and various metal inserts) do not matter.

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Application of sapphire nanostructured substrates for obtaining perfect crystalline semiconductor films and regular metallic nanostructures

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Different microelectronic devices, optics for visible light and X-rays usually require the super-polished substrates of different crystalline materials. In the present report we show the possibilities to use the nanostructured sapphire substrates for this purpose. It is demonstrated that the terrace-like structure of such substrates gives the possibility to obtain single-crystal thin layers of CdTe on top of them. More that such structure of substrates allows creating of oriented gold nanowires on the whole surface of substrates. We developed the laboratory technology to obtain the predicted nanostructure on the top of single-crystal sapphire (fig.1a) and appropriated methods to control the roughness of a surface and deposited coatings less than 0,2 nm.

Making use of fabricated nanostructured sapphire substrates gave us the possibility to find an appropriate surface parameters and epitaxy conditions which provided better structural perfection of CdTe films.

The obtained values of surface nanostructure periods are close to the wavelength of optical range. It was suggested to cover these surfaces with an appropriate material for optical applications. During the research of gold deposition on nanostructured sapphire substrates by the developed technique the conditions of golden nanodots (fig. 1b) and nanowires formation were found. The density for nanodots is about 20-25 per square micron. The period of nanowires is about 40-50 nanometers. Further optical experiments have revealed the peculiarity in the s-polarized optical wave reflectivity. This effect appears when the polarization vector coincides with the surface structure direction and is determined by resonance between s-polarized wave and surface plasmons. In the conclusion we want to note that such substrates are also perspective for use in a nanoplasmoniks and protein crystallization.

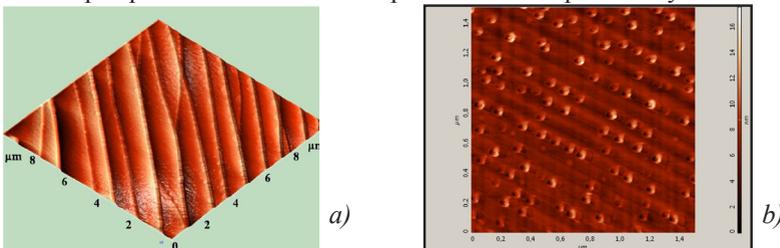


Fig. 1. Image of nanostructured sapphire surface (a); images of golden nanoparticles (b).

Impact of radioactive fallout from Chernobyl and Fukushima on the environment of Leningrad region

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The radioactivity of the environment considerably was affected by the accident occurred at the Chernobyl and the Fukushima nuclear power plants. As a result of these accidents released radionuclides (more than 10 thousand PBq) from discarded nuclear reactor materials spread around the world.

Soon after the Chernobyl accident the investigation was carried out to notify the pollution of Europe by gamma-spectrometric survey from planes. Although this method gives uncertain data of radionuclide activity in the study area, it allows to obtain an overall picture of the contamination. Thus, according to research in the Leningrad region was found ^{137}Cs from Chernobyl in Kingisepp and Lomonosov districts with an estimated activity 1–5 Ci/km² [1].

In order to get a more complete picture of the influence of accidents on radioactivity of the environment of the Leningrad region, in the study was used another method providing more reliable information about the radioactivity, which consists in the investigation of environmental objects by semiconductor Ge gamma-detector. According this method analysis of the sample of topsoil showed a significant expansion of the border of radioactive zones. So the activity of ^{137}Cs of the samples from the contaminated area according [1] is approximately 370 Bq/kg, but there are places outside the polluted zones there activity of ^{137}Cs is more than 620 Bq/kg. The radioactivity of ^{134}Cs with $T_{1/2}=2$ years, which can identify the Fukushima trace, doesn't exceed 0.3 Bq/kg. The map [1] can be corrected using the obtained data in the study region.

In this work was analyzed movement of the radioactive plume from Chernobyl and compared it with depositions of ^{137}Cs in Europe [2] and an updated map of the Leningrad region. On the basis of this was revealed that the number of cesium, which has been laid at the considered territory, is in proportion to the number of precipitation from clouds, which has absorbed the cesium in Chernobyl. On the assumption of this, the peculiarities of atmospheric deposition were considered in the different areas in the study region, regularities of radionuclide deposition in soil were reveal and the most likely places, which may be exposed by radiation from the next accident, was determined.

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Rotation of nonspherical dust particles in weakly magnetic field

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The rotational dynamics of single dust grains in a weak magnetic field is investigated on a kinetic level. The angular velocity of spinning prolate grains varies as magnetic induction increases to 250 G. Spinning dust grains are found to flip over only when the magnetic field magnitude is changing. The results demonstrate that dusty plasma has paramagnetic properties. Qualitative interpretations are proposed to explain newly discovered phenomena.

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Development of a helium flow simulator flexible to changes in geometry of an exhaust channel

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Liquid helium's low boiling point (-452 °F or -269 °C) makes it ideal for cooling the magnetic resonance imaging (MRI) magnets that create the magnetic field by means of which medical professionals need to develop the detailed images of body tissue that can eliminate exploratory surgery and biopsies. In MR facilities using superconducting magnets there is a rare possibility that the liquid helium coolant may suddenly evaporate. If the gases are not vented to the outside, they may pose an asphyxiation hazard. In order to provide safe operation of MR equipment an appropriate exhaust system should be installed to vent gases to the outside in the event of a quench. It's required to estimate most optimal geometry and characteristics of exhaust channel before installation based on model approaches.

ANSYS CFX that is widespread module for fluid dynamics simulation imposes constraints on frequent changes in the geometry of a model required for the above-mentioned problem. For this reason to solve the problem of flow distribution the simulator of helium exhaust channel has been developed according to another approach by which exhaust system was represented as a set of connected components with different geometry: bends, expansions, valves [1]. On the basis of components geometry hydraulic resistance and total pressure losses caused by given components in pipe was calculated [2]. In accordance with graph representation of the model author introduced mass flow and energy conservation laws based on Kirchhoff's laws whereupon resulting system of nonlinear equations was solved by Newton's method.

Given approach make it possible to change geometry in the graph-based model of exhaust channel easy using developed library of components. In spite of all simplifications according to given approach the results of simulation well correspond to the reference points in the Ansys CFX model.

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Innovative non-chemical etching technology

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This work relates to an innovative non-chemical etching technology, using entirely physical process.

“Etching” is a key process of mass production in semiconductor and micro electrical mechanical systems (MEMS) industries. During the process, many kinds of organic chemicals are used. Organic chemicals are very harmful to environment and are difficult to eliminate. Such a fact also leads to difficulties to make medical production.

There are some non-chemical etching process using ion beam, electron beam, and laser beam. However, due to some technical difficulties such technologies are usually used to make samples, not for mass production.

In this work we present an innovative etching method using special type of plasma. The process is entirely physical, and can be used for mass production. According to prior estimation, the etching speed of this method is comparable with that of chemical etching, with limitation of accuracy of tens of nanometer.

By our opinion, such technology is most suitable to making medical productions, and, moreover, allows one to etch future organic or biological materials, which probably will be destructed by chemicals used in nowadays etching processes.

Optimization of flow deceleration by MHD interaction

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This work relates to the technology to control flow by using magneto hydrodynamic (MHD) interaction.

Here we take care about the MHD interaction of gas flow with ionized gas around a cylinder with current passing through its axis to form non-uniform magnetic field, and whose axis is perpendicular to the flow direction. The effect of flow deceleration by MHD interaction is concerned. Such a situation is interested in aviation application .

As showed in the previous work [1], was obtained the distribution of current and Lorenz force. In this work we further consider the power of ionizer. Using results of work [2], we can calculate the electron density in the ionized zone under some given power of electron beam.

As a result we obtained the optimized width of MHD interaction zone, which leads to maximum decelerate the flow under given power of ionizer.

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F. Optics and Spectroscopy

Dimetacyano azobenzene molecules on Bi (111) substrate: the local atomic structure study

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Photoisomerization is a process during which changes are accompanied by corresponding changes in the chemical structure. One of materials with ability to photoisomerization is the azobenzene molecules in a gas phase and a solution.

It is known that the DMC azobenzene molecules change their geometrical structure after irradiation by X-rays or UV during the photoisomerization of trans- and cis-isomers. The two isomers can be switched with particular wavelengths of light - ultraviolet or blue light. The *cis* isomer is less stable than the *trans* (for instance, it has a distorted configuration and is less delocalized than the trans configuration) [1]. This property makes azobenzene molecules suitable for using as building blocks in molecular motors and optical storage devices. On the other hand, deposition of molecules on surfaces leads to a restriction of the molecular switch, which occurs due to the fact that the isomerization process becomes influenced not only by an atomic bonding in the molecule but also by interactions between molecules and surroundings [2].

In the present work the theoretical models of local atomic structure of DMC molecules deposited on a Bi(111) substrate before and after irradiation were studied using density functional theory (DFT). Also, theoretical simulations of the X-ray absorption near edge structure (XANES) spectra were done. As a result of the calculations the low-energy structure for DMC molecules on Bi(111) substrates was obtained.

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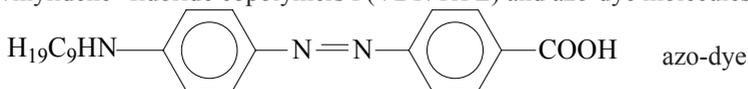
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Multifunctional one-dimensional photonic crystals

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Photonic crystals are currently of great interest because of their peculiar optical properties. In our case 1D-PCs consist of alternating layers of vinylidene fluoride copolymers P(VDF/TrFE) and azo-dye molecules:



$(-\text{CH}_2-\text{CF}_2-)_n(-\text{CHF}-\text{CF}_2-)_m$ - copolymer P(VDF/TrFE)

The sub-layers of azo-dye material provide an effect of the photoinduced optical anisotropy (POA) [1]. The POA effect allows inducing the optical anisotropy by irradiation of the films by linearly polarized light. As a result the photonic band can be made dependent on the light polarization state [2]. Using the external irradiation the patterning on the film's surface can be done.

From the other side, the ferroelectricity of P(VDF/TrFE) sublayers allows electric field control of the photonic band. The computer simulation of investigated effect shows, that the value of the electro-optic effect achieves the optical transmission in several percents (see Fig.1). Such a strong effect can be easily used in optical applications.

Experimentally the 1D-PCs were made both by vacuum deposition and Langmuir-Blodgett technique. The optical anisotropy is induced by polarized laser irradiation ($\lambda=405$ nm, $I\approx 50$ mW/cm², $\Delta t=5$ min). After this recording process the long molecular azo-dye axes are oriented perpendicular to the direction of the light polarization vector, which results in optical dichroism and birefringence. After the POA induction the photonic band strongly depends on the light polarization state.

Thus the POA effect opens new possibilities in controlling the photonic properties of 1D-PCs both by electric field and polarized light irradiation.

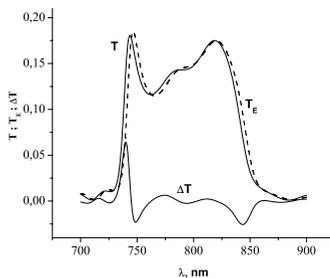


Fig. 1. Transmission spectra of the photonic heterostructure for the linear polarized light (polarization angle +45° to the x-axis). Curves T and TE correspond to the switched-off (T) and switched-on (TE) electric field $E=120\text{V}/\mu\text{m}$, $\Delta T(\lambda)=T(\lambda)-T(\lambda)$ is an electro-optical effect spectrum.

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Formation of dark states via coupling between laser light and sodium HFS

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Interaction between strong laser field and hyperfine level systems leads to formation of dark states [1]. Sodium $3S_{1/2}(F=1,2)$ levels are connected with $3P_{1/2}(F=1,2)$ levels via strong coupling laser. Energy of formed dark states is estimated through measuring of luminescence signal from $7D_{3/2}$ level coupled with dressed states via weak probe laser of changing frequency. Excitation spectrum of $7D_{3/2}$ presents main intense peak with small peaks around. Increase of Rabi frequency of coupling laser makes small peaks scatter whilst the main peak remains in its position. We explain observations using dressed-state formalism. We show that the phenomenon indicates formation of dark states.

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About measuring of spectral lines intensities from volumetric sources using a CMOS-camera

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All emitting plasma sources of light are volumetric. Traditional scheme of measurements in classical non-laser spectroscopy contains a projection of volumetric source on a slit of a spectrograph, light flux dispersion in the spectrograph and signal registration using a CMOS-camera. The big advantage of the CMOS-camera is in simultaneous registration of the full image by matrix in the camera without movement of an image along the slit. Image file analysis allows to retrieve data about pixel brightness in different cross-sections of the source. From this data a large amount of information can be obtained, it allows to investigate different non-stationary processes in details. In the present work an experimental setup was constructed in which one can register an emission of spectral lines from the discharge positive column in noble gases. Due to construction of the tube the length of the positive column under investigation can be 40, 30, 20, 10 cm. In Fig. 1 an example of the image obtained by the camera is given. The program that can retrieve data from RAW-image file was developed. It allows to obtain radial distributions of spectral lines intensities. An example of the radial distribution is given in Fig. 2. The setup has high spatial resolution because of a narrowness of instrumental function (about 4-5 pixels).

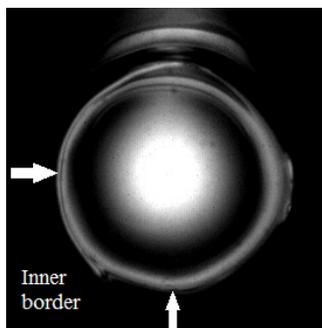


Fig. 1.

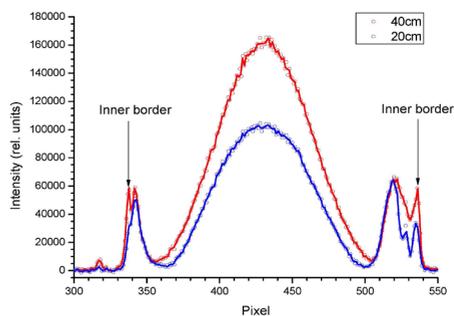


Fig. 2.

