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1

Study of the aging behavior of materials important in nuclear energy field - Incoloy 800 HT and 304L steel- using neutron scattering techniques

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The 800 HT Incoloy is widely used in power generation for steam generators tubing and high temperature heat exchangers for gas cooled nuclear reactors and as a candidate material for fuel cladding in GEN IV reactors. The 304L steel has a high ductibility. Low yield stress and high tensile strength and is used widely in nuclear power plant.
There were manufactured 4 samples of Incoloy 800HTand 4 samples of 304L steel, all of 2x15x25mm dimensions and standing a heat treatment of 60 days at 450, 500, 550 and 600 degrees respectively.
The samples were investigated by neutron diffraction and small angle neutron scattering at the FSD, HRFD and MEREDIT diffractometers, YuMO-SANS and KFKI SANS spectrometers (in function at IBR-2 reactor, Dubna, respectively Budapest). Lattice cell and peak width parameters changes for both sample series (using neutron diffraction measurements) together with information on heat treatment effects concerning precipitate size and volume distribution of alloying elements (using SANS measurements) were found.
Structural properties of the above mentioned materials of significant importance in nuclear energy field, revealed through high temperature heat treatment are described.
Key words: neutron scattering techniques, neutron diffraction, SANS, , Incoloy 800 HT, 304L steel

2

New Rietveld program suited for processing patterns recorded with a inverse- space focusing neutron diffractometer equipped with position sensitive detector

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The efficiency of the neutron spatial focusing high resolution powder diffractometer (SFHRPD) can be significantly increased by using a linear position sensitive detector (PSD) in place of a simple one. This replacement requires a lot of modifications of the soft for data processing including the program of Rietveld refinement.

The principle and the design of the original SFHRPD described by Ionita et al. (1999) were conceived later of 80, early of 90. It is based on a bent plate single crystal monochromator and a flat sample rotated according to a certain function , being the Bragg angle. This dependence which is significantly different from the traditional Bragg-Brentano law, imposed to operate modifications of the Rietveld program. Two of them, rather minor, concern the calculation of the irradiated sample volume and transmission on the Bragg angle . and the parameterization of the dependence of the peak shift on according to Popovici and Stoica (1992). The third modification was imposed by the inappropriateness for this particular instrumental geometry of the texture correction models working at that time in the Rietveld method: the March –Dollase model (Dollase, 1986) and the model of spherical harmonics dependent only on the crystal symmetry (Ahtee et al.,1989). In place was used the model of texture correction representation by generalized spherical harmonics as reported by Popa (1992). This pioneering work given rise to a new application of the Rietveld method namely the quantitative texture analysis (Von Dreele, 1997).

Using a PSD in place of a simple detector a supplementary problem appears for the Rietveld program because of a very peculiar dependence of the instrumental line breadth on the scattering angle. In this scheme the range of the whole pattern is divided in segments of lengths equal to length of PSD and for every segment the sample orientation is set to an angle such that the ideal focusing is realized for the channel sitting the middle of the segment. Obviously for other channels the instrumental breadth is larger, as larger as the distance from the middle channel is higher. The whole picture looks like a garland . The FWHM for every segment of garland was fitted by least square with a three degree polynomial as function of scattering angle .

For the final version of this program were modified the following modules:

was modified the module WIDTH.FOR giving insutrumental line width as a function of scattering angle.

was modified the module ALFAT.FOR giving the sample orientation

Conclusions

The presented Rietveld program is really a valuable one able to process the diffraction data from a diffraction pattern raised with a focusing neutron diffractometer equipped with a position sensitive detector.

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3

Pressure-induced polar phases in relaxor multiferroic PbFe0.5Nb0.5O3

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The structural, magnetic and vibrational properties of PbFe0.5Nb0.5O3 relaxor multiferroic have been studied by means of X-ray and neutron powder diffraction, magnetic susceptibility measurements and Raman spectroscopy at pressures up to 30 GPa. Two successive structural phase transitions from the initial R3m polar phase to Cm and Pm monoclinic polar phases were observed at P = 5.5 and 8.5 GPa. Both transitions are associated with anomalies in pressure behaviour of several stretching and bending modes of oxygen octahedra as well as Fe/Nb localized vibrational modes. The G-type antiferromagnetic order remains stable upon compression up to 6.4 GPa, implying multiferroic properties of pressure-induced phases. The Néel temperature increases with a pressure coefficient (1/TN)dTN/dP = 0.012 GPa-1. The observed pressure-induced phenomena in PbFe0.5Nb0.5O3 are in drastic contrast with conventional multiferroics, exhibiting a general tendency towards a suppression of polar phases and/or magnetoelectric coupling under pressure.

