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Poster abstract	Remarks

1. Study of crystal and magnetic structures of complex ferrites by neutron diffraction method

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The materials based on complex ferrites are widely used in modern industry. These materials exhibit a wide range of physical properties such as magnetism, structural phase transitions, and giant magnetoresistance. Great interest in the ferrites with a spinel structure (FSH) and wide used in various areas are caused by a great number of those magnetic properties. Their physical and chemical properties depend on the distribution of magnetic cations. In particular, the magnetization of these systems is determined by the ratio of cations in the A and B crystallographic sites.

The main aim of the present work was to study crystal and magnetic structures of the FSH nominal composition: $Mn_{0.25}Cu_{0.75}Fe_{1.7}Ga_{0.3}O_4$, $Mn_{0.5}Cu_{0.5}Fe_{1.7}Ga_{0.3}O_4$, $Ni_{0.4}Cu_{0.4}Zn_{0.2}Fe_2O_4$, $Ni_{1.2}Zn_{0.1}Ti_{0.3}Fe_{1.4}O_4$ by means of neutron diffraction. Also granulated powders FSH nominal composition $Mn_{0.676}Zn_{0.224}Fe_2O_4$ (700NM) and $Ni_{0.32}Zn_{0.68}Fe_2O_4$ (1000NN) were investigated depending on particle size. Experiments on neutron diffraction at room temperature was carried out using a diffractometers DN-6 and DN-12 of high-flux pulsed reactor IBR-2 (FLNP, JINR, Dubna). Spectra were recorded using a time-of-flight technique at a fixed angle of scattering $2\theta = 90°$. Analysis of data was performed by the Rietveld method by FullProf program.

Lattice parameters of the compounds studied, the length of the interatomic bonds and valence angles, the distribution of cations in positions A and B in the crystal structure of ferrites were obtained . The magnetic moments of iron and dopants in different positions of the spinel structure were calculated. It is found, that gallium ions predominantly occupy the octahedral B position, while the magnetic ions of manganese is distributed between two crystallographic sites.

It is determined that with increase in the size of granules the bond length Fe-O is almost constant for compounds of $Ni_{0.32}Zn_{0.68}Fe_2O_4$. At the same time, the increase in the size of granules for ferrite $Ni_{0.32}Zn_{0.68}Fe_2O_4$ magnetic moment of tetrahedral (A) and octahedral (B) positions reduced. It is assumed that the structural aspect of this phenomenon is the formation of oxygen defects on the surface of the particles, which leads to instability of the magnetic subsystem of ferrite samples.

2. Poly (ethylene glycol) addition influence on the structure and interaction parameters of anionic surfactant micellar systems

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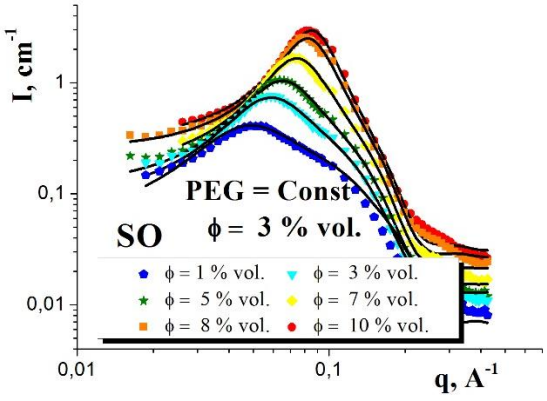
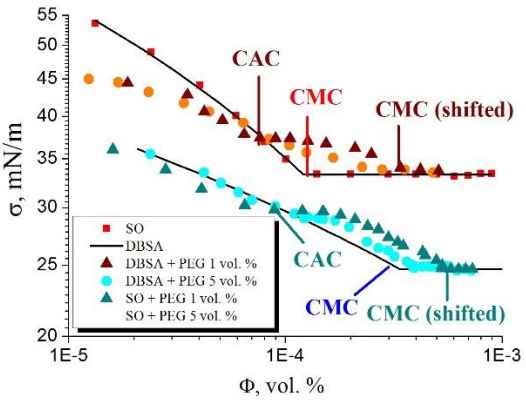
Micellar systems of surfactants plays important role in colloidal chemistry for production stable colloidal solutions [1]. Therefore anionic surfactants sodium oleate (SO) and dodecylbenzene sulphonic asid (DBSA) often used for double layer stabilization of aqueous ferrofluids. In recent works was shown that physicochemical properties of micellar solution have influence on the structural organization of magnetic nanoparticles [2]. In order to improve biocompatibility of ferrofluids, they modify by water-soluble neutral polymer poly (ethylene glycol) (PEG). Therefore, the resulting multicomponent system of micelles-polymer buffer has particular stabilization properties and as consequence, nanoparticles aggregate intend to reorganization [3].

Present work dedicated to investigation of structural of SO and DBSA micellar system after PEG addition together with surface tension study of solution. The presence of a polymer – micelle interaction and polymer-surfactant complex foundation in the range of characteristic concentration, from critical aggregation concentration (CAC) to critical micelle aggregation (CMC) was found (right figure). Further structural investigation using small angle neutron scattering (SANS) technique (left figure) allowed us determine structural and interaction parameters of micelle: number of aggregation (N_{agg}), degree of ionization (α), axial ratio of ellipsoid model (γ), inverse screen length (k_d). The comparative analysis of the above parameters was carried out for systems with different quantitative composition of surfactant-polymer aqueous solution.