Peripheral points of the image are formed by the light fluxes which are non-parallel to the optical axis. This is a defect of this registration scheme. Thereby a usage of corrections that eliminate this defect is needed, especially if the radiation is reabsorbed within the source.

Modelling a method of generation of unipolar pulses from nonunipolar optical pulses by interacting with a quadratic nonlinear medium

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A unipolar electromagnetic pulse is a pulse with nonzero value of the static component of the Fourier spectrum of its real electric field:

$$\int_{-\infty}^{\infty} dt E_i(r, t) \neq 0$$

Here a way to generate unipolar pulses from nonunipolar optical pulses incident normally on a layer of a quadratic nonlinear medium is proposed.

One of the possible applications of unipolar pulses in the future could be, for example, the acceleration of the electrons (in particular in the plasma as proposed in Ref. [1]), which eventually could lead to making of an X-ray source. However, in the scientific literature, many authors express their doubts about that a source of unipolar pulses can be actually constructed, despite the fact that the unipolar pulse is a formal solution of Maxwell's equations. In the contrast to this point of view, in the paper [2] a way to generate unipolar pulses from nonunipolar optical pulses incident normally on a layer of nonlinear medium has been proposed. Using the finite difference time domain (FDTD) method we have made a direct approximation-free numerical integration of Maxwell's equations and recorded the spectra of an incident, transmitted and back-reflected pulses. Indeed, it appears that in the spectrum of the reflected from the boundary "vacuum/nonlinear dielectric" a pulse with significant static component appears. We placed a low-bandpass filter prior to the detection of the reflected pulse and obtained the bell-like shape, as desired.

Then in order to obtain a bigger static component we have modified the geometry of one-dimensional problem. To be more specific, we have replaced the "thick" layer of the nonlinear medium with a multilayer structure and thus increased the number of reflections from the outer boundaries of the nonlinear layers. In short perspective we plan to shift from the one-dimensional problem to a two-dimensional geometry, waiting for more pronounced diffraction effects, which in turn are heavily pronounced for low-frequency radiation.

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Structural and luminescent properties of YAG:Nd³⁺ nanophosphors

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In recent years inorganic phosphors have been extensively investigated for the applications to various types of display panels, such as plasma display panel, vacuum fluorescent display and field emission display. Yttrium aluminum garnet, Y₃Al₅O₁₂ (YAG), is a well-known inorganic compound and is also widely utilized in the optical field. YAG single crystal doped with lanthanides, such as Nd³⁺, is used in solid-state lasers and the poly-crystals of YAG doped with different color centers are employed as phosphors in the cathode ray tube displays.

The aim of the present work is to study the structural and optical properties of nanocrystalline YAG powders doped with neodymium rare-earth ions and determine the synthesis conditions of the most efficient phosphor. Also kinetics of luminescence was investigated and the lifetime of the excited level of neodymium ions (⁴F_{3/2}) was calculated.

Structural properties of nanophosphors sintered at different temperatures were measured by X-ray diffraction (XRD). When the sintering temperature was increased, the diffraction intensities of the sintered powders increased and the width of the diffraction peaks decreased. Morphology of nanoparticles was investigated by scanning electron microscopy (SEM).

Luminescence properties depend on many various factors such as the composition of the host, the method of synthesis, the size and shape of particle grain, the synthesis temperature and the concentration of the ligand.

The dependence of luminescence on the concentration of dopant ions has been studied. The optimum concentration of Nd³⁺ ions was determined to be 0.5 mol.%.

Excitation and emission spectra of YAG:Nd 0.5 mol.% were measured. The most intensive emission transition is ⁴F_{3/2} – ⁴I_{9/2} with maximum at 884 nm.

In order to determine lifetime of the excited state of neodymium the luminescence kinetics has been investigated. We monitored luminescence of the most prominent transition ⁴F_{3/2} – ⁴I_{9/2}. The decay curve was fitted to a single exponential function.

The memory effect appearance in pulsed low-pressure discharge in nitrogen

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If power supply voltage is too low for self-sustained discharge ignition, it nevertheless may be initiated by additional affect (e.g., by the Tesla coil spark). It is known that for the *periodic sequence* of discharge pulses igniting one of the pulses only may be sufficient, all the subsequent breakdowns occurring with no initiating. It implies that discharge pulse facilitates the next breakdown. Another manifestation of this effect was observed when studying time delay between the moment of supply voltage applying and the breakdown [1] (in these experiments short discharge gaps were used). The preceding discharge pulse causes the delay to decrease. For that case, the term *memory effect* (ME) of the discharge gap is used. In this work, we use the same term for describing the influence of preceding pulse discharge on the voltage breakdown. Another important feature of our study is that the discharge in a long tube (similar to one used in discharge lamps and gas-discharge lasers) is considered. Note that no analogous measurements have been done before.

The aim of the present work is to obtain information about the ME in pulsed discharge in a long tube filled with nitrogen at low pressure (1 Torr). For this purpose we performed experiments in which breakdown of the tube of 40 cm length and 3 cm i.d. was produced by sequence of pairs of high voltage pulses 10 ms duration with amplitude up to 3.5 kV. One of the electrodes (the cathode) was grounded. Time interval between the pairs was 200 ms, whereas the time delay between the pulses of the pair was varied from 0.1 to 20 ms. Another variable was the steepness of high voltage applied to the tube.

It was found that the breakdown voltage V_{b2} of the 2nd pulse in the pair may essentially differ from that of the 1st pulse (V_{b1}), i.e. the ME was observed. The most unexpected result was that for some time delays the V_{b2} value was higher than the V_{b1} , that is the preceding discharge inhibited the breakdown (abnormal ME) rather than promoted it (normal ME). The possible mechanisms of the effect are proposed.

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Unidirectional dye laser generation with two-photon pumped by femtosecond pulses

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In work we have studied the generation of laser on solution of organic dye: Rhodamine 6G in ethanol.

Pump was realized by the pulses of femtosecond laser “Pulsar 10” with the following parameters: the wavelength is 790 nm, pulse duration is 50 fs, pulse energy is 1 mJ, the repetition rate is 10 Hz.

The effect of unidirectional generation due to a traveling wave of population inversion is created with a femtosecond pulse propagation in the active medium.

In this report spectral and spatial characteristics of the generation are discussed, comparison with the known characteristics of dye lasers with single-photon pumping is carried out.

In particular, the generation of two-photon pumped by femtosecond pulses followed by filamentation, i.e. process of self-focusing of radiation, leading to the formation of channels of intense radiation as a result of self-organization. Setting the spatial modulator of the pump near the input end of the cell with dye leads to ordering of filamentation.

An example of the spatial distribution across the beam generation during a modulator is shown in Fig. 1.

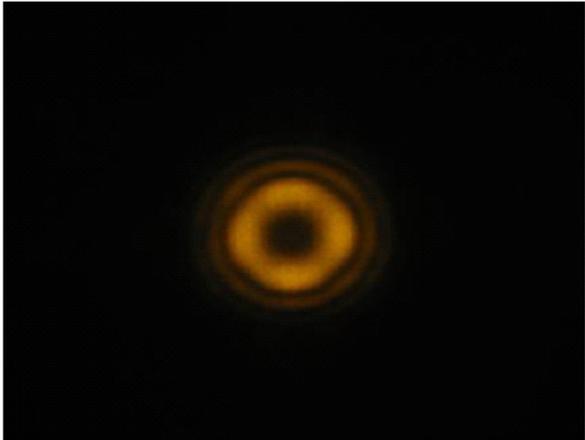


Fig. 1. The spatial distribution across the beam generation during a modulator.

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RIXS spectroscopy to study 5d transition metal complexes

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X-ray spectroscopic methods of local atomic and electronic structure investigation proved to be very effective for a wide range of materials. Element- and sometimes site-selectivity together with the possibility to study non-crystalline materials (like liquids or gases) make them favorable for many scientific tasks in the field of physics, chemistry and materials science. However, for heavier elements like 5d transition metals, standard total fluorescent yield XANES and EXAFS techniques tend to deliver less information compared to the case of lighter elements, because the spectral features are much less sharp due to the dramatic increase of core hole lifetime broadening with the rise of Z (e.g. 0.4 eV and 5.16 eV for Cu and Os L₃-edges respectively). In order to solve this very problem and to gain additional information about the electronic structure of the studied compound, resonant inelastic X-ray scattering (RIXS) experiment can be performed [1]. In this case only the fluorescence photons with the certain energy are detected, due to the presence of analyzer crystal positioned between sample and detector on the Rowland circle. Energy of the detected photons is usually set to be close to the corresponding emission line and can be scanned together with the incoming photon energy, which results in three-dimensional plots (RIXS maps). Such approach gives more information than standard X-ray absorption techniques, because RIXS maps show not only the projection of the unoccupied DOS, but also the occupied one, due to the emission energy scan. Moreover, diagonal plot through the RIXS map (which correspond to constant emission energy, usually set on the maximum of the emission line) results in so-called high energy resolution fluorescence detection (HERFD) XANES spectra, which have much better resolution compared to the standard ones.

To illustrate the benefits of RIXS spectroscopy, experimental RIXS maps, TFY and HERFD XANES spectra for some Osmium compounds (OsCl₃, [Os(bpy)₂(CO)Cl]⁺, Os₃(CO)₁₂ and [(η⁶-biphenyl)Os(bpy)I]⁺), measured on ID26 beamline at ESRF facility are presented together with the results of their theoretical analysis by means of advanced DFT calculations.

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The determination of sizes' levitating particles in the glow discharge of dusty plasmas

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By method of extraction from the discharge chamber study the distribution of dust particles levitating particle size and form-factor. Separately investigated two dust traps that exist in the glow discharge and in the strata above the bottom wall of the tube near the turn of the current channel. Found that in the strata distribution polydisperse particles of arbitrary shape in size is bimodal, due to the simultaneous levitation of particles of two form factors. For polydisperse spherical particles observed levitation of the particle size, due to the separation of particles in wall thickness. If identical discharge particle size in neon is always slightly higher than in krypton, the particle size is trapped in the stratum is much larger than the size of particles in the trap on the wall of the discharge tube. The exact determination of the shape and size of particles allowed to make for dust traps evaluation of the electric field. It is shown that the glow discharge can be used as a device for the separation of dust particles in a wide range of sizes.

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Destruction of polyelectrolyte microcapsules modified with fluorescent dyes by laser irradiation

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Polyelectrolyte microcapsules, fabricated by alternative adsorption of oppositely charged macromolecules on colloidal particles, are prospective technological objects due to their monodisperse size distribution, simplicity of controlling their permeability, and a wide variety of the wall materials. Inclusion of dye molecules into the polyelectrolyte shell of capsules could provide sensitivity to the laser radiation. Irradiation of modified capsules by laser with wavelength corresponded with the absorption band for the dye can result in effective excitation of dye molecules and energy transfer to the capsule shell. It can lead to rearrangement and destruction of the shell. This method for remote release of the encapsulated material can be used for inducing the drug action in particular place of an organism.

Two different fluorescent dyes Rhodamine 6G and Fluorescein isothiocyanate (FITC) were included in the capsules shell. For inclusion of FITC in the shell two different approaches were used – adsorption of the dye and inclusion of chemically bounded dye. Size distribution of the capsules was calculated using the correlation spectroscopy of the scattered light. The capsule suspension was irradiated by laser with wavelength 532 nm, which is within absorption bands of the both dyes. This irradiation had practically no effect on the size distribution of capsules without dye and significantly changed it for capsules with Rhodamine 6G and for capsules with adsorbed FITC. This results show that destruction of the capsules takes place. Difference of effect of laser irradiation on capsules with chemically bounded and adsorbed FITC molecules was shown. Destruction can be caused by effective absorption of the incident radiation by the dye molecules and following transfer of energy to matrix, surrounding the molecules. It is possible when oscillatory frequencies of dye and polymer molecules coincide. In this case transfer of oscillatory energy by inductive-resonance mechanism occurs. It results in local non-equilibrium heating of dye molecules surroundings and breaking of bonds in the capsule shell.

This study was supported by the Program for Basic Research of the Presidium of the Russian Academy of Sciences № 22 and Russian Foundation for Basic Research, Project № 11-03-12164.

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The investigation of the optical switching process in the setting of the laser femtosecond pulse four-wave interaction in the optically-dense Rb vapor

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In the publication [1] you can see the experimental research results of the non-linear beams interaction [1] you can see the experimental research results of the non-linear beams interaction of two continuous-wave Ti:Sapphire lasers tuning to the resonant Rb atom transition frequency. Laser beams are propagated to each other. The induced scattering emission, appearing in such a case, can be switched by the control laser emission signal, what allows authors to talk about the all-optical switch scheme realization. It is worthwhile to say that the switching characteristic time is about a few microseconds, what limits the band pass to 1MHz.

In this report the research results of the optical femtosecond pulse switching process in the optically-dense Rb vapor are given. Laser (“Pulsar 10”) emission pulses with following properties: wavelength 790 nm, impulse time 50 femtoseconds, pulse energy 1 mJ, were sent to the forming optical system, which formed two

pulses converging in the Rb vapor cell center with 0,02 rad angle. Third (signal) beam travels in the plane which is perpendicular to the plane, where two first pump beams are situated. The interaction on the cubic nonlinearity in the Rb vapor leads to the output forth beam forming (nonlinear response) which is the result of the forth-wave interaction of the pumps beams and the signal-carrying beam. The field distribution picture of the long-distance screen which is situated on the cell outlet is given in the Fig. 1.



Fig. 1.

In this report the spectral characteristics of the nonlinear medium response and its' dependence from one of the pump pulses delay and (or) the signal pulse are discussed. The obtained results allow us to claim that the realized scheme discovers the opportunities of the all-optical switch with the femtosecond response time with the THz-band pass creation.