4

Vesicles self-assembly in the mixed phospholipid/bile salt systems

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Phospholid vesicles are important delivery system in cell biology, medicine and pharmacy. Phospholipid / bile salt vesicles used as drug delivery systems through the skin. The process of vesicle formation in the scale of nano is not clear jet. The small size of the stable nano-vesicles requires the large curvature of the lipid bilayer, which could be realized in the presence of detergent molecules. Aqueous bile salt - phospholipid mixtures become more significant as model systems for the investigations of the self-assembly of amphiphilic molecules and the vesicles formation. Small-angle neutron (SANS) and X-ray (SAXS) scattering were used to study the process of vesicle formation in two mixed binary systems: dimyristoylphosphatidylcholine (DMPC) /sodium cholate (NaC) and dipalmitoylphosphatidylcholine (DPPC)/ sodium deoxycholate (NaDC) [1-3]. Both DMPC/NaC and DPPC/ NaDC systems demonstrate similar morphological transformations in the micelle to vesicle transition.

One from the open and discussed problem in the micelle to vesicle transition is morphology of the last structure before vesicle formation (ribbon –like structure or bicelles). Our results shows that for the case of two types of phospholipids (DPPC and DMPC) and two types of bile salts (NaDC and NaC) the last structure before vesicle formation has ribbon-like morphology [2,3].

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5

Wheel steel crystallographic texture investigation by neutron diffraction

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Study of the factors controlling the structure and properties of wheel steel is a very important task because it allows optimizing of steel composition and temperature regimes for mechanical properties improvement [1]. Texture formed as a result of railway wheel usage influences on their strength and operating life [2]. Neutron diffraction is a powerful nondestructive tool for global texture investigation in the volume of the material [3].
In this work the crystallographic texture for a set of wheel steel samples with different regimes of thermo-mechanical treatment and with and without doping by system Al-Mg-Si-Fe-C-Ca-Ti-Ce has been measured by neutron diffraction. The texture measurements have been carried out by neutron diffraction using time-of-flight technique at SKAT diffractometer situated at IBR-2M reactor (Dubna, Russia). The three complete pole figures (110), (200), (211) of α-Fe phase in $5^{\circ}\times5^{\circ}$ grid have been extracted from a set of 1368 spectra measured for each sample (see Fig.1). The samples were cut from wheel hub and wheel rim. The samples from wheels before and after operation were investigated.
It was concluded that the modification of wheel steel results in the reorientation of texture component and the heating destroys weak texture in wheels before operation.

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6

Self-diffusion and relaxation in liquid Ga studied by quasielastic neutron scattering

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The results of liquid gallium investigation by quasielastic slow-neutron scattering are discussed. The experimental data analysis allowed obtaining the temperature dependencies of the diffusion and relaxation characteristics of liquid gallium within temperature range of 313 – 793 K. The comparison of the experimental data and those of the up-to-date literature is held.

Liquid gallium is a medium with a number of unusual properties: the essentially expanded temperature interval of liquid phase existence (303 – 2500 K) and low vapour pressure for T < 1400 K make gallium a possible candidate to a self-cooled target in the photon-neutron converter at the electron accelerator beam. The remarkable possibility of photoneutron source creation without use of fission materials and high estimated neutron flux in the center of Ga target permit to use liquid gallium as a working substance in the device for the neutron-caption therapy [1]. The activity of radiated sample of natural gallium mainly is due to Ga decay with decay period ~ 14 hours, and this is why the compact gallium device is commonly ecological pure one. Moreover, the appropriate thermo-hydraulic properties of gallium as a coolant allow operating with practical meanings of the consumption, velocity rate, and temperature.

Except the liquid gallium applications, there is the scientific reason to investigate such an outstanding substance. The structure factor S(Q) of liquid Ga possesses the asymmetrical shape of the main peak, and the dispersion curve of Ga, e(Q), probably, is two-component [2]. Both the circumstances allow regarding the liquid gallium as a matter having two essentially different densities, probably linked with masses M and 2M. Really, the existence of gallium dimers has been shown at temperatures near 1000 K [3]. The study of self-diffusion in Ga appears to be very informative from this point of view, besides the applications mentioned above.

To study the diffusion and relaxation characteristics of liquid Ga is convenient by the use of quasielastic neutron scattering, the ordinary method of condensed matter investigations.

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7

Neutron scattering and computational studies of water retained in grafene oxide.

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Graphite oxide, which now is called graphene oxide (GO), is the product of chemical exfoliation of graphite using strongly oxidized reagents. Synthesis of GO has been known for more than a century and GO reduction still remains the way of choice for the large-scale graphene production [1]. Now it is generally accepted that GO mostly contains hydroxyl (–OH) and epoxy (–O–) groups randomly spread over its basal planes [2]. The most widely accepted model is the one by Lerf and Klinowski, regarding the structure and hydration behavior of GO as studied by advanced methods of solid-state nuclear magnetic resonance (CP MAS NMR) [3].