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3. SFF analysis of the vesicular systems structure: MPI implementation of the fitting procedure and numerical results

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The separated form factors method (SFF) is an effective approach of investigation of structure of polydispersed systems of phospholipid vesicles on the basis of the small angle scattering data analysis. In this framework, basic parameters of vesicular system are determined by means of minimization of a discrepancy between experimental data on intensity of small angle scattering and the results of the SFF calculations. The minimization procedure is based on the generalized least square method which was employed in the code FUMILI of the library JINRLIB. In this contribution, we utilize the parallel MPI-version of this code, PFUMILI. Effectiveness of parallel implementation is tested on the cluster HybriLIT. Results of numerical analysis of the small angle neutron scattering data collected at the YuMO small-angle spectrometer of the Frank Laboratory of Neutron Physics are presented.

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4. Investigation of crystal and magnetic structure of nanostructured complex oxides of transition metals in wide temperature range

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Special interest in investigation crystal and magnetic structure of complex nanostructured oxides of transition metals caused by great amount of physical phenomena found in such compounds [1, 2].

Complex oxides of iron and manganese have already found wide application in microelectronics [1]. However, the modern synthesize methods, which give opportunity to obtain nanostructured compounds of strictly determined composition, opened a prospect for biophysical applications. Some complex nanostructured oxides of manganese and iron showed itself as promising materials for biomedical applications (in Magnetic Resonance Tomography (MRT), in procedure of magnetic hyperthermia). These facts proof relevance of detailed study of complex nanostructured oxides of transition metals [2].

The knowledge of relationship between magnetic and crystal structure in complex nanostructured oxides, which can be obtained from high-pressure investigations, is very essential for understanding the nature and mechanisms of physical phenomena observed in these nanostructured compounds [1-3].

The crystal and magnetic structure of nanostructured manganite $La_{0.53}Sr_{0.47}MnO_3$ has been studied by means of a neutron diffraction method on diffractometer for investigation microsamples DN-12 of high-flux pulsed reactor IBR-2 (FLNP, JINR, Dubna) in wide temperature range 15K - 320K. The sample of polycrystalline ferrite spinel $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ was chosen and performed neutron powder diffraction measurements at

ambient and high pressures up to 4.7 GPa temperatures using DN-12 diffractometer of high-flux pulsed reactor IBR-2 using the sapphire anvil high-pressure cell. In additional, for studies the role of structural parameters across the paramagnetic-ferrimagnetic phase transition we had investigate structure and magnetic moments evolution in temperature range 300 - 425 K.

With increasing temperature and pressure, a gradual decreasing of the magnetic moments of iron ions in the A and B crystallographic sites and manganese ions were observed.

These effects correspond to magnetic phase transition from ferrimagnetic state to paramagnetic one. The lattice parameters, interatomic bond lengths and angles, magnetic moments of iron and manganese as functions of temperature and pressure were calculated. The structural mechanisms of the magnetic transition in complex oxides of iron and manganese are discussed.

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5. Detection of DNA molecules by SERS spectroscopy with silvered porous silicon as an active substrate

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Progress in an engineering of the SERS substrates has driven a tremendous interest to study DNA by the SERS spectroscopy [1–3]. However, the practical application of this method is still in its infancy comparing to the traditional techniques of the DNA detection. It is mostly caused by severe dependence of the spectral quality and reproducibility on variations of the DNA conformation and/or packing density on the SERS substrates [4]. It has been previously shown that the SERS substrates based on a silvered porous silicon (PS) give rise to a strong enhancement of the signal from a rhodamine 6G [5] and a cationic Cu(II)-tetrakis (4-N-methylpyridyl) porphyrin resulting in an extremely high sensitivity [6]. In this work, we investigate the effect of such substrates on the spectra of the herring sperm DNA to choose optimal conditions of the SERS measurements resulting in a reliable DNA study.

The Raman and SERS spectra were measured with a 3D laser scanning confocal CARS microscope. An adsorption of analyte molecules was realized by a drop deposition method of herring sperm DNA in 0.01M NaCl water solution on the silvered PS.

The results on the DNA study by the SERS spectroscopy with the silvered PS presented here were partially similar to those with solid SERS substrates that gave surface enhancement from DNA but with aweak reproducibility of the spectra. This was typical for the measurements in random points on the SERS substrate. However, from the results of this work it is likely that the classical spectra of the DNA molecules can be found by the SERS substrate mapping [7]. Moreover, the prospects for the DNA detection by the SERS spectroscopy with lasers of 473, 633, and 785 nm wavelengths are very encouraging. The most promising result is in the detection of the DNA molecules at very low concentration (10^{-10} M) with the silvered PS. According to our knowledge, detection of such a small amount of DNA has not been reported elsewhere. It shows an advantage of the developed silvered PS compared to other solid SERS active substrates. Thus, the SERS substrate based on PS is a very unusual material that can help to overcome some of the existing problems in the DNA study by SERS spectroscopy.