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Laser-induced modification of trisulfide of arsenic glass to produce a diffraction grating inside it

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Chalcogenide semiconductor glasses exceed silicate ones in a number of parameters like a refractive index, a wide window of transparency in the infrared (IR) region. Due to this parameters chalcogenide glasses are widely used as a IR visualizers, a working element in optical storage devices, etc. These materials are considered to be promising for use as optical media for the various elements of integrated optics.

In this work we prepared diffraction grating inside the sample of amorphous trisulfide of arsenic (As_2S_3) using a continuous laser irradiation from a semiconductor laser. The wavelength of laser is 785 nm. An influence of the laser radiation on structural changes of the sample has been investigated. It has been found that a number of heteroatomic bonds (As-S) decreases while a number of homoatomic ones (As-As, S-S) increases. In this experiment dependence of laser parameters like laser power and rate of scanning on the structure of the sample was studied. The power was changed from 25 mW to 100 mW. It has been discovered that the best quality lines were produced with 100 mW-powerful light. After this, speed of the assembler was changed from 1 to 10 $\mu\text{m/s}$, the better one was 1 $\mu\text{m/s}$. At the speed of 10 $\mu\text{m/s}$ there was not any modification.

Finally we built the diffraction grating inside the sample of amorphous trisulfide of arsenic.

Dependence the structure angular velocity of the concentration of particles in the dust structure

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The mechanism of rotation of dusty structures formed in striations in magnetic field has not unique interpretation in present time [1-3]. One of the hypotheses assumes that the dust particles get the momentum from the ions moving from structure center and turning under the influence of magnetic field [3]. The increasing of dust particle concentration in structure results in the increasing of the value of negative volume charge inside the structure and therefore in the rising of electron temperature and ionization rate. Growth of the plasma concentration inside structure cause the rising of ion diffusion flux from structure which lead to increasing the magnitude of ion drag force acting on the particles in the structure.

In this work the experimental investigation of dust structure rotation in small magnetic field (less then the values at which the structure rotation deceases) are presented [3]. The dependence of structure horizontal section density on magnetic field is obtained. This dependence has ascending character in the range of magnetic field from 0 to the value corresponding to maximum of angular velocity of rotation of structure. The same result is obtained in three gases: Ne, Xe end Ar.

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NEXAFS study of the unique copper-containing biomineral from endemic Baikal Lake sponges

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The investigation of chemical structure peculiarities and identification of mineral and organic constituents within nanostructured biocomposites is a challenging task in modern material science. Recently, were discovered blue colored endemic sponges from Baikal Lake, which synthesized unknown copper-based biomineral. At present, chemical states of copper atoms within this structure are unknown. The determination of the copper location within organic templates and inorganic minerals is a crucial task.

The main aim of present research is investigation of chemical structure and composition as well as valence state of the copper within this unique copper-based biomineral by near edge X-ray absorption fine structure (NEXAFS) spectroscopy [1].

During this investigation comparative NEXAFS studies (Cu2p-, C1s- and N1s-spectra) of different copper compound including minerals (Chrisocolla, Malachite, Azurite), biominerals (moolooite), benchmark samples (CuO, mix CuO+Cu₂O, copper phosphate, Cu-metal) and native Blue Sponge dried in standard condition were carried out at the Berliner Elektronenspeicherring für Synchrotronstrahlung (BESSY) using radiation from the Russian-German dipole beamline (RGLB).

In the result of comparison and interpretation of Cu2p spectra of Blue Sponge, Cu-compound, minerals and biomineral we assume that copper atoms within copper biomineral produced by endemic Baikal Lake Blue Sponges is bivalent. Moreover by the comparison the spectra of Cu and non-Cu-containing sponge, we suggest that Cu-atoms interact with the protein side chain nitrogen atoms.

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X-ray study of the C₆₀ high temperature modification at Ar moderate pressures

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The C₆₀ modification under pressure and high temperature were studied for more than one decade, however there are still on the pressure-temperature transitional phase grey areas diagram of C₆₀, even at low pressures. The disordered graphite-type (sp²-bonded) carbon phase synthesized from fullerite under moderate pressures from 0.1-0.2 GPa at high temperatures 900–1300 K can be identified from structural data as nanographite which has unique properties such as high hardness and elasticity with a density less than that of graphite [1]

The set of new nanocarbon samples were produced by hot isostatically pressing (HIP) in piston-cylinder high-pressure device using high-temperature (600-1300 K) treatment of pure C₆₀ (99.9%) in atmosphere of Ar at moderate (0.1-0.2 GPa) pressures attainable for large-volume high-pressure apparatus. The samples for the investigation by TEY-method were prepared by pressing in the surface of the In-metal. The NEXAFS-experiments were performed at BESSY-II using radiation from the Russian–German beamline.

In the result of the investigation we can assume, that during HIP modification at moderate pressures 0.1 GPa and temperature above 1100K in Ar the fullerite crystal lattice is distracted, and the fullerenes are transformed into peapods-like structure, which mostly consist of hexagons. The NEXAFS C1s-spectra of the modified C₆₀ and HOPG and nanotube are in good agreement. Besides the hypothesis about peapods formation is clearly correlated with fullerene fusion model introduced by S. Ham et al. [2] using a finite sequence of generalized Stone-Wales transformations, which involve only bond rotations and avoid bond breaking.

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Influence of the solvent-solute interactions on geometry and spectroscopic parameters of hydrogen bond studied by means of computer simulations

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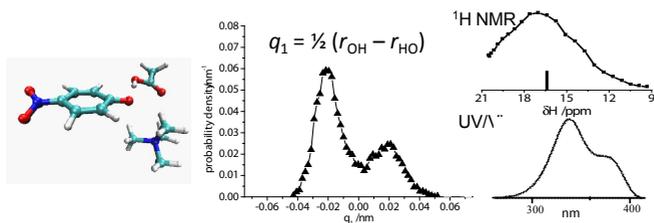
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We studied influence of solvent-solute interactions on geometry of a strong hydrogen bond formed between *p*-nitrophenol and acetate anion dissolved in CD₂Cl₂ with tetramethylammonium as cation (Fig. left). We carried out *ab initio* molecular dynamics calculation of the system using CP2K [1] simulation package. We show that a wide ensemble of H-bond geometries exists in the solution (Fig. center), and this structures interconvert into each other. Using hydrogen bond correlations [2] we calculated distributions of NMR and UV-vis absorption spectroscopic parameters of the studied system (Fig. right). This work is supported by the German-Russian Interdisciplinary Science Center (G-RISC) funded by the German Federal Foreign Office via the German Academic



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Quantum-chemical investigation of the Ru(II) chloro-bis(bipyridyl) complexes with substituted pyridine ligands

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Ruthenium(II) complexes with polypyridine ligands have a unique combination of photophysical, photochemical and redox properties, and chemical stability. The interest in these compounds is mainly due to their prospective use as “antenna complexes” in solar energy conversion, biotechnology, design of luminescent sensors and photochemical molecular devices. Directed synthesis of new complexes with a set of predetermined characteristics requires understanding the interrelation between the composition of the coordination sphere and the electronic structure of the compounds and their photophysical parameters measured in experiment. The study of series of complexes in which the composition of the inner coordination sphere is purposefully varied is an efficient method of obtaining the information.

In the preceding investigation [1] absorption and luminescence spectra of ruthenium(II) complexes $\text{cis-}[\text{Ru}(\text{bpy})_2(\text{L})\text{Cl}]^+$ [bpy=2,2'-bipyridyl; L= NH_3 , pyrazine, pyridine, 4-aminopyridine, 4-picoline, isonicotinamide, 4-cyanopyridine, 4,4'-bipyridyl, or trans-1,2-bis(4-pyridyl)ethylene] in alcoholic (EtOH–MeOH 4:1) solutions are studied at 77 K. The linear correlation between the energy of the lowest state ${}^3\text{MLCT } d\pi(\text{Ru}) \rightarrow \pi^*(\text{bpy})$ of the complexes and the parameter pK_a of the free 4-substituted pyridines is established.

In current work several quantum-chemical calculations of $\text{cis-}[\text{Ru}(\text{bpy})_2(\text{L})\text{Cl}]^+$ [bpy=2,2'-bipyridyl; L=4-picoline, pyridine, 4-cyanopyridine complexes were performed using Gaussian 03. Calculations were performed within the bounds of DFT, using 6-31G(d) and LanL2DZ basis. Operations performed: frequency analysis, geometry optimization, single-point energy calculation and an excited state calculation using the time-dependent DFT method. The interrelation between the energy of the lowest state ${}^3\text{MLCT } d\pi(\text{Ru}) \rightarrow \pi^*(\text{bpy})$ of the complexes and the feature of the coordination bond between L and Ru were consider.

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Investigation of the decay properties of the $1s2s^2$ state in Li-like bismuth

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We present the experiment for studying the radiative decay modes of the $1s2s^2$ level in Li-like bismuth (Bi^{80+}) [1].

The experiment was performed with the initially Be-like bismuth ions colliding with N_2 gas target at an energy of about 100 MeV/u. By measuring coincident events of the projectile K-shell ionization and thus resulting x-ray emission, a high selectivity for the investigation of the decay properties of the $1s2s^2$ state in Li-like bismuth is reached [2, 3].

We obtain a strong hint that an exotic two-electron one-photon (TEOP) transition is observed for the first time in a Li-like heavy ion (Bi^{80+}). This transition is of special interest because it provides access to the thorough investigations of the contribution of the relativistic and correlation effects on the atomic structure of few-electron systems.

According to the theoretical predictions, there is M1 transition, that has the second largest rate (but it's still less by one order of magnitude, then TEOP has), and its energy is close to the one of TEOP [4].

Possible systematic errors caused by geometrical uncertainties are estimated and discussed. Therefore it's impossible at this stage to give an absolutely certain answer concerning the experimental TEOP and M1 transition energies. We suppose that accurate measurements of the target chamber geometry are needed for this purpose.

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Features of spectrum registration in analytical atomic emission digital spectrography

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The development of atomic-emission spectrum analysis in the last decades occurred in the direction of creation and using of new recording devices based on solid-state multichannel semiconducting detectors of optical radiation. These devices used with a computer can combine the advantages of the photographic method of simultaneous recording of a certain spectral region and the photoelectric method of spectral lines photometric measurements. The result of this modernization is that spectral devices made 20-60 years ago become instruments of new generation in which the spectrum registration and spectral information processing are based on digital technology. Therefore such devices are in fact becoming digital spectrographs, and the direction of their use in optical spectroscopy can be described as “atomic emission digital spectrography”.

Often digital spectrographs used for productivity boosting of analysis and increasing of its execution velocity. Meanwhile techniques of spectrum recording, which had been previously developed for the photographic registration, are used.

It should be noted that the digital spectrum registration involves not only the setting of total exposure time T_T , but base exposure time T_B . The value of each of these parameters has a singular influence on the intensity of the recorded spectrum, and the precision of the analytical line intensity measurements.

In addition, the photometric measurements of analytical lines in the registered spectrum requires the selection of one of several procedures for measurement, each of which shows its specific features with respect to detection limits decreasing, improving of analysis precision, and concentration range.

The report presents results of research carried out by means of the spectral device MFS-8 combined with the photodiode linear detector MAES (VMK “Optoelektronika”, Novosibirsk). Obtained data allow us to determine how to optimize the above parameters for digital registration of spectrum for different spectroanalytical tasks.

Diffraction efficiency measurements of the Holoeye Pluto SLM fed by blazed-profile pattern

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At the moment, thin dynamic holograms (DHs) find numerous applications in solving various problems of applied optics, for instance, dynamic holographic correction of distortions in optical and laser systems, processing of optical information, etc. It is known, however, that the diffraction efficiency (DE) of a thin holographic grating recorded by the conventional “direct” method, i.e., as a pattern of interference of two laser beams, to the +1st and –1st orders of diffraction cannot exceed 33% for a sinusoidal profile and 40% for a rectangular grating (square wave). Correspondingly, the use of such a hologram as a corrector yields high energy losses in the optical system. This problem can be solved by means of holographic grating profile asymmetrization. In particular, for a phase transmission grating which profile is formed by right triangles and the phase modulation depth is 2π , its DE to the +1st or –1st order can reach 100%.

However, diffraction efficiency of currently popular electronically-addressed spatial light modulators (EA SLM) is less than theoretical 100% when driven by blazed-profile pattern. Apart from diffraction into higher orders caused by the lattice structure of the LCOS display itself, which leads up to about 40% losses, DE of the Holoeye Pluto SLM is stated to be about 75% using 8-level blazed profile and about 83% for 16-level blazed profile with 0 order intensity taken as a reference (100%). To measure the real DE of the Pluto SLM, which we’ve got in possession, a simple experimental setup was build. The Pluto SLM was illuminated by the collimated plain beam of He-Ne laser (633 nm) and fed by blazed-profile grating with variable phase modulation depth using Holoeye SLM Application Software. The output beams were focused by converging lens onto Lasercheck power meter with external diaphragm installed to split and measure intensities of the 0 and $\pm 1^{\text{st}}$ orders. Using the data obtained in this experiment we calculated the DE of the Pluto SLM and plotted graphs of the DE versus depth of modulation.

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Application Kerr effect for remote sensing of electric fields storm clouds

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Quantitative knowledge of the magnitude as well as spatial and temporal structure of electric fields above a thunderstorm, both prior to and immediately after a lightning discharge, is crucially important for understanding the electrodynamic effects of tropospheric weather on the upper atmosphere. At present such fields can only be measured with local methods, either at ground level or by balloon-borne instruments launched near or within the cloud. Such measurements do not allow accurate estimation of the overall structures inside and outside the cloud. The launch, operation, and recovery of balloon- or aircraft-based experimental apparatus also pose logistical problems, especially in the thunderstorm context. Using remote sensing techniques can be overcome the problems described above.