The studied graphene oxide sample was synthesized by S. V. Tkachev et al., at the Institute of General and Inorganic Chemistry RAS in Moscow [4]. The powder sample, subjected to neutron scattering studies, was obtained from the aqueous dispersions of the pristine GO after a severe centrifugation and heating in a dry box for 6 days at 65-700C. The composition of the final GO keeping it at the following level (mass %): C(58,0±1,0), H(1,5±0,5), O(39,0±1,0), N (0).

Neutron scattering study was performed at the high flux pulsed IBR-2 reactor of the Frank Laboratory of Neutron Physics of JINR by using the NERA spectrometer [5]. The inverted-geometry spectrometer NERA allows simultaneous recording of both inelastic incoherent neutron scattering (IINS) and neutron powder diffraction (NPD) spectra. Experiments were performed at temperature range of (293 – 6) K. The NPD spectra have shown that a separation of the GO flakes depends on humidity and average interlayer distance at room temperature change within the values (6.9 – 8.1) Å. The integral intensity of IINS spectrum which correspond to separation of GO layers on the distance 8.1 Å is twice higher than at the distance 6.9 Å, what confirm presence of water molecules between the layers of GO.

By combining the state-of-the-art ab initio calculations with IINS neutron scattering experiment we were able to shed more light on the vibrational dynamics of GO and the interlayer water. We may conclude that the proposed structural models have delivered satisfying qualitative description of the related IINS spectrum, which was found to be mainly driven by the dynamics of the interlayer water molecules. Despite of the static and configuration limitations, a sufficient overall reproduction of the spectral features was found [6].

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8

AGGREGATION IN MIXED NONIONIC C14E7 AND ANIONIC CsDS SURFACTANTS MICELLAR SOLUTIONS

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The aim of this experiment was investigated of aggregation in mixed of two surfactants - nonionic C14E7 (heptaethylene glycol monotetradecyl ether) and anionic CsDS (cesium dodecyl sulfate) micellar solutions in heavy water at 25oC by small angle neutron scattering (SANS) method. The variations in the size and shape of micelles with composition was observed in heavy water dilute solutions of non-ionic surfactant (c1=0.17%,c2=0.5%,c3=1%) as result of surfactants headgroup steric and electrostatic interactions [1-3] when nine different amounts of anionic surfactant CsDS was added to these solutions.

9

Thermal analysis of new thioester derivatives of terpenoids

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I present the properties of a new series of thioesters: 4-(4-nonyloxybenzylothio) benzoates modified menthol (9OSBm), thymol (9OSBt) and carvacrol (9OSBc). The chemical structure and purity of all substances were established by 1H NMR, 13C NMR and FT-IR spectroscopy. Polymorphism was characterised by differential scanning calorimetry (DSC), polarizing optical microscopy (POM) and transmitted light intensity (TLI).
Only one of all presented compounds – 9OSBm has polymorphism of crystal phases Cr2-Cr1. Replacement of the cyclohexyl ring of menthol part on aromatic ring which is in thymol and carvacrol in these thioesters does not affect the appearance of the mesophases. Probably isopropyl group of terpenoids is steric hindrance and makes the arrangement of molecules in the layers impossible. All samples are stable and do not decompose after the transition to the isotropic phase.

10

RECONSTITUTION OF REACTOR VESSEL SURVEILLANCE SPECIMENS

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This paper reports the results of residual stress studies in surveillance specimens reconstituted by electron, laser beam and arc stud welding techniques. The studied specimens were reconstituted using a Leybold Heraeus electron beam welding unit, 45 kW continuous wave (CW) CO2 laser and KOKO stud welding machine. The material used in this study was 18MND5 steel. The Charpy impact tests showed good agreement between the original and reconstituted specimens. In order to evaluate feasibility of various welding methods the residual stress in test Charpy specimens welded by various techniques were analyzed using high resolution neutron diffraction on FSD diffractometer. The lowest level of the residual stress was found for electron beam welding specimen as compared to laser beam welding and arc stud welding specimens. This confirms well known fact that among all the welding methods the electron beam welding technique results in lowest level of residual stress in welded joints.