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6. Structure of magnetic fluids at interface with silicon by neutron reflectometry

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Ferrofluid(FF) is the colloidal system of magnetic nanoparticles with solvents of different polarity. Layers of surfactants are frequently used to stabilize such systems. Great interest in these systems is related due to the possibility of their use for controlled drug delivery, diagnosis and treatment of various diseases, for example cancer. Therefore, the study of biocompatible FF are very relevant. At the same time behavior of magnetic nanoparticles in the bulk and at interfaces can be very different due to specific adsorption properties, which should be considered in a variety of applications. It also remains an open question regarding the possible differences in the stability of magnetic fluids in bulk and at interfaces.

The main aim of this study is to get values of structural parameters of biocompatible ferrofluids, the study of their stability in the volume and near the surface. Information about the structure of FF in bulk was obtained from small-angle neutron scattering experiments. Neutron reflectometry experiments were done to investigate behavior of magnetic fluids with different methods of preparation and concentration at the interface with silicon. Influence of gravity on the adsorption properties of magnetic particles was also checked. It was shown that only single magnetic nanoparticles, coated by surfactant molecules, are adsorbed to the surface of the silicon from bulk of ferrofluids. X-ray reflectometry make possible to study free liquid surfaces or interfaces air/FF. It is reported about structural organization nanoparticles at this interface. Influence magnetic field with horizontal and vertical to surface direction was shown. Comparative analyses is held for all interfaces of study and volume.

7. Preparation of the lithium ion battery electrodes for operando X-Ray and neutron diffraction investigations

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Improvement of the performance characteristics of lithium-ion batteries (LIB) requires understanding of the nature of the structural processes occurring on the electrodes [1]. In this case *operando* studies of the electrode materials crystal structure by X-ray and neutron diffraction methods are very important and complementary. Investigations of commercial electrodes in ready-to-use batteries are useful but do not allow studying new electrode materials. So, it is necessary to produce the electrodes at conditions of a small laboratory. Such electrodes should satisfy the tasks of specific experiment.

This report is devoted to the problems of synthesis of new cathode materials ($xLi_2MnO_3 \cdot (1-x)LiMO_2$, $0<x<1$, M = Mn,Ni,Co [2]) and electrode preparation. The methodology of cathode and anode manufacturing was worked out in the Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research (FLNP JINR). Based on the literature data [3] and our experience, the most suitable equipment was selected and the supporting components (carbon-conductive additives and polymer binders) of the electrode were chosen. Conditions for electrode preparation were optimized. As possible large amount of sample is needed for obtaining of qualitative diffraction pattern. So, there must be a lot of studied material and as small as possible amount of carbon and polymer additives in the electrode. In the same time, the stable operation of electrodes in LIB is very important. Our electrodes satisfy the requirements of diffraction and electrochemical experiments simultaneously.

The electrodes were investigated in special LIB designed in FLNP JINR for *operando* neutron and X-ray structural analysis. Values of capacity of the cells assembled with our electrodes ($LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$, $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ and others based) are close to the values calculated on the basis of the maximum achievable capacity of electrode material. Stable operation of our electrodes is demonstrated for commercial cathode materials and laboratory synthesized material.

The examples of *operando* experiments on High Resolution Fourier Diffractometer at the IBR-2 pulsed neutron reactor and X-ray diffractometer PANalytical Empyrean show high quality of the diffraction spectra obtained using the electrodes prepared in FLNP.

This work was supported by the Russian Science Foundation (project #15-13-10006).

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8. Optimization of neutron reflectometry experiments for planar interfaces

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Neutron reflectometry (NR) is a non-destructive method for study different planar interfaces in surface chemistry (surfactants, polymers, electrochemistry, lipids, proteins and mixtures adsorbed at liquid/fluid and solid/fluid interfaces), surface magnetism (ultrathin Fe films, magnetic multilayers, superconductors) and solid films (Langmuir–Blodgett films, thin solid films, multilayers, polymer films) [1,2].

However, a lot of experiment are conducted for "in operando/in situ" study of changes at planar interfaces. Usually such changes are not so pronounced. Thus in this case, initial structure of samples should be optimized to get maximum change in specular reflectivity curves, which is most completely providing the information about interface of interest.

This work is aimed to find the method for optimization initial parameters of samples to increase the sensitivity of the NR experiment, i.e. finding maximum ratio between initial and final NR curves of the sample. Some examples of interfaces modeling and selection the best configuration to study small changes at the interface [3] are presented in the given work.

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9. Fullerene-based complexes in solutions for anticancer therapy: structure characterization and toxicity tests

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Applications of fullerene water solutions (FWS) in medicine and cosmetics [1,2] are of current interest due to their antioxidant, antitumor and antibacterial properties. However, up to now there is no consensus to the question about influence of these systems in living organisms. In the literature both positive and negative health influences have been reported depending on the type of primary organic solvents used in the technique preparation and the cluster size distribution in the final solutions, as well as on the chemical modification of fullerenes resulting in a wide class of biologically active derivatives. In particular, there are indications [3] that cytotoxicity and antibacterial properties of FWS correlate with the aggregate formation. The latter also has an impact on the environment, since after utilization the FWS interacting with natural salts coagulate, which significantly complicates their removal.

The present paper is devoted to the comparison of the efficiency of fullerene C60 water solutions with respect to their application for the treatment of oncological diseases. Different methods of preparation of fullerene water solutions were considered. At the initial stage of research, the detailed structure analysis for each solution in water and after fullerene transfer in saline solutions included several methods (small-angle X-ray and neutron scattering, dynamic light scattering, atomic force microscopy, transmission electron microscopy, UV-Vis spectroscopy). At the next stage, cytotoxicity in vitro tests with mammalian fibroblasts of Chinese hamsters, line V-79, revealed good survival at fullerene concentrations up to 5 μg/ml. Subsequent investigations of the complexation of fullerenes with several anticancer drugs for potential enhancement of their activity concerned were presented.