A recently developed remote sensing method for measurement of near thunderstorm electric fields by electrically induced birefringence (Kerr) effects on natural sky polarization, providing detection of electric fields near or above thunderclouds [1]. The birefringence results in a difference in index of refraction for waves polarized parallel and perpendicular to the applied field given by $\Delta n_k = nKE^2$ where n is the index of refraction, K is the Kerr constant, and E is the applied electric field. Thus phase shift is a measure of the electric field.

Besides Kerr effect in atmosphere there are other phenomena can cause birefringence. Strong air currents also can change natural sky light polarization [2]. The value of the birefringence caused by the air flow $\Delta n_f = \beta G$ where β is coefficient of air flow birefringence, G is velocity gradient of wind.

We have calculated the phase shift caused by Kerr effect in a typical storm $\varphi_k \approx 10^{-5}$ (rad) and by air flow $\varphi_f \approx 2 \times 10^{-6}$ (rad). Since the values of the phase shifts are comparable the effect of air flow on natural sky light polarization cannot be neglected. Measure the electric fields storm clouds using the method proposed in [1] is impossible. However, modifying this method may exclude the influence of the gradient wind speed.

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Combination of the conformational probes method and real-coded genetic algorithm for spectroscopic study of polymers

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We used the method of conformational probes [1] and hybrid real-coded genetic algorithm [2] to study the influence of impregnation with supercritical carbon dioxide on secondary relaxation transitions in glassy polymers which is successfully applied for membrane separation processes.

The conformational probes method is based on introducing small molecules (probes) in a polymer and following study of conformational dynamics in the probe molecules at different temperatures. For each polymer-probe system, freezing of conformational transitions is observed by FTIR at a certain individual temperature, T_f . Relaxation transitions observed in the polymers at the temperatures T_f are assigned to certain types of molecular mobility of their lateral groups and other fragments of macromolecules. We determined the temperatures of the freezing of conformational equilibria of probes in polymers investigated before and after the proceeding of impregnation with supercritical carbon dioxide.

The method of conformational probes requires investigation of temperature dependence of ratio of intensities of analytical conformationally-sensitive FTIR absorption bands. However, for some polymer-probe systems the analytical absorption bands of the probes are strongly overlapped. For correct determination of the intensities of conformationally-sensitive absorption bands of probe the deconvolution of spectral contours into components is necessary. We supposed the use of hybrid real-coded genetic algorithm for the treatment of FTIR spectra.

Using the offered technique we had been processed experimental spectra of polymer-probe systems and decomposition on elementary components of an investigated site of a spectrum was received.

This work was supported by Human Capital Foundation (<http://www.hcfoundation.ru>).

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Spectroscopic Identification of the Sizes of Scattering Nanoparticles in Polymer Composites

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The sizes of particles of a filler in polymeric composites are studied by the FTIR and Raman spectroscopy, optical and electronic microscopy methods. The composites are researched using the developed in the laboratory spectroscopy of Tver State University spectroscopic method for determining the average size and size distribution of filler particles, as well as the nature of their aggregation in the bulk polymer matrix. A basic idea of the method consists in a separation of the absorbed and scattering components of the passed through a sample radiation. Scattering component allows estimating the average size of the scattering particles, particle size distribution and their aggregation. Main requirements of this nondestructive technique to a sample are pore or filler particle size being in micrometer region and some difference in refractive indices and density of polymer matrix and filler.

Polymeric composites with fillers of the various nature were investigated in the work. Compositions were made in such a way that the difference of indicators of refraction of “*n*” of a matrix and a filler varied in studied systems. Composites with a polymeric matrix from PVA were prepared from 5 % of solution of polymer and water suspensions of powders of a filler of various concentration.

IR spectra of polymeric films are registered with FTIR spectrometer “Equinox 55” (“Bruker”) within 400 – 7000 cm^{-1} . Raman spectra of polymeric films are registered with Raman spectrometer “X” within 1000-5000 cm^{-1} . Films’ thickness is 10 μm . Sizes and particle distributions in polymer matrix volume are controlled by optical microscope “Neophot 30” (“Carl Zeiss”) and scanning electron microscope SEM “Hitachi SU8030”. Analysis of microphotographs was accomplished by software “Image Pro” to estimate particle distribution in the volume and on the surface of polymeric material.

It was attempted to apply a technique of determination of the sizes of particles of a filler in the polymeric matrix developed for IR spectroscopy to Raman spectroscopy. In Raman spectra the scattering effect similar to scattering in IR spectra is found out. For Raman spectroscopy also as well as for IR spectroscopy the difference in refractive index between a polymeric matrix and a filler is important. Preliminary data received of Raman-spectroscopy show quite good coincidence of the average size of particles for samples of polymeric composites. However the spectroscopic technique of an assess of particles of a filler demands completion for application to Raman-spectroscopy.

This work was financially supported by German-Russian Interdisciplinary Science Center (G-RISC) № C-2012a-2.

Influence of anharmonic interactions of vibrations on the spectral transition intensities in the H-bonded complex of acetone with hydrogen fluoride

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Intensities of spectral transitions between vibrational states of polyatomic systems provide detailed information about the motion of nuclei and the electron density distribution. Such information is especially important in the studies of molecular complexes because it allows researchers to understand the nature of complexation. Accurate measurements of this quantity are usually associated with significant experimental difficulties, and the calculation of transition intensities requires the use of complicated methods.

This study is devoted to the quantum-mechanical calculation of intensities associated with transitions to the doubly excited C=O and singly excited H-F stretching vibrations in the H-bonded complex $(\text{CH}_3)_2\text{CO}\dots\text{HF}$. These transitions can resonate because their frequencies are close. The main purpose was to examine the influence of anharmonic interactions of these two vibrational modes with each other and with the H-bond stretching vibration and the bending vibration of the HF subunit on the intensities of the H-F fundamental transition and the C=O first overtone transition. Using the GAUSSIAN 03 package of codes, we calculated 4D surfaces of the potential energy and dipole moment in the space of four vibrational coordinates, and then solved by the variational method a number of vibrational Schrödinger equations in 1 – 4 dimensions. Comparison of the intensity values obtained from solutions of Schrödinger equations with different combinations of interacting degrees of freedom can show how the inter-mode coupling affects spectral properties, in particular, the transition intensities. It was found that the interaction of the H-F stretch with all other degrees of freedom decreases its intensity (at most by a factor of 1.5). In contrast, the C=O first overtone intensity is increased by a factor of about 15 due to the anharmonic coupling to the H-F stretch; however, an additional interaction with other intermolecular vibrations can reduce this intensity transfer.

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Investigation of the excitation spectrum in Be-like bismuth

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We present the experiment for studying the L-series of transitions in Be-like bismuth (Bi^{79+}) [1]. The experiment was performed with the initially Be-like bismuth ions colliding with the supersonic N_2 gas-jet target at an energy of 98.168 MeV/u.

According to the theoretical calculations [2], the probabilities of the simultaneous ionization and excitation or simultaneous excitation and capture of an electron are extremely low and can be neglected. Therefore we have only three main processes: ionization, excitation or capture. In the experimental setup we have x-ray detectors, dipole magnetic analyzer and particle counters. By measuring coincident events of the projectile K-shell ionization and resulting x-ray emission as well as the coincident events of the capture of an electron from the target molecules and resulting x-ray emission, a high selectivity for the investigation of the excitation spectrum in Be-like bismuth is reached.

The L-series of the transitions in Be-like bismuth is analyzed and compared with the energy and intensity [3] predictions of relativistic theory based on the one-electron (Dirac) model with the population of energy levels up to $n = 5$. All transitions are identified and classified by their principle quantum numbers and full angular momentum. It's found that despite the high nuclear charge and thus the strong interaction of the electrons with the nuclei, this approximation is appropriate to describe the spectrum only qualitatively, but more accurate models (taking into account the electron correlations and the population of the higher energy levels) are necessary for the quantitative analysis.

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G. Theoretical, Mathematical and Computational Physics

Schwarzschild solution in R-spacetime

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We consider the Schwarzschild metric in the background R-spacetime. At first we begin with the AdS-Schwarzschild solution of Einstein equations and transform it to Beltrami coordinates. Then we take the limit of $c \rightarrow \infty$ and get R-Schwarzschild metric. The test particle's equation of motion in R-Schwarzschild metric is analyzed. Finally we calculate the gravitational radius of the Earth and time variation of the moon orbit radius.

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Two-photon approximation in frames of quantum mechanics

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A quantum mechanics theory of the multiphoton decay of excited states in a hydrogen atom is presented. The “two-photon” approximation is considered on the basis of [1, 2], which is limited by the one- and two-photon transitions including cascade transitions with two-photon links. The method of two-photon approximation for multiphoton transitions is applied to the decays of the 4d, 4s and 3p states. This may be helpful for a strict description of the recombination process in the hydrogen atom and, in principle, for the history of hydrogen recombination in the early universe.

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Renormalization of the General Effective Theory: Scalar Self-Energy

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There are at least two approaches of constructing a consistent physical theory. One approach is a way of symmetry. One can postulate an exact symmetry (like colour symmetry in QCD) or an approximate one (phenomenological symmetries) to be physical and to construct the action invariant under this symmetry. Another approach can be called 'general'. One should restrict the form of the action just by the requirements of the unitarity, causality and covariance of the S-matrix. In this approach there is no additional symmetry and all the constraints on the coupling constants are imposed by the experiment.

Of course in first approach it is easier to construct a possible action because of the renormalizability: usually there are just several interaction terms consistent with given symmetry and the requirement of renormalizability. But in the second approach the action is renormalizable by construction (as it was mentioned by S.Weinberg [1]). And on one hand there is a lot of freedom for coupling constants but on another hand there should be a finite set of coupling constants being observable on the experiment.

One can divide the whole set of coupling constants in the action into two subsets: 'minimal' constants that are physically observed and 'redundant' parameters that are not observable (see [2]). One should carry out the renormalization procedure step-by-step in the loop order. And all the parameters should be classified on each step.

V.V.Vereshagin and I are investigating the renormalization procedure in the approach of general effective theory. In current report we explicitly construct the general action for the scalar fields and show how to classify the parameters on the tree level and on the first loop order for the two-legged S-matrix element.

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The simulation of cholesteric liquid crystal structure depending on external magnetic field and temperature

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The application of liquid crystals in display systems and in information transfer is based on the reorientation of liquid crystals in the external field. This effect is known as Frederiks transition. It is that the orientation variation of liquid crystal in external electric and magnetic fields are threshold phenomena. Mostly detailed it is described for nematic liquid crystals. In nematics Frederiks transition the most often is phase transition of the second order. As for cholesteric liquid crystal situation is more complicated, because there may be either phase transition of the first or the second order.

Also it is interesting to describe orientational structure distortion of cholesteric with temperature. As far as the pitch is the function of the temperature the director on the surface of the sample can deviate from the direction of alignment. When this deviation reaches the critical value abrupt transition of the cholesteric helix occurs in the layer between configurations differing from one another by one half-turn of the helix in the layer.

In the first part of the work we investigated the structure dependence of cholesteric liquid crystal on the parameters of the system and the applied magnetic field. The presence of a helix spatial structure makes the problem mathematically very complicated, because it is necessary to solve system of nonlinear differential equations of the second order. Therefore the computer modeling was performed by means of minimization free energy of the system. In the numerical calculation two different types of boundary conditions were considered: solid boundary condition, that is the anchoring energy considered as infinite and soft condition when the anchoring energy is finite. In both cases spatial orientation of the director in the bulk of liquid crystal was calculated. Also the region of fields near the threshold was properly examined. Especial attention was paid to analysis of the crystal structure at various anchoring energies on the surface. In this case noticeable asymmetry of director orientation was observed.

In the second part a helix pitch behavior was examined by computer simulation with the temperature variation. Numerical calculations were performed using the Rapini anchoring potential. The obtained results permit not only observe the transition between configuration of system, but also quantitatively investigate its parameters in the process.

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Evaluation of centrality classes based on Glauber Monte-Carlo model in heavy-ion collisions at high energy

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Fluctuations in physical observables in heavy-ion collisions have been a topic of interest for some years as they may provide important signals regarding the formation of quark-gluon plasma (QGP). For studying fluctuations and searching delicate effect it is necessary to determine precisely measurement's parameters (to fix the centrality classes) when the observable's fluctuation is minimal.

This work is connected with heavy-ions experiments in CERN at LHC energies and proposes the method of estimating the centrality classes where the fluctuations are minimized based on the analysis of RHIC experiments (WA97 [1], WA98 [2]). The main goal of this work is minimization of trivial fluctuations of observables by determination of the centrality classes width influence on the fluctuations of observables.

For that purpose the Monte-Carlo generator of Pb-Pb collisions at 2,76 TeV was created based on Glauber Model. We consider MC simulations due to the possibility of extraction of the information about impact parameter and number of nucleons participated in collisions. Using connection between multiplicity and number of nucleons participated in the collision we can evaluate the multiplicity which is measured on the experiments. This data makes the distinctions for different classes of centrality evident.

We compared two methods of determination of centrality classes by impact parameter and multiplicity. Analysing the distribution of number of participated nucleons (N_{part}) in different centrality classes we can evaluate the value of RMS (root mean square) and mean value of N_{part} in each centrality class with the different widths. As a result, for all values of multiplicity and the impact parameter including the central and peripheral collisions the value of centrality selection bins was determined in percentage wise of widths in the minimum bias cross section where the fluctuations of the observable values are minimized. Using this method one can make analysis of the reconstructed data for different experiments of NN collisions at high energy (like ALICE [3]) to determine conditions where the observables fluctuations will be minimized.

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Exchange coupling in metallic magnetic nanosystems

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Development of spin-polarization scanning tunneling spectroscopy makes it possible to control the magnetic moments of nanosystems at the atomic scale. It results in discovering of the new types of magnetic structures in magnetic overlayers and 3d-clusters supported on metallic surfaces. The investigation of magnetic order in such nanosystems as well as the study of the possibility to tune the exchange coupling between atoms are of great importance for development of magnetic memory with ultra-high storage density. Therefore, the analysis of the theoretical models for explanation of exchange coupling mechanisms has large theoretical and practical interests.