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НЕЙТРОННАЯ СПЕКТРОМЕТРИЯ НЕЛИНЕЙНЫХ ЩЕЛЕВЫХ КОЛЕБАНИЙ КРИСТАЛЛИЧЕСКОЙ РЕШЕТКИ НИТРИДА УРАНА ПРИ ВЫСОКИХ ТЕМПЕРАТУРАХ

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Методами компьютерного моделирования и рассеяния нейтронов исследуется микродинамика высокоамплитудных нелинейных колебаний кристаллических двухатомных решеток типа нитрида урана при температурах 600 оС-2500 оС вблизи порогов диссоциации и разрушения топливного материала. В спектральной щели между полосами частот акустических и оптических фононов обнаружены резонансы гармонических поверхностных колебаний нового типа и заполняющая щель полоса их генетических продолжений - нелинейных поверхностных колебаний. На нейтронном спектрометре ДИН-2ПИ в щели обнаружены резонанс и полоса этих поверхностных колебаний, а также высшие обертоны оптических колебаний. Показано, что солитоны и бисолитоны инициируют образование и схлопывание динамических пор с генерацией таких поверхностных колебаний на границах полостей, испарение атомов и атомных кластеров, образование трещин и разрушение материала. Показано, что массоперенос азота в трещинах и по границам зёрен может осуществляться мик-родинамическим механизмом сёрфинг – диффузии атомов азота на высокоампли-тудных солитонных волнах.

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Analysis of charging/discharging processes in Li-ion batteries by neutron diffraction

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Ex-situ and in-situ neutron diffraction experiments were performed at HRFD time-of-flight (TOF) diffractometer (IBR-2 long-pulsed reactor, JINR) to characterize the entire battery system based on $LiFePO_4$ and V-added $LiFePO_4$ electrodes during electrochemical cycling and to find additional information about crystal structure of electrodes. Another purpose of this work was checking possibilities for in-situ experiments with real Li-ion batteries at the IBR-2 pulsed reactor. An important advantage of TOF method is the possibility to work at the fixed geometry of the experiment, which allows selecting the optimal battery orientation relative to the directions of the incident and scattered neutron beams and, thus, to minimize the difficulties associated with complex internal structure of the battery. It was shown that charge/discharge process of Li-based real Li-ion battery can be effectively studied by TOF technique at the IBR-2 pulsed reactor.
Three full charge/discharge cycles were realized at room temperature (~17°C) with slow rate. The step-like appearance of several LiCn phases was observed and the volume fractions of $LiFePO_4$ and $FePO_4$ structural phases at different states of charge were determined. The analysis of changes in cathode material microstructure when doped with vanadium showed a significant increase in the density of defects, which correlates with better electrochemical properties of V-added $LiFePO_4$ compared to pure $LiFePO_4$.

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The structural aspect of luminescent properties forming in composite phosphors Y3Al5O12:Ce3+/Lu2O3 and Lu3Al5O12:Ce3+/Lu2O3: neutron diffraction results

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The crystal structure and spectral luminescent properties of composite phosphors Lu3Al5O12:Ce3+/Lu2O3 and Y3Al5O12:Ce3+/Lu2O3 synthesized by colloid chemical approach have been studied by means of neutron powder diffraction and optical spectroscopy methods. We found the formation of stable defect structures on the phase boundary between phosphors Lu3Al5O12:Ce3+, Y3Al5O12:Ce3+and Lu2O3. In the study of Y3Al5O12:Ce3+/Lu2O3 significant enhancement of integral luminescence intensity and shift of its maximum to longer wavelength region was revealed on Lu2O3 doping.

We found, that the modification of luminescent properties by Lu2O3 doping in Lu3Al5O12:Ce3++Lu2O3 is drastically different is comparison with Y3Al5O12:Ce3++Lu2O3 due a redistribution of optically active Ce3+ ions between initial Lu3Al5O12 and lutetium oxide Lu2O3 phase during the colloid chemical synthesis, resulting in suppression of luminescence intensity. The obtained results demonstrate that oxide doping effects on structural and luminescent properties of “garnet+oxide” system have a complex character, and one needs to take into account several factors. They include not only diffusion processes of Ce3+ ions between system components, but also possible formation of new structural phases and stable defect regions at phase interface, and optically active or inactive state of activator ion in a specific structural environment.

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The magnetic structure of HoCo2 and ErCo2 compounds studies at high pressures

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The magnetic properties of RCo2 compounds, where R is a rare-earth or yttrium were intensively investigated from both experimental and theoretical point of view. At ambient temperature, these have a cubic structure with space group Fd3m, but below the Curie temperature Tc, the cubic structure becomes distorted. When R is nonmagnetic (R=Y, Lu and Sc) the compounds are an exchange-enhanced paramagnet and exhibit metamagnetic behavior in externally applied magnetic field only, but the RCo2 compounds with R=Gd, Tb, Dy, Ho, Er, Tm are ferrimagnetically ordered. The moment on the cobalt sites close to ~1.0 μB over the RCo2 series and is described as being induced by the molecular field exerted by the localized 4f moments. The pressure studies on RCo2 compounds can give additional information on the magnetic behavior of cobalt in ordered phases.
In this work, studies of ErCo2 and HoCo2 compounds have been performed by neutron diffraction at high pressures up to 5 GPa and in temperatures range from 10 K to 300 K. At ambient conditions, both compounds have a cubic structure with space group Fd3m. At cooling down to temperature 80 K in HoCo2 and at 37 K for ErCo2 compound structural phase transition from cubic Fd3m to tetragonal I41/amd and rhombohedra R3c, corresponded, have been observed, which is also accompanied by magnetic transition from the paramagnetic state to the ferrimagnetic. The Curie temperature decreasing and Co magnetic state suppressing for both compounds at high pressure have been found.