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10. Raman, CARS and up-conversion luminescence imaging of bio- and nonorganic samples on the multimodal optical platform

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Imaging of small crystals which is highly demanded remains a challenge, especially in case of membrane protein crystals. The studies are carried out at the multimodal optical platform for performing Raman, CARS, SHG, and transmitted light imaging of bio-samples. Here we describe a new extremely sensitive method of the imaging of protein crystals which is based on polarized coherent anti-Stokes Raman scattering (P-CARS). As the first step to understand the CARS imaging potential we performed studies with in meso grown bacteriorhodopsin (bR) crystals. We used bR in the present study because it is the most studied membrane protein. Very small crystals of the in-plane size about 2 μm and the thickness less than 1 μm are well resolved with signal integration time of 3μs/pixel [1].

Highly-contrast epi-SECARS micro-images of Au-nanoparticle-binded organic reporter molecule distributions at a surface of novel SERS-active metamaterial junctions, based on nanoparticles spread over a nanostructured CeO2 faceted dielectric film, deposited on an Al sublayer, were recorded at two-color picosecond excitation of the surface in the NIR spectral range. For this, a newly-built scanning confocal laser-based micro-CARS spectrometer was employed. The investigations showed that at Raman resonant laser excitation of the molecules/Au-NP conjugates immobilized on the surface strong SECARS signals can be generated with laser powers not deteriorating the conjugates. Coupling CARS with the plasmonic metamaterial structures under investigation provided excellent chemical imaging contrast (up to 400) for biochemically-relevant thionitrobenzoic acid and mercaptophenylboronic acid reporter molecules. Taking into account easy handling and utmost long-term stability of the investigated metamaterial junction at ambient conditions, it might be considered as a promising perspective for a single-molecule-sensitivity SERS/SECARS biosensor [2]. We also performed experimental study of feasibility to detect surface enhanced CARS (SECARS) signals at picosecond excitation of DTNB molecules in NIR spectral range; mapping of the SECARS intensity at the characteristic Raman frequency of DTNB molecules (1344 cm^{-1}), i.e. recording a micro-image of the surface at the

corresponding anti-Stokes wavelength.

Also, results are presented on the giant plasmonic enhancement of the upconversion luminescence (UCL, SE-UCL) in the system of $NaYF_4$ co-paired with Yb^{3+}, Er^{3+} and Yb^{3+}, Tm^{3+} ions adsorbed on the surface of porous silicon with an immersion layer of silver nanoparticles.

In the future of the applied research, it is planned to synthesize "core-shell" nanostructures with a core of $NaYF_4$:Yb,Tm and SiO_2 shell with silver nanoparticles or porphyrins for highly-contrast optical imaging of biological objects, and testing them in studies of photodynamic cancer treatment as well. This demonstrates not only the importance of this study but also some novelty of the research within the given area.

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11. New ring detector for small-angle scattering of thermal neutrons for Real-Time Diffractometer (RTD)

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The development of the detector is based on the design and experience of working with a one-dimensional coordinate-sensitive ring thermal neutron detector [1, 2], which allows measurements of the spatial distribution of thermal neutrons scattering from samples in 8 discrete coaxial rings.

The new detector is designed to measure small-angle scattering of thermal neutrons at the IBR-2 reactor, Real-Time Neutron Diffractometer (RTD) (channel No. 6a). Structurally the detector is divided into 9 independent equidistant coaxial rings. The cathodes of each of the rings are divided into 16 independent sectors, the same for each ring. The cathodes are located with inner side of rings and have a rectangular shape, their length being a function of the radius of the corresponding ring. Thus, each separate cathode segment takes position ~ 1/16 of the total angle 2π of any ring counter.

This innovation made it possible to introduce a new coordinate as a measurement parameter.

Due to its feature in design, the detector is a suitable tool for any researches in which angular or axial anisotropy of the scattering of slow neutrons can be observed.

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12. Clusterization aspects of fullerene C_{60} and C_{70} in toluene/N-methyl-2-pyrrolidone mixture according to SANS, SAXS and DLS data.

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Since fullerenes were discovered potential applications of fullerene solutions in various fields including electronics, optics, cosmetics, and pharmaceutics were intensively studied [1-3]. Despite of a wide application of fullerene solutions, the processes of their aggregation are still not clear in both weakly polar solvents and their mixtures with polar solvents [4]. Having a good solubility in different nitrogen-containing solvents, the systems based on the fullerenes C_{60} and C_{70} show a high sensitivity of optical properties to the change of liquid medium, an addition of miscible solvents to them.

N-methyl-2-pyrrolidone (NMP) is a comparatively good solvent for molecules C_{60} and C_{70} and it is also mixable with water. This solvent is suitable for fullerene transferee into aqueous media that is important for employing biological functionalized fullerenes in medical applications [5, 6].