In the refs. [1, 2] using X-ray magnetic circular dichroism authors demonstrated that a ferromagnetic coupling between paramagnetic Fe-porphyrin molecules and ultrathin Co(Ni) film on Cu(100) substrate can be changed to an antiferromagnetic one through the introducing of intermediate layer of atomic oxygen. The theoretical interpretation of this phenomenon was based on the *ab initio* calculations with additional parameter of the Coulomb interaction (LDA+U). Nevertheless, such approach don't give insight to the dependence magnetic properties on the gas adsorption, which is necessary for controlled management of exchange coupling parameters.

We developed the theory based on model microscopic Hamiltonian for itinerant electrons model which take into account on site Coulomb interaction in mean field approximation [3]. The number of d-electrons and magnetic moment are determined self-consistently via matrix elements of Green functions. For the calculation of Green functions we uses the recursion method. It is shown that the exchange coupling between the atoms strongly depend on the number of d-electrons N localized on the atoms of transition elements. In the case Fe, Co and Ni ($N > 7$) this coupling is ferromagnetic. The interaction with atomic O decreases the number of d-electrons on 3d- atoms and the sign exchange coupling can be changed. It allows to manage the exchange coupling between magnetic moments via control of the filling of d-states.

This work was partially supported by grant RFBR 12-02-31716

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Optimization of calculations using Sector Decomposition approach: three-loop calculation of renormalization constants of ϕ^4 -theory

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Method of renormalization group is now generally accepted approach in the research of second type phase transitions and of critical phenomena. It allows us to justify the critical scaling and to make calculations of the critical indicators as the decomposition in the formal small parameter (ϵ - Wilson decomposition). The main technical problem in this approach is the calculation of renormalization constants. These values are determined by multiple integrals that are singularly depended on ϵ , that is why it is very difficult to find them numerically. Nevertheless, Sector Decomposition method was intensively developing during recent years, and now it allow us to overcome such difficulties using explicit allocation of residues at the singularities of ϵ . To make this calculations, we need to divide the space of integration into several sectors, which will allow us to isolate a singularity of integrand. The resulting integrals are very well suited for numerical calculations. The main disadvantage of Sector Decomposition method is a very large increase in the number of sectors with the increasing order of perturbation theory. The choice of sectors is ambiguous, thus it is profitably to find such realization that will reduce the number of sectors. There are several "strategies of decomposition", each of which has its own advantages and disadvantages.

An approach which allows us to reduce the number of sectors using the most complete account of symmetry of Feynman diagrams that define the renormalization constants has been developed at the Department of Statistical Physics in the Faculty of Physics in St. Petersburg State University. In this paper the efficiency of this method is verified by the calculation of renormalization constants of the most famous ϕ^4 -model. This calculation is performed in the three-loop approximation. The allocation of the singularities and the recognition of symmetries during decomposition were performed manually, without using any computer program. The numerical taking of integrals was implemented only on the last step of calculations. Such computations revealed a number of nuances that will be thoroughly considered in the future, when the fully automated program of calculation will appear. This program is the necessity in the higher orders of perturbation theory. The calculated renormalization constants coincide with great precision with the previously known constants in the literature. The number of sectors in the decomposition is lower than in all known strategies.

Solving the time-dependent Dirac equation with the B-spline basis set method

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Investigations of heavy ions provide a unique tool for tests of relativistic and quantum electrodynamics effects at strong fields [1].

In the present work we have considered the $U^{91+}(1s)$ - U^{92+} collision and solved the time-dependent Dirac equation in a central field, which is the sum of the potential of the target nucleus and the potential of the projectile nucleus. The projectile potential is treated within the monopole approximation which includes only the spherically symmetric part with respect to the target. The target $U^{91+}(1s)$ is at the rest at the origin. The projectile U^{92+} moves along a straight-line trajectory with a constant velocity and the impact parameter b .

Nowadays a great amount of calculations in atomic physics and quantum chemistry are based on finite basis set methods. This paper represents the use of the dual kinetic balance (DKB) approach with basis functions constructed from B splines [2]. The absence of spurious states is a significant advantage of this approach. The time-dependent Dirac equation is solved using the DKB basis functions and the expansion coefficients are defined employing the Crank-Nicolson propagation scheme [3].

The probabilities to observe the electron at the ground or excited states or to be ionized as functions of the impact parameter b have been calculated. The obtained results are in a good agreement with the previous calculations [4].

The extension of the method beyond the monopole approximation will be considered in future work.

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Lagrange alternative to the construction of meson spectra

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In this work we consider the highly excited mesons. A particular interest in this kind of particles in QCD is explained by several reasons; the one crucial for us is the assumption that the highly excited hadron can be represented quasiclassically.

Commonly the structure of mesons in the quasiclassical approach is described as a pair of ultrarelativistic quarks interacting via a confining linear potential. Apparently, the meson state can be imagined as a quark and an antiquark connected by a flux tube of the chromoelectric field (a gluon string). This hypothesis implies asymptotically linear Regge like trajectories $M^2 \sim \sigma \cdot n$, where M is the meson mass, σ denotes the tension of the flux tube, and n is an integer ($n \geq 0$) called the radial quantum number.

We introduce some classical field models describing an infinite tower of radial meson excitations.

Firstly, we consider the complex scalar field. The spontaneous breaking of the global symmetry in the model gives rise to an infinite number of Goldstone bosons.

As we intend to operate under the Higgs mechanism, we add the gauge field in the Lagrangian density of the model. In this model the spontaneous symmetry breaking of the local gauge symmetry leads to the generation of mass terms for the gauge bosons and no Goldstone bosons appear. I.e. each massive vector boson gets its longitudinal polarization “absorbing” the corresponding Goldstone boson.

The advantage of the method discussed consists in avoidance of at least one problem (the breaking of the string at 1fm) arising in the hadron string models.

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Crossing the boundary between parity breaking medium and vacuum by vector particles

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In Quantum Electrodynamics the interest to possible Lorentz and CPT Invariance Violation was raised up after the seminal paper [1] where the very possibility to have a constant vector background generating Lorentz and CPT parity breaking in the large scale universe was conjectured and falsified. The latter was employed to modify QED supplementing it with the Chern-Simons (CS) parity-odd lagrangian spanned on a constant CS vector.

Spontaneous Lorentz symmetry breaking may occur after condensation of massless axion-like fields [2] at large space scales comparable with star and galaxies sizes or in collisions of heavy ions [3]. In both cases there is a boundary between parity-odd medium and vacuum.

The aim of the present work is to study the effects of propagation of photons and vector mesons through the boundary with the help of results obtained in [4]. The solutions in different half-spaces will be matched both in the case of space-like and time-like Chern-Simons action by means of the Bogolubov transformations. Accordingly the two different Fock vacua happen to be mutually coherent states. The boundary mirror/transparency properties will be illustrated. In particular, the most significant effects will be discussed. They can help to register local parity violation in a finite volume of heavy ion fireball with nontrivial axial charge and/or of a star with cold axion condensate degrading to its boundary.

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Instrumental measurements of freak waves in the southeast area of Sakhalin Island

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Know quite a lot of freak waves attack ships in the ocean, when they reached the height of 30 meters. Such waves are dangerous for marine structures such as oil and gas platforms.

Abnormally large waves (freak waves) are waves of large amplitude, suddenly appearing on the sea surface and just as quickly disappear. The main feature of such abnormally large wave is its high altitude and slope compared to the surrounding waves. The study of freak waves in the ocean, where the results of observations they reach great heights, is rather time-consuming task due to the difficulty of instrumental measurements and unpredictable occurrence of such waves.

Therefore, to study the physics of abnormally large waves should be used to measure in the coastal and offshore. These studies are conducted in a number of areas on the coast of Sakhalin Island. In this work, the analysis used 12 high-frequency recordings for 18 days near the Ostry cape (southeast Sakhalin). Each record contains about 200,000 waves. The main tool of instrumental wave measurement are autonomous wave recorders ARV-K12. These instruments are unique equipment developed since 2006 LLC SKTB “ELPA” (Uglich, Russia). Bottom pressure sensor detects pressure fluctuations, which generally do not coincide with fluctuations in sea level. As is known, the surface waves decay with depth, so if you use the hydrostatic relation, the bottom pressure sensor to underestimate the amplitude of the waves. In this article, the wave height was calculated as the distance from the base to the crest of the wave (i.e., secondary extrema in the record, which do not cross the middle line of the wave, not included). To account for the non-stationary process, as it is in oceanography, the record was broken into quasi-stationary parts of 20 minutes is used to calculate the average and the significant wave height (the average height of the one third highest waves). The data presented experiment on surface waves offshore Sakhalin Island in the Ostry cape in 2006 that the freak waves in the coastal waters of the Russian occur in about 2 times per day.

The comparison with the simulation results indicate that the registration unrest in increments of 1 second is found only 2% to 6% of the calculated freak waves.

Supersymmetrical Separation of Variables for Scarf II Model: Partial Solvability

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Supersymmetrical quantum mechanics gave a new impetus to the development of new analytical methods in the study of different quantum models. One of the directions of the research within this framework is the investigation of two-dimensional quantum models which are not amenable to the standard separation of variables. Only a few two-dimensional models are now exactly solved or quasi-exactly solved such as two-dimensional generalizations of Morse, Pöschl-Teller, and periodic Lamé models. Supersymmetrical (SUSY) separation of variables is based on supersymmetrical intertwining relations with second-order supercharges and shape invariance property.

In our papers we have investigated the two-dimensional model with potential which is naturally associated with solvable one-dimensional hyperbolic version of Scarf model (Scarf II). There are two variants of SUSY separation of variables. The first variant is applicable if the supercharge allows the standard separation of variables as it happens for supercharges with Lorentz metric. This method leads to quasy-exact solvability of the model. The second variant works if one of the intertwined Hamiltonians allows the standard separation due to the specific choice of parameters, but its superpartner still does not. Such situation gives a chance to solve the problem completely – to find energies and wave functions of all bound states.

However we have not only applied these two methods to Scarf II model but we also have extended our results by construction the hierarchy of Hamiltonians. As a result we have calculated a complete spectrum of the model Scarf II with arbitrary negative integer parameter and we also have obtained a part of the spectrum for arbitrary parameter of the model.

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A comparison of methods of the approximation of the spectral surface in 2D-correlation spectroscopy

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This work was devoted to developing of two-dimensional correlation spectroscopy method using the continuous approximation of the two-dimensional surface of the spectral amplitude of two-dimensional correlation spectra in the process of two-dimensional correlation spectra analytically. This approximation is described on the example of the experimental data obtained from the ozonolysis of ethylene on the surface of fine ice at 77 K.

At approximation of the spectrum the task was to select the peaks. To solve this problem “wavelet” analysis – the convolution of the spectrum with the derivative of Gaussian (“wavelet Regehr”) has been applied .

The chosen method was compared the peak search with the discrete derivative of the spectrum. Our methodology with application of described approximation has been applied to the construction and analysis of symmetric and antisymmetric two-dimensional correlation spectra. This modification allows to describe synchronous and asynchronous two-dimensional correlation surface more accurately than in terms of standard discrete methods, largely due to separation of the signal from the noise.

In particular, in the analysis of dynamic spectra recorded during the experiment, the asynchronous spectrum allows more detail to see the correlation between the bands at 1020 and 1036 cm^{-1} , corresponding to the secondary ozonide and molecular ozone, respectively. These data are indicate the presence of a secondary ozonide, which is an intermediate product of ozonolysis reaction of ethylene and support the assumption that the process proceeds according to Criegee.

Treatment of the two-center time-dependent Dirac equation in a rotating coordinate frame

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Heavy ion collisions can be used as a good tool for tests of quantum electrodynamics in the supercritical Coulomb fields [1].

In this work a new method of heavy ion collisions treatment is presented. The approach is based on numerical solving the time-dependent two-center Dirac equation using the finite basis set of Hermite splines. The collision process is treated in a rotating reference frame. It allows to use two-dimensional grid instead of three-dimensional one.

The $U^{92+}-U^{91+}$ collisions are considered using the developed method. The charge-transfer probabilities are calculated at the projectile energy

$E_{\text{lab}}=6$ MeV/u for various values of the impact parameter. The results of the calculation are in a good agreement with recent calculations by our group [2] obtained within the approach employing atomic-like Dirac-Sturm orbitals. This work can be useful for the current and future experiments at GSI (Darmstadt).

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Homogenization of the Cauchy problem for a parabolic equation with periodic coefficients

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The paper concerns homogenization theory of periodic differential operators. We consider a matrix elliptic second order differential operator. The principal part of this operator is given in a factorized form. The operator also includes zero and first order terms with bounded coefficients. The coefficients are periodic in space variables and independent of time. We do not need any smoothness assumptions on coefficients.

We study homogenization in the small period limit for a periodic parabolic Cauchy problem. Our goal is to prove convergence of the solutions of the problem with rapidly oscillating coefficients to the solutions of the “homogenized” problem with constant coefficients.

The problem reduces to the study of the operator exponential. We find approximation for this exponential in the L_2 -operator norm in terms of exponential of the effective operator. The error estimate is order-sharp, and the constant in this estimate is controlled explicitly in terms of the problem data. This approach allows us to prove the convergence of the solutions and to obtain an error estimate in L_2 -operator norms.

The method is based on the abstract operator theory approach for selfadjoint operator families. This approach was developed for elliptic problems in [1, 2]. We apply the scaling transformation, the Floquet-Bloch theory and the analytic perturbation theory. It turns out that the homogenization procedure is determined by the spectral characteristics of the periodic operator near the bottom of its spectrum.

The homogenization problem for parabolic equations has been studied by this method in [3] in the absence of lower order terms. We study a more general problem in the presence of lower order terms.