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Neutron Imaging Station at IBR-2

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New neutron imaging station has been developed and started at beemline 14 of IBR-2 high flux pulsed reactor recently. It consists from beam shater, vacuumed neutron guide with builtin collimation sistem, rotation table and neutron detector based on CCD camera. The obtaned neutron flux is aproximetly 5*10^6 n/cm^2/s at the sample position. The achievable spatial resolution is about 200 um due to high L/D ratio equaled to 200. The current state of the instrument and recent experimental results, covering neutron imaging of technological, natural heritage and geophysical objects are reviewed.

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Study of polymorphic transformations in the complex molecular crystal of fluconazole at high pressure

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One of the major problems of condensed matter physics is the investigation of the high pressure effects on the structure and properties of pharmacological components. Synthetic drug fluconazole C13H12F2N6O is the object for the research due searching for polymorphic transformation in it. Fluconazole is highly active component in pharmaceuticals against a variety of fungal pathogens that cause systemic mycoses. Investigation of structural changes in fluconazole at high pressure is very important due modeling of tableting processes, which can effect on the quality of final product.
In our work we have been prepared by means of the energy-dispersive X-ray diffraction experiments at pressures up to 4 GPa on the beamline F2.1 (HASYLAB-DESY, Hamburg) using the multianvil X-ray system MAX80. In additional, a Raman spectra at ambient temperature and pressures up to 4.4 GPa were collected using a LabRam spectrometer (NeHe excitation laser) with wavelength of 632.8 nm, 1800 grating, confocal hole of 1100 mkm, and a 50x objective.
The X–ray diffraction and Raman spectroscopy data indicates polymorphic phase transition from initial form-I of fluconazole to new high-pressure form-II at pressures of 1.6 GPa. We choose structure model for new pressure induced phase as triclinic symmetry with P1 space group. The lattice parameters of form-II have been obtained. The baric coefficients for lattice parameters and unit cell volumes of both polymorphic forms of fluconazole have been calculated.
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Aqueous solutions of magnetoferritin: structure and applications

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Magnetoferritin represents a synthetic derivate of ferritin, iron storage protein, with external diameter of 12 nm. It consists of magnetite or maghemite in the core surrounded by protein shell of apoferritin. Nanosize, superparamagnetic behavior and biological origin provide to magnetoferritin significant potential for application in nanotechnology, industry and biomedicine (as a drug carrier in targeted transport, a standard in diagnosis of various diseases, a contrast agent in MRI). The structure of such biological complex in aqueous solution was investigated by small-angle neutrons (SANS), including contrast variation, and X-rays (SAXS) scattering for different loading factors (average number of iron atoms per complex). With the LF growth, the scattering curves exhibit a higher polydispersity, relative increase in the total scattered intensity, a partial smearing and a shift of the match point in the SANS contrast variation data (Fig. 1) which are pointed out to corresponding effective increase in the relative content of magnetic material against the protein moiety of the shell. It was obtained that at LFs above 156, the apoferritin shell undergoes structural changes as compared to the native hollow state of apoferritin. It could be expected that the structure of the magnetoferritin package was changed due to the magnetic core presence and the shell stability is affected by iron oxide. The obtained results are important for understanding of synthesis procedure and further application of magnetoferritin.

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Neutron diffraction study of the crystal and magnetic structure of the natural pyrrhotite. Data from Epsilon and DN-2 spectrometers.

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We present the data of neutron diffraction experiment on natural pyrrhotite from the two different impacts performed at different temperature on DN-2 spectrometer (high intensity data) and Epsilon diffractometer (high resolution data). Our results are compared with results obtained from synthesized pyrrhotite and samples from other impacts.

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STRUCTURE OF WATER MAGNETIC FLUID AT THE INTERFACE WITH SILICON BY NEUTRON REFLECTOMETRY

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Recently it was observed by small-angle neutron scattering (SANS) that comparatively small and compact aggregates of nanoparticles in the initial water-based magnetic fluid (MF), where nanomagnetite (characteristic particle size below 10 nm) is coated with double layer of sodium oleate (length about 2 nm), transfer to large and developed associates after poly(ethylene glycol) (PEG) is added to the system with the ratio above 1:1 with respect to the magnetite content [1]. In the given work the structure of magnetite/sodium oleate/d-water MF at the silicon interface before and after PEG addition was investigated by neutron reflectometry. The volume fraction of magnetite in the studied ferrofluids was about 1 %. The ratio PEG/magnetite was 1.5 w/w.