The change in the absorption UV-Vis spectrum of the systems C_{60}/NMP and C_{70}/NMP varying the composition of the systems by admixing water of another extra solvents is well-known as solvatochromic effect. The phenomenon could be related with the appearance of donor-acceptor complexes between C_{60} (C_{70}) and solvents molecules on the cluster surface. At the same time it has a temporal character that can be connected with aggregation of fullerene monomers in the systems or their reorganization. Thus, the two effects competing determine the existence of the solvatochromic effect in C_{60}/NMP and C_{70}/NMP systems.

Solutions of the fullerenes C_{60} and C_{70} in polar and non-polar solvents and their mixtures are characterized by various effects, such as the unexpected aggregation in “good” fullerene solvents, or solvatochromic effects in solvent mixtures. The question under study in the present work is at what extent the solvatochromism (change in the absorption UV -Vis spectrum with time) is determined by the cluster formation in toluene (ε=2.4)-NMP(ε=32) mixture.

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13. On determination of the core-shell structure in magnetic nanoparticles by neutron and X-ray scattering

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The theme of a comprehensive study of condensed matter containing nano-objects is regularly filled out by the persistent activity of numerous research groups. In particular, many attempts are made in the present day material science to improve methods of controllable

synthesis of complex colloidal systems containing nanoparticles with a characteristic size in the range of 1–100 nm. Especially, this concerns magnetic fluids (or ferrofluids) where magnetic nanoparticles (MNPs) are dispersed and stabilized in liquid carriers. MNPs have much prospect in biology and medicine due to their promising applications.

Studies on the synthesis of MNPs, such as Fe_3O_4, $CoFe_2O_3$, $NiFe_2O_3$, etc. [1,2], are of great interest because of the possibility of their wide using in various fields of technology and science, including medicine [3,4]. Creation of new magnetic fluids with specified properties for biomedical purposes involves the development of new methods for synthesis of the magnetic nanoparticles with ability to predict and adjust their properties. It is considered a method which allows us to produce powders of magnetic NPs consisted of Fe_3O_4, $CoFe_2O_4$ and composite $CoFe_2O_4$/ Fe_3O_4 with core-shall internal structure [5]. Varying the thickness of "$CoFe_2O_4$-shell" around "Fe_3O_4–core" it is possible to affect on averaged magnetic properties of NP. With this respect, Small-Angle Neutron (SANS) and X-ray (SAXS) Scatterings are ones of the actively used methods to probe at the nanoscale the structure of various complex colloidal solutions including magnetic fluids [4,6].

To observe the core-shell structure in composite nanoparticles is an actual aspect of material study at nanoscale and, nevertheless, it meets many practical obstacles because of the direct detecting thin crystallite-shell around nano-sized crystal-cores lies at the edge of resolution of typical diffraction techniques. The main idea is to make a conclusion analyzing the data on the small-angle diffraction together with other complement methods, X-ray powder diffraction (XRD) and dynamic light scattering (DLS), and in comparison results for a composite material "$CoFe_2O_4/Fe_3O_4$" with MNPs consisted of single compounds, "Fe_3O_4," and "$CoFe_2O_4$".

The presented investigation unites the study of the powders with dried MNPs and their dispersions in liquids.

The SANS, SAXS and XRD were applied to testify nanostructured powders of magnetite, cobalt-ferrite and their composite. Characteristic size of MNPs and agglomeration state have been specified experimentally. The difference between SAS spectrum from core-shell composite MNPs and single-phase analogues was shown in comparison. The SANS (and SAXS) spectrum for composite powder could not be expressed as the sum of partial terms, corresponding to scattering spectra from magnetite and cobalt-ferrite samples. This can exclude a possible presence of mechanical mixture single-phase MNPs in the "$CoFe_2O_4/Fe_3O_4$" sample.

To distinguish the form-factor and to avoid scattering on large inhomogeneities Ferrofluids (FF) the same kind of MNPs were prepared. To prevent aggregation in aqueous media the MNPs were covered by molecules of Polysorbate-80 (Tween-80). DLS tests on FFs shows the presence of single-particle fraction in volume against of agglomeration. Structures of water-based ferrofluids were analyzed in a framework of SAXS and SANS data. Contrast variation approach within the SANS was used to try to resolve the scattering on the magnetic cores of MNPs. All magnetic liquids under study were quite stable colloidal systems.

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14. Simulation of interprocessor interactions for MPI-applications in the cloud infrastructure

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A new cloud center of parallel computing is to be created in the Laboratory of Information Technologies (LIT) of the Joint Institute for Nuclear Research (JINR) what is expected to improve significantly the efficiency of numerical calculations and expedite the receipt of new physically meaningful results due to the more rational use of computing resources. To optimize a scheme of parallel computations at a cloud environment it is necessary to test this scheme for various combinations of equipment parameters (processor speed and numbers, throughput of a communication network etc.). As a test problem, the parallel MPI algorithm for calculations of the long Josephson junctions (LDJ) is chosen. Problems of evaluating the impact of abovementioned factors of computing mean on the computing speed of the test problem are solved by simulation with the simulation program SyMSim developed in LIT.