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BV Formalism vs Auxiliary Fields in Supergravity Quantization

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Supergravity Lagrangians for physical fields are invariant under supersymmetry transformations only on the mass shell. Extending this symmetry to off-shell is required for consistent quantization of the model. Therefore we want to obtain Lagrangians invariant under the transformations off-shell.

There are different methods of obtaining an off-shell invariant Lagrangian. One of the methods is to introduce auxiliary fields to the model. But this method doesn't respond to the origin of the fields. Thus we miss systematical procedure for obtaining off-shell invariant Lagrangian in this approach. In simple models we are able to guess the auxiliary fields but in more complicated cases this is not yet done. It is not clear whether we can do it someday. In particular, for $N=1$ $d=4$ supergravity such fields are proposed in paper [1], but for $N=8$ $d=11$ supergravity such fields are not known. Fortunately there is another way to obtaining the necessary model extension developed by Batalin and Vilkovisky [2]. Off-shell invariant Lagrangian can be obtained for any gauge theory in this approach.

These two approaches should yield the same physical results, so it must be a relationship between these two approaches. It is interesting to study this connection. This will expand the understanding of both the auxiliary fields and Batalin-Vilkovisky approaches.

Specifically equivalence of approaches can be understood considering simple supergravity case. Paper [3] demonstrates the equivalence of two approaches for simple supergravity but some modification of Batalin-Vilkovisky formalism occurs that would be possible for the theory of rank two. For generalization to more complicated models we consider general BV formalism. It would allow us to obtain an invariant Lagrangian without singularity for $N=8$ $d=4$ supergravity by using the Batalin-Vilkovisky approach and to understand whether it is possible to get auxiliary fields for theory with rank higher than two.

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Calculation of propagator asymptotics in logarithmic dimensions for the models φ^3 and φ^4 by means of renormalization group method

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Using the renormalization group equation [1]:

$$\left(-p \frac{\partial}{\partial p} + \beta(g) \frac{\partial}{\partial g} + 2\gamma(g) - 2 \right) f(p, g) = 0,$$

we study the asymptotic behavior of propagator $f(p, g)$, where p is a momentum, g is a coupling constant.

For the φ^3 -theory ($L_{\text{int}} = (\lambda/3!) \varphi^3$) in the logarithmic dimension ($d=6$) it holds: $\beta(g) = b_2 g^2 + b_3 g^3 + \dots$, $\gamma(g) = c_1 g + c_2 g^2 + \dots$, where $g = \lambda^2$. The solution is the following:

$$f(s, g) = f_0 s^{-2} (-\ln s)^{\frac{2c_1}{b_2}} \left(1 + \sum_{n=1}^{\infty} \sum_{m=0}^n W_{nm}(g) \frac{\ln^m(-\ln s)}{\ln^n s} \right),$$

where $s = p/\mu$, μ is a scale parameter. The coefficients W_{nm} are universal, they do not depend on g and they are expressed in term of b_2 , b_3 and c_1 . The coefficients W_{nm} with $m < n$ are not universal, they depend on g and can be calculated in framework of perturbation theory.

For the φ^4 -theory ($L_{\text{int}} = (g/4!) \varphi^4$) in the logarithmic dimension ($d=4$) we have: $\beta(g) = b_2 g^2 + b_3 g^3 + \dots$, $\gamma(g) = c_2 g^2 + c_3 g^3 + \dots$

The solution has a form:

$$f(s, g) = f_0 s^{-2} \left(1 + \sum_{n=1}^{\infty} \sum_{m=0}^n W_{nm}(g) \frac{\ln^m(-\ln s)}{\ln^{n+1} s} \right).$$

The coefficients W_{nm} are also universal, they are expressed in term of b_2 , b_3 and c_2 . The coefficients W_{nm} with $m < n$ are presented as perturbation theory series in the coupling constant g .

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Reconstruction of quarks propagators in the effective Lipatov theory

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The inclusive gluon production on the nucleus is one of the basic processes in high-energy collisions off nuclear targets. Our scientific Group is specifying in the calculations of inclusive cross-sections of quark – two quarks scattering. Both the target and the projectile are nuclei with the interaction dropped to the level of this quarks number.

A powerful and constructive technique for the calculation of all Feynman diagrams in the Regge kinematics is provided by the Lipatov effective action [1]. In the inclusive production on two centers, in the lowest order, there appear diagrams with production of the observed gluon (P) from the splitting vertex of a reggeized gluon (R) into two or three reggeized gluons. The splitting vertex $R \rightarrow RRP$ entering Fig. 1, a was calculated in [2] and its contribution together with all accompanying ones to the inclusive cross-section was found in [3].

The total inclusive cross-section of quark – nucleon scattering turns out to be in the 10th order of g. To finally find the total inclusive cross-section one has to calculate contributions from diagrams of the type which involve a still more complicated vertex $R \rightarrow RRRP$.

This report is devoted to the study of this vertex and its contribution together with all accompanying diagrams to the production amplitude of this process.

These attendant diagrams include the contributions with factors like a product of delta function and a pole in the principal value sense and a product of two delta functions. What is more that delta function is considered as a part of a quark propagator dropped into it because of the rapidity cut-off or in other words – the Regge kinematics. The principal value also emerges in the vertices with splitting reggeons by the same reason. In this report I'd like to explain this process and the reconstruction of the quarks propagators with the simplification of $R \rightarrow RRRP$ and $R \rightarrow RRP$ vertices in the process under consideration. This observation substantially simplifies the calculation of the inclusive cross-sections. The calculation of the inclusive cross-sections the current work of our scientific Group.

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Holographic model for heavy quarkonia

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In the last few years a great attention was paid to the so-called phenomenological AdS/QCD theories. The essence of these models is to use the AdS/CFT correspondence to describe QCD via its 5-dimensional dual theory. The exact structure of this 5D theory, describing all specific features of QCD is not clear, but some simple models have been proposed [1, 2], which already give promising results.

The aim of the present work is to describe spectrum of heavy quarkonia such as bottomium. It requires to introduce new AdS/QCD model with appropriate effective potential. Once such model is constructed our next goal is finding a “dynamic model” of quarkonia, which has to reproduce light mesons spectra as well.

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Estimate of the dilepton invariant spectrum in $B^+ \rightarrow \pi^+ \mu^+ \mu^-$ using data in $B^0 \rightarrow \pi \ell^+ \nu_\ell$ and heavy quark symmetry

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The physics of B -meson plays a fundamental role both in the precision tests of the Standard Model (SM) and in the search of New physics. In this connection it is important to determine different characteristics of B -meson decays, such as branching fractions (BFs), differential distributions, CP -asymmetries, etc. with high accuracy. The interest in B -physics is greatly stimulated by the experiments at the B -factories, BaBar and Belle, and the LHCb at the LHC, which provide a huge amount of new and accurate experimental data concerning B -meson and b -baryon decays.

Experimental data and theoretical calculations of the $B^0 \rightarrow \pi \ell^+ \nu_\ell$ and $B^+ \rightarrow \pi^+ \ell^+ \ell^-$ decays are discussed. Based on the data of the BaBar and Belle collaborations, the $f_+(q^2)$ form-factor shape has been extracted in terms of four different form-factors parametrizations. It was found that the least χ^2 was achieved with the Boyd-Grinstein-Lebed (BGL) parametrization [1].

Predicting the total branching ratio in the decay $B^+ \rightarrow \pi^+ \ell^+ \ell^-$ involves some approximations due to modeling the $f_0(q^2)$ and $f_+(q^2)$ form factors in the large q^2 range. The numerical value of the branching fraction $\text{Br}(B^+ \rightarrow \pi^+ \mu^+ \mu^-) = (1.96 \pm 0.21) \times 10^{-8}$ [2] was reproduced under the assumption that the small- q^2 shape of the form factor can be extrapolated into the large- q^2 values. This result is in agreement with the experimental one $\text{Br}(B^+ \rightarrow \pi^+ \mu^+ \mu^-) = (2.3 \pm 0.6(\text{stat}) \pm 0.1(\text{syst})) \times 10^{-8}$ measured recently by the LHCb collaboration [3]. To reduce the number of unknown independent form factors in the $B \rightarrow \pi$ transition, the heavy quark symmetry (HQS) was applied and the expression for the decay rate was obtained. This rate is valid only for small- q^2 values but involves only one independent form factor $f_+(q^2)$. In the framework of the SM, the prediction for the partial branching fraction $\text{Br}(B^+ \rightarrow \pi^+ \mu^+ \mu^-) = (0.81 \pm 0.24) \times 10^{-8}$ have been obtained for $q^2 \leq 8 \text{ GeV}^2$, which can be checked by the LHCb collaboration.

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pA collisions at LHC in Modified Glauber model

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One of the main possible evidences of the quark-gluon plasma formation in collisions of ultra-relativistic heavy nuclei at the Large Hadron Collider (LHC) is a decrease of the total multiplicity of charged particles compared to the predictions of superposition of the independent nucleon-nucleon collisions. Usually a simple geometric Glauber model is used to define the relevant initial conditions of the collisions. However, this model is not justified in case of a so-called “soft processes of particle production”.

We present the further developments, such as the repulsive nucleon core and multiple nucleon-nucleon collisions of the modified Glauber model (MGM) [1]. A broad class of available experimental data on the multiplicity of charged particles in Au-Au collisions is analyzed. The analysis of the total multiplicity yield in Pb-Pb collisions at the Large Hadron Collider and forecast for p-Pb collisions are made based on the new version of the MGM. The main result of the model is the prediction of “nucleon stopping” in collisions of proton and lead nucleus. In this connection, we expect to observe a considerable (2 fold) decrease of the average number of nucleon participants and the average multiplicity of charged particles compared to the predictions of the standard Glauber model.

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Recoil effect on g-factor of few-electron ions

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The effect of finite nuclear mass on g-factor of boronlike and lithiumlike ions is investigated in the present work. The recoil correction to g-factor to first order in m_e/M is calculated for boronlike ions. The inerelectronic-interaction correction to the recoil effect is considered within the perturbation theory of the second order. Numerical results are calculated for lithiumlike ions.

The nuclear size correction to the nuclear recoil effect on the energy levels is evaluated by averaging the recoil operator with relativistic wave functions calculated for the finite nucleus.

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Study of C60 Fullerene Antioxidant Effect Using Density Functional Theory and Computer Modeling

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Recently it has been discovered that repeated admiration of fullerene C60 expands the lifetime of rats almost two times [1]. This effect is ascribed to the attenuation of oxidative stress, which is increasing with age. Despite the fact that fullerene C60 is well-known for its potential applications in various fields of biology and medicine, some mechanisms of its action are still unknown.

This work is devoted to the theoretical simulation of interactions between fullerene and several molecules and ions. The purpose is to simulate processes that may take place in the organism, which may be crucial for understanding the very mechanism of these processes. Researches are done in a collaboration with the laboratory of Experimental Mutagenesis of Research Institute of Biology (Rostov-on-Don, Russia).

For the theoretical simulations of abovementioned processes Density Functional Theory was used realized in Amsterdam Density Functional 2010 code (ADF 2010). Different basis sets and exchange-correlation potentials were used for calculations. Also, molecular dynamics simulations were applied to some systems.

As a result, possible mechanisms of interaction between fullerene and protons H^+ were considered. It was shown that it is possible for a proton to penetrate into fullerene. In contrast, such ions as Na^+ and Cl^- cannot get into a fullerene. Also, the possibilities for interaction between fullerene and fatty acids, such as oleic, palmitic, linoleic, stearic acids and tocopherols were studied.

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Considering perturbation theory as hamiltonian system

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When we want to calculate some field theory, or quantum system, we usually use perturbation theory. But if we use only N first members of row, we replace equations, which we got from some hamiltonian or lagrangian, to other equations. Using exact lagrange and hamilton equations guarantees us positive and normed on 1 probabilities, preservation them in time and right commutators. But considering only first N orders of perturbation theory satisfy these requirements only approximately. And usually is said, that it is not a problem, because it is only approximation.

But some theories, like gravity, are checked only in few orders of perturbation theory. So we can try to build some more simple theory, which will be equal to initial exact theory in first N orders and arbitrary in higher orders but doesn't have such problems, as described above. And if such building is possible, we can use this simpler theory as a new exact theory.

We will consider some different ways of building this theory:

- 1) Theories appearing directly from lagrangian
- 2) Theories appearing from hamiltonian, which we got from exact lagrangian

We will use as usual way $L \rightarrow H$ Heisenberg's equation, and limited by first orders of perturbation theory we get modified correct ways.

Net charge fluctuations in AA collisions in the color strings approach

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Net charge event-by-event fluctuations have been proposed as an indicator of the formation of quark-gluon plasma in high-energy nucleus-nucleus (AA) collisions [1, 2]. The theoretical predictions of the value of the fluctuations [1–3] are not directly consistent with the experimental results from RHIC [4]. At present the preliminary results extracted from the ALICE experimental data have rather ambiguous interpretation in the framework of existing models [5]. Here, we test the experimental data against an alternative string-inspired model.

In this model [6] the mid-rapidity particle production is due to the decays of the color strings. We assume that all strings, formed in AA collisions at given conditions, are identical. In the string model one has an approximate conservation of the charge locally in rapidity. So we assume each string emits positive and negative particles in the central rapidity interval with the same mean values and variances, but due to “leakage” of the charge on the borders of the interval the number of positive particles does not equal to the number of negative ones event-by-event. In string models the positive charge of initial nuclear protons is associated with their valence quarks and is concentrated at projectile and target rapidities. The transport of this charge into the mid-rapidity region is the second cause of the deviation of the charge from zero in this region.

The measure of the dynamical net charge fluctuations, v_{dyn} , is expressed in terms of the parameters characterizing the individual string and their event-by-event distribution.

The model calculations are compared with the experimental data. It is shown that under the natural values of the model parameters the obtained results are consistent with the data.