Despite rather strong diffuse scattering still the specular reflectivity curves for the aqueous ferrofluids before and after PEG addition can be excluded from 2D scattering maps and compared with the reflectivity curve from the D2O–silicon interface. A deviation of the neutron reflectivity curves from the Fresnel behaviour is observed for both ferrofluids which is connected with formation of some layer of colloidal particles at the silicon interface. The additional band in the reflectivity curve for the magnetic fluid after PEG addition observed in a q-range of 0.4-1 nm-1 indicates to different adsorption layers of nanoparticles for the two kinds of ferrofluids. The detailed analysis to obtain the quantitative information about the scattering length density profile of the adsorbed nanoparticles is in progress. Mainly, it concerns the fact that a significant effect of SANS contributing to the off-specular scattering was concluded. It should be taken into account at the raw data treatment while the reflected signal is extracted from the raw 2D data. The task is to get the size characteristic of the adsorbed aggregates, as well as their composition, and to compare the results with those for the aggregates in bulk known from the previous SANS experiments. It should be noted that no response of the system on the presence of an external magnetic field (up to 500 Oe) could be observed, which is probably due to a comparatively small concentration of magnetite in the studied ferrofluids.

[1] M.V.Avdeev, A.V.Feoktystov, P.Kopcansky, G.Lancz, V.M.Garamus, R.Willumeit, M.Timko, M.Koneracka, V.Zavisova, N.Tomasovicova, A.Jurikova, K.Csach, L.A.Bulavin // J. Appl. Cryst. 43 (2010) 959–969.

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Парциальные частотные распределения атома водорода для воды, адсорбированной аэросилом и катионитом СГК-7

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Представлены парциальные частотные распределения (ПЧР) атома водорода молекулы воды, адсорбированной на поверхности аэросила и в катионите (ионообменной смоле) СГК-7, полученные с помощью неупругого рассеяния нейтронов.

Использовались образцы аэросила со степенью гидратации в интервале от 4,9 % до 900 % (степень гидратации c = [m(H_2O) / m(SiO_2)]•100 %, где m – общая масса соответствующих молекул в образце).

Образец ионообменной смолы СГК-7, гидратированной как в тяжелой, так и в легкой воде имел степень гидратации около 90 %.

Измерения спектров неупругого рассеяния нейтронов образцами при комнатной температуре проводились на спектрометре ДИН-2ПИ для начальной энергии нейтронов E0=4,2 мэВ.

Посредством итерационной процедуры с помощью комплекса программ PRANA с учетом многофононного и многократного рассеяния из экспериментальных дважды-дифференциальных сечений было определено ПЧР колебаний атомов водорода g(ε) в области межмолекулярных колебаний для воды, адсорбированной на поверхности аэросила и в катионите СГК-7. Проведен сравнительный анализ ПЧР с использованием данных, полученных для чистой воды.

Наблюдаются общие черты распределения частот колебаний адсорбированной и объемной воды: четко выражена полоса заторможенных вращений (либраций) при энергии колебаний ε = 70 мэВ и полоса заторможенных трансляционных колебаний молекул воды вместе с окружением (ε = 5-7 мэВ).

Для аэросила со степенью гидратации 4,9 % по сравнению с чистой водой и для гидрогеля для передачи энергии ε примерно 6 и 25 мэВ по отношению ко льду и адсорбированной аэросилом воде при температуре 10 К обнаружено существенное уменьшение интенсивности в низкочастотной трансляционной области, что свидетельствует о заметных нарушениях в сетке водородных связей.

Либрационная полоса ПЧР адсорбированной воды по сравнению с объемной водой смещена в сторону более высоких энергий, что может быть результатом возмущения ближней упорядоченности и усиления межмолекулярного силового поля.

На основе ПЧР рассчитан ряд микродинамических и термодинамических характеристик адсорбированной воды, которые были сравнены с данными для объемной воды: автокорреляционная функция скорости протона, среднеквадратичная амплитуда колебаний атомов (фактор Дебая-Уоллера), средняя силовая постоянная межатомного взаимодействия, средняя кинетическая энергия, теплоемкость.

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The crystal and magnetic structure of nanostructured manganites La0.67Sr0.33MnO3 at high pressure and temperature.