The simulation of the LDJ calculations in the cloud environment enable users without a series of test to find the optimal number of CPUs with a certain type of network run the calculations in a real computer environment. This can save significant computational time in countable resources. The main parameters of the model were obtained from the results of the computational experiment conducted on a special cloud-based testbed. Computational experiments showed that the pure computation time decreases in inverse proportion to the number of processors, but depends significantly on network bandwidth. Comparison of results obtained empirically with the results of simulation showed that the simulation model correctly simulates the parallel calculations performed using the MPI-technology. Besides, it confirms our recommendation: for fast calculations of this type, it is needed to increase both, – the number of CPUs and the network throughput at the same time. The simulation results allow also to invent an empirical analytical formula ex-pressing the dependence of calculation time by the number of processors for a fixed system configuration. The obtained formula can be applied to other similar studies, but requires additional tests to determine the values of variables.

15. Influence of high pressure on the crystal and magnetic structure of $La_{0.5}Ba_{0.5}CoO_3$

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The crystal and magnetic structures of cobaltite $La_{0.5}Ba_{0.5}CoO_3$ have been investigated by the neutron diffraction method at high pressure up to 4.6 GPa in the temperature range from 10 to 290 K. Under normal pressure, the crystal structure of this compound has a cubic symmetry with the spatial group $Pm\bar{3}m$, which is kept throughout the investigated pressure range. Ferromagnetic ordering is observed when the temperature is reduced to T = Tc = 178 K. This magnetic ordering and Curie temperature do not change at high pressure up to 4.6 GPa. It is assumed that the stability of the ferromagnetic phase for $La_{0.5}Ba_{0.5}CoO_3$ is provided by preservation of the Co^{3+} ions concentration in the intermediate-spin state in the total investigated range of the pressure.

16. Monte Carlo simulations of SESANS-TGF experiments

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The realization of a wide and different type of experimental possibilities at IBR-2 reactor in Dubna is a scientific priority of the Frank Laboratory of Neutron Physics.

At present, there is only one small-angle neutron scattering (SANS) instrument, YuMO operating at the IBR-2 pulsed reactor. The Q-resolution of this instrument is limited by $7x10^{-3}$, that doesn't allow the studies of large-scale structures and limits experimental possibilities suggested for users. This fact makes necessary the construction of a new high-resolution SANS instrument.

Here we are considering new opportunities, which are opened by the development and implementation of a new Spin-Echo SANS method based on the use of time-gradient magnetic fields (TGF NSE), matches well to the pulsed neutron structure of IBR-2. The time-gradient magnetic fields are realized as a periodic sequence of the saw-teeth-like magnetic pulses that are synchronized with the reactor pulses.

A virtual SESANS instrument with TGF for the IBR-2 pulsed reactor was assembled using the VITESS software package for the Monte Carlo simulations. Results of simulated experiments on new SESANS-TGF virtual instrument are presented. These results allow to determine possibilities of new Spin-Echo SANS method.

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17. Verification of the "XiO" TPS using Radiochromic Films

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The objective of the present study was to verify all the stages of proton pencil beam scanning technique applied at the Proton Therapy Center (PTC), Prague, Czech Republic.

A proton beam irradiation simulation was carried out using "XiO" treatment planning system (TPS) developed by ELEKTA, Sweden, which is currently used on daily bases at PTC.

To evaluate the 2D dose distributions of different clinical treatment plans measured in an anthropomorphic phantom, from Alderson, and compare them to computer simulation predictions from a TPS we used Gafchromic EBT2 films, Ashland, USA.

A simulated target has been drawn on CT images of the phantom in a high heterogeneity region. The target irradiation was first simulated from 3 irradiation angles (240°, 305°, and 110°) and in the second case only from one direction, angle 240°, dose 2.5 Gy.

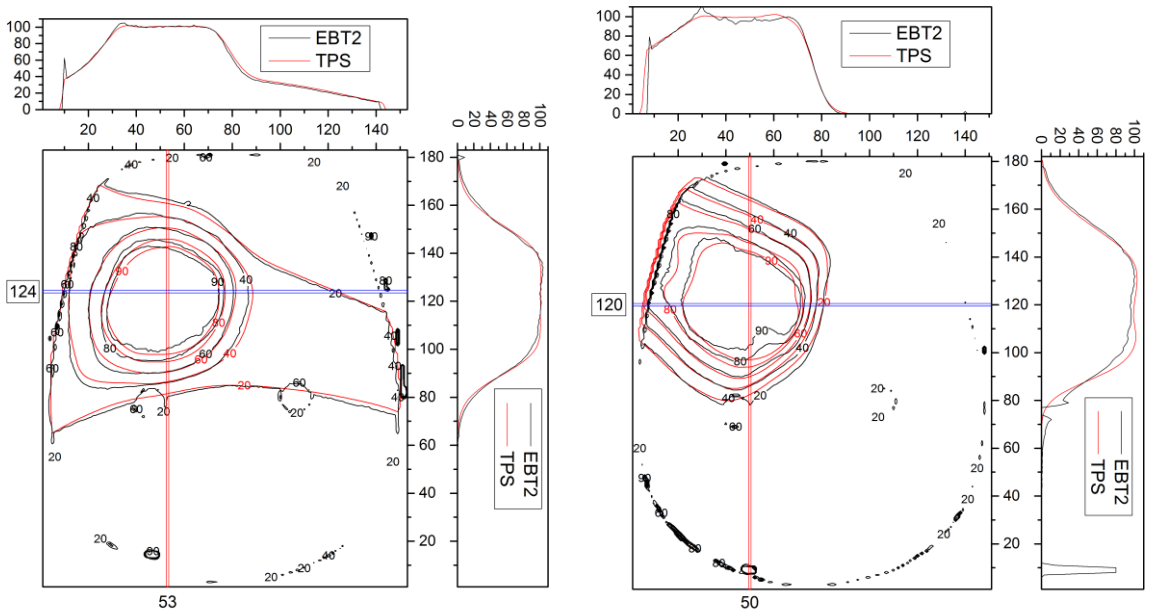
Radiochromic films cut in the shape of phantom's slice were placed between the slices containing the target. The films were calibrated for a dose range from 0 Gy to 3 Gy.