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The direct QED evaluation of the “two-photon” decay width in H-like ions

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The evaluation of the “two-photon” decay width is important in the theory of cosmological hydrogen recombination and in the atomic spectroscopy field of research. The interest to the theory of the multiphoton transitions in hydrogen during the last decade was triggered by the accurate measurements of the asymmetry in the temperature and polarization distribution of the Cosmic Microwave Background (CMB) [1, 2]. The launching of the Planck Surveyor enables to perform the measurements with accuracy 0.1% . It is a challenge to the theory to perform the calculations of the properties of CMB with the same accuracy. For this purpose the adequate theory of the cosmological hydrogen recombination should be developed. The modern theory of this recombination starts from the works by Zel'dovich, Kurt and Sunyaev [3] and by Peebles [4]. As it was first establishment in [3, 4] where 2s-1s transition was found to be the main channel for the radiation escape and formation of CMB. Apart from 2s-1s transition, as it was noted recently in [5] the two-photon decays from the excited states with the principal quantum number $n > 2$ also can contribute at the 1% level of accuracy. In view of this it became important to introduce the “two-photon” decay width via imaginary part of two-loop self-energy. Definition of the one-photon width of the atomic level as the imaginary part of the oneloop self-energy Feynman diagram is well known. Usually authors prolongate this result to the definition of the “two-photon” width, see for example [9]. However it is not obvious and have to be proved. In our work we give the analytical derivation of the “two-photon” width of the energy level in H-like ions in frames of Quantum Electrodynamics theory via imaginary part of two-loop self-energy.

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H. Biophysics

Conformational, optical and electrooptical properties of cellulose pelargonates, trideconates, valerianates, and acetovaleriates

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To a great extent, the interest in the cellulose esters (CE) is associated with their use as binding agents, additives, modifiers, film-forming materials in the processing of plastics, woodworking, and leather working. The feasibility of attaching various side radicals to the backbone cellulose chain, which substantially change characteristics of polymer molecules, stimulate further study of these compounds. Synthesized anew cellulose pelargonates, trideconates, valerianates, and acetovaleriates of various molecular weight are studied in chloroform (CF), dioxane, and tetrachloroethane (TCE) solutions by the methods of isothermal translational diffusion, rapid sedimentation, flow birefringence (Maxwell effect), viscometry, and equilibrium electric birefringence (Kerr effect).

The Mark-Kuhn-Houwink equations were obtained for all under investigation samples of cellulose esters in CF and TCE. The values of the equilibrium rigidities are determined, which are in the range from 12.5 to 28.0 for all studied samples. The influence of the solvent nature and the temperature on the formation of the conformational characteristics of the studied macromolecules is analyzed. It is demonstrated that the equilibrium rigidities of macromolecules decrease as the solvent polarity and temperature increase. The rigidity of the studied polymers, as well as of the other cellulose esters, is governed by the hindered rotation about valence bonds due to interaction of the side groups.

To study the optical characteristics of cellulose esters, we chose TCE as a solvent due to the fact that the refractive index increment does not exceed $0.02 \text{ cm}^3 \times \text{g}^{-1}$ for CTD in TCE. Hence, the role of the optical micro- and microform effects is negligibly small in this case. We determined the proper values of the optical shear coefficient, optical anisotropy of the Kuhn segment, and optical anisotropy of the monomeric unit of the polymers studied in TCE. The optical shear coefficient is negative. The aliphatic side substituents make negative contribution to the optical anisotropy of the studied polymer macromolecules. The longitudinal component of the dipole moment of the monomeric units of CP, CV and CAV coincides with that obtained for other cellulose esters with the aliphatic side substituents. This is due to the fact that the dipole structure of the cellulose esters with the aliphatic side substituents is governed by their backbone chain (with the attached ester groups) and is independent of the length of the aliphatic substituents which do not contain the polar groups.

Hydrodynamic properties of the micelles of surfactants and their polymerized counterparts

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Forming micelles of Surfactants (TDTAB, AOT, DsNa, Triton X-100, AMPS-DDA) and polymerized micelles in solutions were investigated by dynamic light scattering method. TDTAB is investigated at concentration 1,02 and 2,04/dl. AOT has been investigated at concentration 0,3/dl. DsNa is investigated at concentration 0,3 and 0,7/dl. Triton X-100 has been investigated at concentration 0,3/dl. AMPS-DDA(dodecylammonium-2-acrylamido-2-methylpropane) has been investigated in a wide range of concentration from 2,65 to 10/dl. Solvent of all Surfactants is water. Measurements passed above CMC-1. There were spirits, chloroform and DMFA as a solvent for PM.

The sizes of micelles of Surfactants are found in solutions. It has been noticed that at concentration AMPS-DDA in a solution 2,65g/dl there is a sharp change of the sizes of micelles, that speaks about the closed aggregation of the system. After a solution filtration, at it is present a component in the size of more than a size of a pore of the filter that speaks about system self-organizing. Growth of the sizes PM in a series of spirit-DMFA-chloroform, is shown, it is connected with diphilic of polymeric systems. The model of self-organizing PM in environments with various polarity is offered.

Behavior polyzwitterion molecules in aqueous solutions of different ionic strength

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Ionic polymers including polyelectrolytes and polyzwitterions take particular attention of scientists, due to unique physical and chemical characteristics.

There is a range of theories and the significant experimental data-base concerning polyelectrolytes in contrast to polyzwitterions which are poorly investigated due to their low solubility.

This paper considers the theoretical research of how does the polyampholyte behaves interacting with the salt solutions of different ionic strength. The analysis of correlation of the swelling ratio and the low-molecular salt concentration was carried-out in the framework of the perturbation theory and the mean-field approach.

According to the perturbation theory, the second virial ratio was being looked for with the allowance for volumetric interactions of the electrical attraction and repulsion contribution in the polyzwitterion chain. The constitutive equation for polyzwitterion was obtained by minimizing the macromolecular free energy which was figured out within the mean-field approach.

The correlation indexes for polycarboxybetaines in solutions of different ionic strength were compared for both theoretical and experimental approaches.

Formation of photosensitive DNA-surfactant complexes

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Compaction of DNA molecules to sizes necessary for entering cells is nowadays the most powerful tool for gene therapy. Nonviral approaches are highly promising as alternatives, avoiding the risk of viral gene modification and other problems of currently known viral gene delivery systems. It is desirable to achieve simple and reversible control over the compaction process. Moreover controllable DNA conformation changes can yield a plethora of new decisions for externally switchable nanobiosystems. Here we suggest the development of photo-reversible compaction of DNA molecule using light-sensitive surfactants.

The study of DNA interactions with light-sensitive surfactants was started several years ago with the G-RISC kind support. The azobenzene containing surfactants (fig. 1) were synthesized at the University of Potsdam, experimental part was carried out in collaboration between University of Potsdam and Saint-Petersburg State University. The DNA-surfactant interaction was characterized by UV-Vis and fluorescence spectroscopy, low-gradient viscometry, circular dichroism, gel-electrophoresis and dynamic light scattering.

It was shown that DNA coil size can be controlled by light when complex formation is performed under definite conditions. Intriguing preliminary results on theoretical modeling of the photosensitive system which were obtained at Saint-Petersburg State University by R. Ramazanov correlate with an experimentally predicted interaction mechanism.

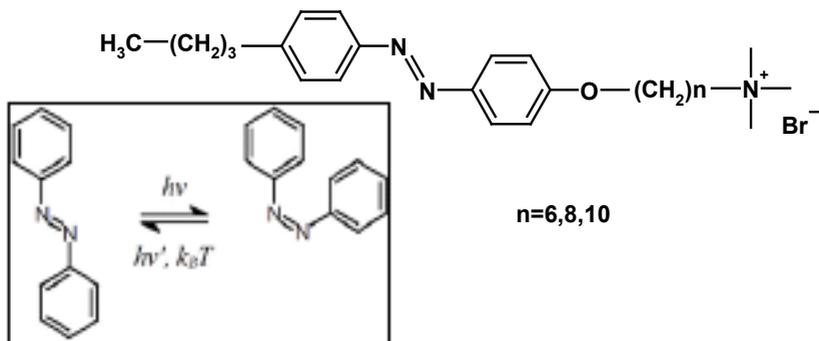


Fig. 1. Chemical structure of the surfactants. Inset: *trans-cis* isomerization of azobenzene unit under irradiation.

Conformational and optical properties of comb-like polymers in organic solvent

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The complex and comparative investigations of polymerized micelles in dilute solutions were studied via the methods of molecular hydrodynamics and optics. The object of investigations were samples of poly (12-acryloylaminododecanoic acid) PAAD and poly (12-acryloyloxydodecanoic acid) PAOD, in which long aliphatic fragment linked to the main polymeric chain by amid or ester groups respectively. Special interest was to establish the influence of these groups on the physical properties of molecules and to compare the physical properties of macromolecules PAAD and PAOD with comb-like polymers (N-acryloyl-11- aminoundekanoic acid) (PAAU), studied previously. All investigations were carried out in mixed organic solvent dioxane-cyclohexanol.

Values of intrinsic viscosity of PAAD and PAOD are in the range from 0,6 to 1,6 dl/g. By the obtained values of translation diffusion coefficient and intrinsic viscosity were determined the molecular weight, which are in the range $(0.3 - 9.3) \times 10^6$.

Recently was shown, that macromolecules of PAAD have high equilibrium rigidity. For PAAD Kuhn segment value is close to PAAU ($A = 8.5 \pm 1.5$ nm). At the same time estimated value of equilibrium rigidity PAOD is significantly lower ($A = 5 \pm 1$ nm). That indicates that the replacement of the amide group on the ester leads to almost twofold decrease of equilibrium macromolecules rigidity.

The average value of the optical shear coefficient for PAADK was $\Delta n / \Delta \tau = -4.4 \times 10^{-10} \text{ cm}^2 \text{ g}^{-1}$. This value is almost identical to the value obtained for PAAU ($\Delta n / \Delta \tau = -4.7 \times 10^{-10} \text{ cm}^2 \text{ g}^{-1}$). The average value of the optical shear coefficient for PAOD was $\Delta n / \Delta \tau = -6.7 \times 10^{-10} \text{ cm}^2 \text{ g}^{-1}$.

This work was supported by the Russian Foundation for Basic Research (project nos. 12-03-00687-a).

Molecular dynamics study of a galactan chain in water

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Carbohydrates (saccharides) represent an important class of biological molecules. Saccharides participate in processes of cell recognition and adhesion. However, for historical reasons the carbohydrates have been studied to a considerably lesser extent as compared to nucleic acids or proteins.

The aim of this work is to investigate a three-dimensional structure of a single galactan chain in aqueous solution. We consider this work as a first step towards characterization of the structure and properties of arabinogalactan, a branched polysaccharide that is found in many plants. Galactan constitutes a main chain of arabinogalactan and is built from β -D-galactopyranose units connected with (1-3)-glycosidic bonds.

To study the structure and properties of galactan in water we employed atomic-scale computer simulations. The simulations were carried out with the use of Gromacs suite [1]. The GROMOS 45A4 force field for carbohydrates [2] and SPC water model [3] were employed. Galactan chains of 8, 16, 24, 40 and 56 monomeric units were studied. Each system was simulated for 250 nanoseconds. Overall, molecular dynamics simulations show that galactan molecules have tendency to form a helix-like structure with relatively high internal flexibility.

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Kerr effect and the structural transitions in the isotropic phase of smectic comb-like polymers

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The isotropic phase of mesogens is characterized by the presence of pretransitional phenomena including the electro-optical properties. Electro-optical Kerr constant K monotonically varies over a wide temperature range, this dependence is described by $1/K \sim (T-T^*)$. Recently, in the isotropic melt of methacrylic polymer with chiral side groups we found abrupt change of K which we attribute to the isotropic-isotropic phase transition [1]. In other studies using calorimetry [2-4] and dielectric spectroscopy [5] was established the existence of such transitions in the isotropic melts of liquid crystal substances. In all cases, the transition was implemented only in chiral smectic molecular systems.

In this work melts of smectic comb-like polymers with different structures are investigated. For the first time the presence of the isotropic-isotropic phase transition was detected in non-chiral smectic polymer CBO-5-PA with an acrylic main chain and mesogenic cyanobiphenyl side groups. Thus, it can be assumed that these transitions in smectic polymers can be realized with different molecular architecture.

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Kerr effect and the structural transitions in the isotropic phase of smectic comb-like polymers

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I. Resonance Phenomena in Condensed Matter

Competition between hydrophobic and hydrophilic interactions in carboxylic acid aqueous solutions

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Aqueous solutions of ions and organic molecules are the basis of a living tissue. Hydrophobic and hydrophilic interactions play an important role in formation of structure of solutions with organic molecules. One of the most informative techniques of investigation of the hydration properties is an analysis of concentration and temperature dependences of NMR-relaxation rates.

The aim of this work is an investigation of the hydrophobic and hydrophilic interactions in acetic acid and propionic acid ($\text{CH}_3\text{-COOH}$ and $\text{CH}_3\text{-CH}_2\text{-COOH}$ respectively) aqueous solutions. These molecules are characterized by uncharged hydrophobic methyl and methylene groups and hydrophilic carboxylic group.

Measurements of spin-lattice and spin-spin relaxation times of solvent nuclei were carried out using the spectrometer Bruker SPX 4-100.

The analysis of the concentration and temperature dependences of the spin-lattice relaxation rates of the solvent nuclei gives us information about microstructure of solution: the number of water molecules in hydration shell (coordination number) of whole molecule and in the shells of the molecular functional groups, averaged activation energy and activation energies of water molecules in different substructures of the solution. The difference between propionic and acetic acids only in the methylene group allows to obtain the detailed information about water structure near this group: the relaxation and correlation times, the coordination number and activation energy.

The obtained structure parameters allow us to study the temperature and concentration features of the hydrophobic and hydrophilic interactions between the functional groups and water molecules in the acid solutions. The method used in the work may be applied for aqueous solution of other classes of organic molecules.