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Apart from potential application, the complex manganites are attractive for great number of scientific research. It is widely accepted that interplay between magnetic, transport and electronic properties in these compounds results from a complicated balance of the ferromagnetic (FM) double exchange and the antiferromagnetic (AFM) superexchange interactions coupled to lattice distortion effects and orbital degrees of freedom. Due to strong correlation between magnetic and transport properties of La1-xSrxMnO3 compounds, the knowledge of relationship between magnetic and crystal structure or nanostructured features, which can be obtained from high pressure investigations, is very essential for understanding the nature of physical phenomena observed in these nanostructured compounds. Due to correlation between order parameters, knowledge of the structural evolution of magnetic phase under pressure is also important to understand a mechanism of formation of unusual magnetic properties of this compound.
In our work, the magnetic and structural properties of nanostructured manganites La0.67Sr0.33MnO3 with nanoparticle size 20 nm and 50 nm have been studied at pressure up to 5.7 GPa and in the temperature range 4-300K at neutron diffractometer DN-6 on pulse high-flax reactor IBR-2. The high pressure will obtain using sapphire anvil cells and close-cycle refrigerator will used for low temperature experiments.
As result, in manganite La0.67Sr0.33MnO3 with particle size 50nm the some portion of AFM phase at the low temperature 4 K at ambient pressure have been observed. In both compound the magnetic phase transition from ferromagnetic (FM) to antiferromagnetic (AFM) state at high pressure have been found. The unit cell parameters and volume, magnetic moments of FM phase as function of pressure and temperature have been obtained.
The work was supported by RSF grant N 14-12-00182.

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Residual stress investigation in the crack region of the gas pipeline tube

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The main objective of this study was to determine the crack reasons of gas transport tube during its long term operation. The residual stresses near the crack region were measured by three methods: high resolution neutron diffraction, magnetic anisotropy and the Barkhausen noise technique. Neutron diffraction data indicate practical absence of the residual stresses in the studied region. On the contrary the magnetic methods of MMA and Barkhausen noise give a strong signal at the outer surface near the crack.

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FORMATION AND GROWTH OF CLUSTERS IN NON-POLAR AND POLAR FULLERENE SOLUTIONS: EXPERIMENTAL AND THEORETICAL ASPECTS

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The properties of fullerene solutions remain an interesting field of research in modern physics, chemistry and medical science. A lot of non-trivial effects are observed in fullerene solutions, such as cluster formation, solvatochromic effects, non-linear dissolution processes, and others. For the last several years our research group has performed experimental and theoretical studies of solutions of C60 and C70 of different polarity.
Inseparable with the cluster formation of fullerene in polar and low polar solvents is the solvatochromic effect. It has been explained to be the consequence of complex formation between solvent and fullerene molecules. The dissolution processes and solvatochromic effects in fullerene solutions where studied by UV-Vis spectroscopy and SANS experimental methods. For non-polar solutions, the kinetics of C60 dissolution where studied by UV-Vis and modeled by classical laws. The cluster growth in non-polar solution is explained to be a consequence of non-equilibrium preparation. The effect of excess radius of gyration, observed by SANS in fullerene solution in CS2, is explained. The cluster size in polar fullerene solutions was measured to be in the range of 10-100 nm by SANS. The description of kinetics of cluster growth in this work is made via different models originally based on the theory of nucleation. These theoretical models reveal the kinetics of cluster growth on the whole time scale of cluster state evolution for polar fullerene solutions. In addition, the small angle neutron scattering curves for fullerene solutions are modeled with the use of the cluster-size distribution functions.

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Micelle formation in surfactant solutions in the presence of polymer by small-angle neutron scattering

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Mixed polymer-surfactant systems are very interesting not only for academia researchers but also for industry. Polymer and surfactants are very often used in combination in cosmetic, medicinal, and pharmaceutical preparations. Particularly, complex surfactant-polymer solutions are used for the synthesis of highly stable and controllable water-based ferrofluids (magnetic fluids (MF)). Poly(ethylene glycol) (PEG) is frequently used for increasing of biocompatibility of MF. At the same time, the introduction of PEG into initially stable MF can result in their structural reorganization. Such effect was recently observed [1] by small-angle neutron scattering (SANS) in MF where nanoparticles of magnetite (size below 10 nm) are placed in water and coated by double layer of sodium oleate (SO). In particular, comparatively small and compact nanoparticle aggregates (size at level of 40 nm) in the initial samples transfer to large (size above 120 nm) and developed (fractal dimension 2.5) associates after PEG is added to the system with the ratio above 2:1 with respect to magnetite content [1]. It should be noted that smaller amount of added PEG did not lead to aggregates reorganization.

The goal of the given work is to reveal by means of SANS the structure and interaction in complex aqueous micellar solutions of surfactant (SO and dodecylbenzene sulfonic acid (DBSA)) with PEG. SO and DBSA are actively used for stabilization of aqueous MF.