The irradiated films have been scanned (Epson 11000XL Pro scanner) and transformed into a matrix of doses using measured calibration curve.

The result containing the 2D dose distributions of the imaginary target in the phantom calculated (TPS) and measured (EBT2) are presented in Fig. 1.

Quantitative comparisons between the TPS and the EBT2 film data were carried out using gamma index procedures.

Our tolerance criterion for geometric accuracy was 3 mm and 3% for the values of dose. The first and second target coincides with the calculated one with at least 95.8% and 85.7% accuracy (≥10% in the region of doses), respectively. The result is within the accuracy of the experiment.



a) b)

Fig. 1. a) 1st target irradiated under 3 directions, b) 2nd target irradiated from one direction. The comparison of the dose distributions. Profiles at the isocenter of the target

18. Increasing Bandwidth of Data Acquisition Systems on IBR-2 Reactor Spectrometers in FLNP

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The present paper considers development of a new fiber-optic adapter with a USB 3.0 high-speed interface for a data acquisition system based on MPD [1] and De-Li-DAQ-2D [2] modules developed earlier in FLNP and widely used on IBR-2 reactor neutron spectrometers at present. In addition, it considers software implementation of USB3.0 stack protocols for operation with such data acquisition units.

Modern detector systems with point detector elements currently used on and being developed for FLNP spectrometers can be connected to data acquisition systems based on MPD-240 and De-Li-DAQ 2D modules, respectively. The MPD-240 module enables data acquisition from a maximum of 240 elements with a maximum load of up to 8 mega events per second. This requires the bandwidth of computer communication channels of up to 50 MB/s, which is impossible with a USB 2.0 interface.

A ten times bandwidth increase has been realized by development of the new fiber adapter FLINK USB 3.0 enabling a link between the fiber optic interface of the modules and the interface USB 3.0 of the computer, as well as allowing use of the FTD3XX library of the FT600 chip to provide the USB Super Speed to FIFO bridge with a new communication adapter.

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19. Investigation of the magnetic and structural properties of nanosized simple oxides

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To establish the correlation between structure and magnetic properties of simple oxides the magnetic structural phase transitions in NiO and MnO have been studied by neutron diffraction. Complete separation of the antiferromagnetic and nuclear diffraction peaks in these oxides makes possibility for detailed analysis of the magnetic structure and structural phase transitions. The effect of size reducing of the crystallites on the magnetic structure of simple oxides was also studied. For this purpose 4 samples NiO with different crystallite size of 1500 nm, 138 nm, 100 nm, 12 nm were investigated by high resolution neutron diffraction.

The experiments were carried out in a wide temperature range from 5 to 563 K on the Fourier diffractometer of high resolution (HRFD) at the pulsed reactor IBR-2 (JINR). HRFD has a high resolution of the order of 0.001, which allows precision to investigate small distortions of the structure that occur in NiO. In both oxides, a structural transition occurs with a decrease in symmetry from cubic to rhombohedral, and the magnetic with the formation of the antiferromagnetic structure of G-type.

From high resolution neutron diffraction data the magnetic space group (P2s-1) of the rhombohedral distorted NiO has been determined.

The temperatures of structural and magnetic phase transitions as well as the temperature dependence for the rhombohedral distortion and the magnitude of the ordered magnetic moment were obtained. It was found that in MnO structural and magnetic transitions occur at the same (within experimental error) temperature (T_N = Tc = 123 ± 3 K). However, in NiO noticeable difference between structural and magnetic phase transition is observed (ΔT=56 ± 9 K, T_N = 539 ± 7 K, T = 483 ± 5 K).

20. Growth of the silicate clusters in basic TEOS/ethanol/water solutions

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The study of the structure of branched polymeric materials is of current interest because of its great role in modern technologies. The classical material most widely used to produce silicon-based branched polymers is silicon tetraethoxide (TEOS) [1]. After hydrolysis in alcohol-water solutions, it forms silicate clusters, which results in a wide class of different structures [2-4] depending on the number of parameters like pH, H_2O/TEOS molar ratio, total TEOS concentration *etc*.

In present research small-angle neutron scattering with the inner and outer contrast variation (H/D substitution) was applied to clusters in hydrolyzed solutions of TEOS in ethanol. The task was to find out characteristics of the distribution of the scattering length density inside the clusters and conclude how much hydroxyl and ethyl groups are included in the final aggregate structure (both bulk and surface), as well as how far this depends on the conditions of the synthesis. Obtained data indicate that the structure of clusters does not contain closed hydroxyl groups. Thus, the overwhelming majority of the hydrolyzed bonds participate in the condensation reaction to form Si-O-Si structure units. The temporal dependence of cluster growth was investigated together with the dependence of the structure of a liquid nanosystem under study on the parameters of synthesis.