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Electronic structure and electric field gradient distribution in the layered perovskite NaLaTiO₄

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During last decades the layered perovskites, such as NaLaTiO₄, have been intensively studied due to their photocatalytic properties. According to recent researches layered perovskites with hydrated interlayer space exhibit more efficient photocatalytic activity for water splitting [1, 2]. The photocatalytic properties of these materials are governed by both the cation types and number of layers. From this perspective the study of water intercalation into layered perovskites (where the water molecules are located? how do they bound to the host ions lattice?) is very important.

It is obvious that when entering into the interlayer space the water molecule disturbs the charge density distribution around the host ion. If the nucleus of the host ion is quadrupole (that means the nucleus spin $I > 1/2$) experimentally information about the charge distribution around it can be derived from electric-field-gradient (EFG) measurements, for example, by nuclear magnetic resonance or nuclear quadrupole resonance methods, combined with calculations. However, before start an experiment it is important to verify if such a characteristic is sensible to the changing in the coordination of water molecules around the quadrupole nucleus under study

In this contribution we report on the result of our theoretical studies of the NaLaTiO₄ layered perovskite carried out applying the density functional theory. The EFG value at the Na site was calculated within both band and cluster approaches. The cluster approach is more flexible and can be used to simulate local disorder [3]. To choose correctly the basis set and cluster size we used the EFG at the Na site calculated within the band Full-Potential Linearized Augmented Plane Waves (FLAPW) method as a reference point.

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Main magnetic field stability research of a low-frequency MRI installation

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There are the various sources of a magnetic field used in MRT-tomographs. As a rule, in modern tomographs superconducting magnets which are characterized by high time stability of a magnetic field, are used. But such magnets are the extremely expensive. For working out of more budgetary versions of tomographs other sources of a magnetic field are used: constant magnets, electromagnets, solenoids. The magnetic field of two last sources depends on following factors: sizes of a feeding current and temperature of surrounding space. If these factors change not controllably, so that field created by these sources, have instability in time and if a value of a magnetic field are not controlled, received MRT images have characteristic artifacts. The purpose of the given work is creating a program in LabView, which writes the FID and echo in a separate file. Division of the data in Mathcad 14. Construction of images and estimation of the stability of the field. Development of methods for auto-imaging. Experimental verification of this methods. To eliminate the given problem an engineering software Mathcad 14 is used. Our program uses series of test images to calculate size of the basic magnetic field average value and its disorders (dispersion). A matrix of k-spaces (experimental results) transmits on an input of this program. As a result it is possible to see, the level of stability of given magnetic field, in the form of numerical data and schedules. We developed two auto-correction methods: In the first case, we propose for each row of the image to make correction to the corresponding carrier frequency. In this case, the instability of the field and the “right” and “wrong” lines will be corrected. Finally, we obtain a picture in which each row of the image in k-space has its own carrier frequency. In the second case, we propose to identify lines, taken at an unstable field and do not consider them at all. For imaging use balanced lines in the matrix, previously having made the complex conjugate. Then, finally we get the right image without artifacts. During this work the corresponding program has been written. The program was investigated for 3 variants of change of a field in time. A program in Lab View, which writes the FID and echo in a separate file, a program for the separation and processing of data in Mathcad 14. Get a series of images for different variants of stability field. The methods of auto-image, in the case of unstable field were developed. Thus results of work can be used as preliminary check of stability of a magnetic field straight ahead of experiment.

We have plans for future - to improve the program to automatically reconstruct inaccurate images (obtained with an unstable field.) Conduct a series of experiments and debugging programs and algorithms.

The contribution of Super Fine Interaction at spin selective recombination

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More of physico-chemical exothermic process in condense phase followed by emergence excited “hot” particles. This excitation can be the origin of excited hyperfine states in hydrogen atoms in the Universe which are the source of the space radio frequency emission ($\nu = 1428,5714$ MHz).

The present work provides insight into the impact of Super Fine Interaction (SFS) on products of spin selective recombination. The both hydrogen atoms are initially in the ground singlet state $|S_H\rangle$. These atoms are producing molecules H_2 have been proved to be created in *para*-hydrogen state only. However, if atomic pairs (H+H) are in triplet electron states, they can't recombine and produce separated atom H. That the probability of excitation is determined by the probabilities P_T of the triplet hyperfine states. The other hydrogen atoms leave the contact state begin in the ground singlet states.

Another interesting problem is the spin depended recombination in magnetic field. Magnetic field makes state the mixture of singlet and triplet states of hydrogen atoms. The admixture of the triplet state decreases the probability of recombination.

Results of work:

1. “Unsuccessful” attempts of spin selective recombination can be the source of excited hydrogen atoms.
2. Strong magnetic fields decrease the recombination probability and populations of hydrogen excited states.

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Features of the ^{23}Na quadrupole NMR - relaxation in aqueous solution

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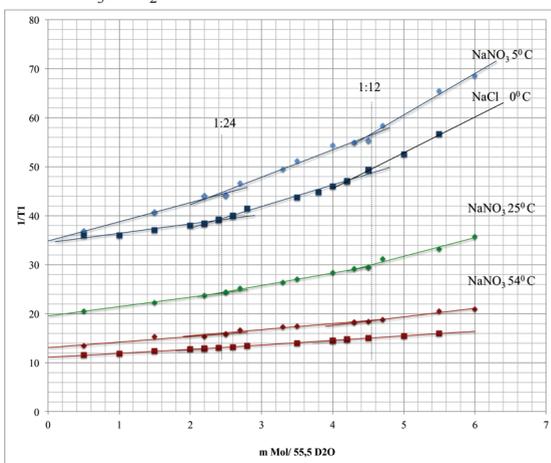
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Introduction

A method is presented for determining microstructural parameters of diamagnetic aqueous solutions with NMR and quantum chemistry; it is based on the analysis of the concentration and temperature dependences of the relaxation rates of various nuclei of solvent molecules and ions. The results, obtained for ^{23}Na ion, make it possible to find out several laws which describe the formation of ion hydration shells: monatomic ions are surrounded by the highly symmetrical shells, hydration shells of cations are characterized by two layers usually.

^{23}Na NMR-relaxation

The slope of the experimental curve changes at concentration $m = 2,3$ mol ($[\text{NaNO}_3]:[\text{D}_2\text{O}] = 1:24$). The main reason is the disappearance of zone of free solvent in the solution.



The first hydration shell of the sodium consists of 6 water molecules, second shell – 12. The NO_3^- ion coordinates 6 molecules. The bend at concentration $m = 4,6$ mol ($[\text{NaNO}_3]:[\text{D}_2\text{O}] = 1:12$) indicates complete disappearance of the second layer of the hydration shell of the ion Na^+ .

Fig. 1 Concentration dependences of the spin-lattice relaxation ^{23}Na nuclei in aqueous solutions at different temperature.

Quantum-chemical calculation

Using the density functional approach with the B3LYP hybrid functional and the 6-31G basis set, two equilibrium structures of the $\text{Na}^+(\text{D}_2\text{O})_{18}$ complex with two completely filled hydration shells of the ion were obtained. The calculations confirm experimental results. Thus we were able to obtain fundamental knowledge using two complementary and independent methods.

A study of the cation mobility in [bmim]Cl ionic liquid using temperature dependence of spin-lattice relaxation times

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The dependence on molecular mobility through the fluctuations of local magnetic fields is a remarkable property of the nuclear magnetic relaxation. It allows the experimental study of such mobility by measuring nuclear magnetic relaxation times. In liquid matter the typical molecular movements leading to the fluctuations of local magnetic field are translational and rotational molecular diffusion. One can determine the correlation time and activation energy in the wide range of temperature by the nuclear magnetic resonance relaxation.

The object of this study is ionic liquids (ILs) – which have the melting point below 100 °C. They are objects of interest because of its notable properties: they are unflammable, have negligibly small vapor pressure, thermically stable, non-toxic and sustainable. Also such kind of matter has good conductivity and unique properties as a solvent.

The goal of present work is to measure spin-lattice relaxation times T_1 for the [bmim]Cl ionic liquid at 90MHz in temperature range of 22-95 °C and to determine the correelation time and activation energy using this data which are supposed to be in average correlation time and activation energy referring to the whole molecule. The acquired results were to be compared with previous literature results obtained for ionic liquids under similar experimental conditions. The results obtained are:

- 1) The minimum of spin-lattice rexation times was attained for considered ionic liquid and the correlation times were directly determined.
- 2) The activation energies for the cation movement in [bmim]Cl were determined from Ahrenius approximation as well as from the whole curve. It was shown that for correct determination of the activation energy it is necessary to use the separate activation energies at high and low parts of temperature dependence.
- 3) Comparison of the obtain results with the literature ones was performed for similar systems. Strong influence of the anion upon correlation times and activation energy was revealed.

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Hydration properties of biological nanostructures in complex solutions

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A clear understanding of interaction of amino acid functional groups with different environment allows us to understand the formation of the spatial structure of proteins in complicated biological solutions and live tissues. This is the subject of this work.

Investigated systems are aqueous solutions of amino acids. The water structure in the solution can be described as the superposition of different substructures: hydration shells of functional groups (methylene, amino, carboxyl, etc.) and pure solvent.

NMR relaxation rate of the solvent nuclei is the sum of contributions of each substructure with weights which are equals to the relative concentrations of the substructure [1]. Deuterium relaxation in D_2O solutions with organic molecules with different functional groups, and results of quantum chemical calculations make it possible to determine these contributions. Studying of hydration properties of the functional groups was carried out. For example, the activation energies of motion in different substructures and the deuteron relaxation rates were calculated for water near COO^- , NH_3^+ , CH_2 and CH_3 groups.

Quantum chemical calculations (Hartree-Fock and DFT) of the investigated systems [organic molecule + $(H_2O)_n$] ($n > 30$) were performed. Microstructure of the water clusters around amino acids, coordination numbers and length of hydrogen bonds were studied. In case of the hydrophilic interaction the length of the hydrogen bond between COO^- , NH_3^+ functional groups and the nearest water is equal about 1.8 Å, for hydrophobic interaction the distance between proton of CH_2 and CH_3 groups and oxygen of the nearest water molecule - 3 Å.

The substructures of water may be divided by hydration type: a – the activation energy in water structure is greater than in bulk water $E_{struct} > E_0$ and b - $E_{struct} < E_0$. It was shown that solvent molecules near the hydrophilic groups COO^- and NH_3^+ are referred to the first type and the water near the hydrophobic CH_2 and CH_3 to the second one.

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NMR study of complexes of 1,1-dinitroethane with proton acceptors in aprotic medium

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The very first reference to C-H \cdots B (B is a proton acceptor group) hydrogen bonds goes back to 1936 [1], but only in the 1962 these weak interactions [2], often not even considered as hydrogen bonds [3], were accepted widespread. In this work we focus on unusually strong C-H \cdots B bonds, formed by 1,1-dinitroethane (DNE) with various proton acceptors. Proton donating ability of DNE (pKa = 5.1) is sufficiently high to form complexes of various structures, including those with proton transfer, i.e. ion pairs of the C $^-$ \cdots HB $^+$ type [4].

Usually investigation of hydrogen bond made by means spectroscopic studies (NMR, IR) or *ab initio* calculation. Different correlation between NMR parameters with interatomic distances have been successfully used to define the geometry of the hydrogen bonds. To date there are a few experimental data about correlation between $^1J_{\text{CH}}$ coupling in the proton donor group and interatomic distance C \cdots H. In this work we would like to fill this gap by reporting results of ^1H , ^{13}C and ^{14}N NMR study of DNE dissolved in aprotic solvents of different proton accepting abilities (CCl_4 , CDCl_3 , CD_2Cl_2 , $(\text{CD}_3)_2\text{CO}$, $(\text{CD}_3)_2\text{SO}$) as well as in complex with such organic bases as di- and triethylamine. Interestingly, molecular and zwitterionic complexes of 1,1-dinitroethane with bases can coexist in solution in the NMR slow exchange regime. Also we discuss the reasons of broadening carbon signals in ^{13}C NMR spectra.

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¹H NMR study of hydrogen diffusion in hydrides of ternary Ti-V-Cr alloys

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Metal hydrogen systems have been extensively studied last decades due to their ability to be used as hydrogen storage materials. A good hydrogen storage material has to fulfill a number of criteria, such as a high hydrogen storage capacity, a low hydrogen desorption temperature, a high hydrogen sorption kinetics, a reversibility of the hydrogen sorption reaction etc. **Despite a comparatively low hydrogen storage capacity** (up to 3.8 wt% for selected compositions) Ti-V-Cr alloys exhibit low temperature of the hydrogen release and rather high hydrogen sorption kinetics [1]. The latter can be further improved by alloying with Zr₇Ni₁₀.

Kinetic properties of hydrogen storage materials are governed by their microstructure. Nuclear magnetic resonance (NMR) is a powerful tool to determine both the microstructure of the hydrides, including positions of hydrogen atoms and their nearest neighboring, and the hydrogen mobility in the metal lattice [2].

In this contribution we report on the results of our experimental study of the hydrogen diffusion in ternary Ti-V-Cr alloys of various compositions, T_{0.5}V_{1.9}Cr_{0.6}H_{5.03} and T_{0.33}V_{1.27}Cr_{1.4}H_{1.13}, pure and with addition of 4 at.% of Zr₇Ni₁₀. The self-diffusion coefficients were measured by ¹H NMR in ultrahigh static field gradient (SFG-NMR) instrument [3] in Darmstadt Technical University (the Prof.F. Fujara's group).

It was found:

(i) in all studied compounds the hydrogen diffusion is limited and run inside crystallites;

(ii) the activation energy is lower in the vanadium rich compounds;

(iii) the addition of Zr₇Ni₁₀ does not affect T_{0.5}V_{1.9}Cr_{0.6}H_{5.03}, but leads to decreasing of the self-diffusion coefficient in T_{0.33}V_{1.27}Cr_{1.4}H_{1.13}.

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