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21. HLIT-VDI - a new service of the HybriLIT ecosystem for work with applied software packages

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A new service - HLIT-VDI – has been developed for shared use of applied software packages on the HybriLIT cluster using GUI (graphical user interface). By means of this service, it is now possible to work with applied software packages such as Wolfram Mathematica, Maple, Matlab, GEANT4, etc. via remote access to the virtual machines (VM) in the framework of the HybriLIT cluster. The developed service allows carrying out computations in the frames of VMs and massive computations using the resources of the cluster.

22. Neutron reflectometry study of structure and glass transition in thin films of polystyrene-fullerene nanocomposites

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Glass transition in different systems and materials remains one of the most intriguing phenomena for both experimental and theoretical investigations in the area of condensed matter physics. A particularly interesting field of research in this respect is the investigation of glass transition of polymers [1]. Different polymers are applied in modern technologies and new fields of application are emerging. One of the most actively evolving research fields is connected with thin polymer films. Applications of thin films increase in technologies involving dielectric coatings, resist layers for lithography, electronic packaging, optical coatings, non-linear optical devices, lubricating surfaces, etc.

Neutron scattering studies of polymers structure in glassy and liquid state have been performed during last 30 years and have proven to be very supportive [2]. The recently performed investigations of polymer thin films and glass transition of bulk polymer systems gave new insights. Presently, the most interesting topic is the study of polymer nanocomposites, and their glass transition, as new materials for technological applications [3].

The presented poster summarizes our recent research on polymer thin films glass transition, including the latest experiments performed by us at the GRAINS instrument of the IBR-2 reactor. The initial investigations of polystyrene (PS) and PS thin films glass transition via neutron reflectometry (NR) were performed in 2015. The first results have shown that the conducted and planned experiments are achievable from methodological part.

The late experiment was aimed at obtaining the new scientific results for the glass transition in polymer thin films and polymer/carbon nanoparticles mixtures films. At the GRAINS instrument (reflectometry from liquid-containing interfaces) the specular reflectivity was measured and analyzed for free surface of d-PS/C_{60} and PS/C_{60} samples in the temperature range covering the transitional region between molten and amorphous glassy states (40-135 ºC). The analysis allowed analyzing the influence of nanoparticles on glass transition temperature of thin films, as well as speculating about the internal structure of these thin films, a highly debated subject in the literature at present.

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23. Data management system of the UNECE ICP Vegetation Program

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The aim of the UNECE International Cooperative Program (ICP) Vegetation in the framework of the United Nations Convention on Long-Range Transboundary Air Pollution (CLRTAP) is to identify the main polluted areas of Europe, produce regional maps and further develop the understanding of the long-range transboundary pollution. The Data Management System (DMS) of the UNECE ICP Vegetation consists of a set of inter-connected services and tools deployed and hosted at the Joint Institute of Nuclear Research (JINR) cloud infrastructure. DMS is intended to provide its participants with modern unified system of collecting, analyzing and processing of biological monitoring data. General information about DMS and its abilities are presented.

24. Temperature resumption and correlation of inhomogeneous magnetic states in the structure Nb(70nm)/Ni[65%]Cu[35%](7nm)//Si

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In theoretical work [1] a special domain state of a ferromagnetic thin layer in contact with a superconductor was predicted. This phenomenon is known as cryptoferromagnetism or "hidden" ferromagnetism. It appeara as the domain's characteristic size decreases by several orders of magnitude 10^3-10^5. This is possible only under the influence of superconductivity and for a ferromagnetic layer with thickness of the order of correlation length of superconductivity in a ferromagnet. Direct methods for experimental detection of the described state are: polarized neutron reflectometry, off-specular scattering, grazing incidence small-angle scattering and diffraction. Using later, one can detect inhomogeneities with correlation length 1-100 nm.

In previous works [2,3], we investigated the layered structures V/FeV/Nb, where FeV is a ferromagnetic layer, and V and Nb are superconducting. The relaxation of magnetic state of V/FeV/Nb structure was investigated in [3]. At the temperature T = 2K correlations in the behavior of the domain structure and the system of atomic-magnetic clusters were observed. It was found that the domain structure interacts with the cluster system. In this case, influence of superconductivity appeared as increasing domain walls density (decreasing of the domain's size) and as increasing of coherent oscillations of the magnetic moments of the clusters.

In this work we investigate structure Nb(70nm)/Ni[65%]Cu[35%](7nm)//Si in the temperature range 1.5 K - 10 K and magnetic field 25 Oe - 200 Oe. The superconducting transition temperature was T_C = 8.8 K. Dependence of the intensity of specularly reflected neutrons on temperature shows the inhomogeneous state at 9K repeated at 4K. The analysis showed that scattering occurs because of a magnetic lattice with an interplanar distance d<2.3 nm. Dependence of neutron scattering intensity on temperature in the region surrounding the reflected beam shows that scattering also occurs on a lattice of clusters with magnetic moments directed against magnetic field. Interplanar spacing in the lattice was 4 nm. Two types of scattering correlate at 9 and 4 K. Possible explanation for resumption of the formation of a magnetic lattice is that at T≈Tc the structure is formed due to a proximity effect, and at T = 4K the entire ferromagnetic layer becomes superconducting. Note that the temperature 9 K is above T_C = 8.8 K for the structure, but not below T_C for bulk Nb. It is not excluded that the magnetic lattice is antiferromagnetic and it is the cryptoferromagnetic state.

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