First step in such study was investigation of pure aqueous solutions of PEG [2] and surfactants [3] themselves. Some part of the polymer molecules in concentrated polymer solutions is found to form aggregates with size exceeding 30 nm. The form-factor of Gaussian coil is used to describe low concentrated PEG solutions. The interparticle interaction effect is well observed for PEG solutions with concentration higher than 3% where. In pure surfactant solutions a typical increase in the micelle size with the growth in the surfactant concentration within a range of 0.06-0.52 mol/l (2-17 vol. %).) is found, which can be related to the transition from spherical to rod-like micelles. The obtained data are used for estimating surfactant micelle concentration in water-based MF stabilized with DBSA.

Despite the fact that PEG addition into surfactant solutions should effectively increase the distance between micelles, a decrease in the micelle interaction radius takes place, which points to some kind of screening. Effect of screening of interaction takes place at PEG addition above 5 vol. %.

The obtained results are important specifically for understanding the synthesis procedure of highly stable water-based magnetic fluids with controllable properties.

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Development of the neutron sonde microscopy for the investigations of magnetic microstructures

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To investigate local magnetic microstructures with high spatial resolution, the narrow neutron beam (sonde) of micron width is needed. Therefore different focusing devices are developed (refractive lenses, curved crystal monochromators, diffraction gratings, etc.). But these devices have restrictions and cannot produce a neutron beam narrower than 50 mkm. Planar waveguides are more simple and effective devices which transform a conventional neutron beam into a very narrow (about 0.1 mkm) and slightly divergent (about 0.1°) neutron microbeam. It is tri-layer film structure where the middle guiding layer (channel) with low neutron optical potential is enveloped by two layers with high potential. We present experimental results on the investigations of planar waveguides, neutron channeling in waveguides and application of the polarized neutron microbeam for the investigation of a magnetic amorphous microwire.

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Структурно-динамическое исследование модифицированного реакторного уран-оксидного топлива

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С использованием нейтронных спектрометров HRFD и DIN-2PI на реакторе ИБР-2 (ОИЯИ, Дубна) в интервале температур 20-1000 ⁰C измерены структурно-динамические характеристики (тип и параметры кристаллической решетки, размер кристаллитов, уровень микродеформаций, плотность фононных состояний) модифицированного реакторного уран-оксидного топлива. Аналогичные данные получены для образцов двуокиси урана, изготовленных по стандартной технологии. Полученные данные используются для анализа свойств модифицированного топлива.

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Программный продукт для on-line обработки экспериментальных данных спектрометра ДИН-2ПИ

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Список современных программных продуктов, которые могут быть использованы для визуализации и первичной обработки экспериментальной информации, получаемой на спектрометрах неупругого рассеяния, обширен. Однако, их адаптация для использования на спектрометре ДИН-2ПИ требует существенных доработок. Кроме того, такое программное обеспечение, как правило, является платным. В результате анализа современных бесплатных программных продуктов было принято решение реализовать обработку экспериментальных данных на основе библиотеки ROOT. В настоящее время разработана первая версия приложения, в которой реализованы стандартные процедуры обработки данных, позволяющие выполнять on-line обработку экспериментальных спектров до уровня закона рассеяния (динамического структурного фактора) S(Q,ω).

Следующая версия приложения будет учитывать конструкционную особенность спектрометра ДИН-2ПИ - дискретный диапазон углов детектирования и наличие, вследствие этого, «мертвых» зон в области динамических переменных – передачи импульса и энергии нейтрона. Такое ограничение зачастую существенно снижает полноту экспериментальной информации и, соответственно, полноту анализа исследуемого явления. Поэтому предлагается получить информацию в непрерывном диапазоне динамических переменных путем проведения 2-х экспериментов с одним и тем же образцом, но с двумя различными значениями начальной энергии нейтронов. Правильный выбор значений начальной энергии должен обеспечить перекрытие исследуемых диапазонов передач импульса и энергии. Проблема состоит в объединении информации, полученной в разных экспериментах. Решение этой проблемы потребует разработки способов оптимального использования данных, полученных с различным разрешением и статистической точностью, и решения задач экстраполяции экспериментальных значений, точнее, выбора метода их экстраполяции. Результатом разработки такой методики станет возможность получения динамического структурного фактора исследуемого вещества в виде карты интенсивности в непрерывном диапазоне динамических переменных, ограниченном минимальным и максимальным углами рассеяния нейтронов.

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Nonreciprocal unpolarized neutron reflection in noncoplanar magnetic field of two magnetic mirrors in the external field

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It is known the unpolarized neutron scattering in systems with noncoplanar magnetic induction spatial distribution can be nonreciprocal [1]. In this work we investigate system consisting of two magnetic mirrors in external magnetic field. The nonreciprocal effect in this system is expected to be about of 50% of the initial neutron beam intensity.

The mirrors prepared by magnetron sputtering of CoFe thin film on smooth glass substrates. Thickness and roughness are controlled by x-ray small angle reflectometry and atomic force microscopy. Magnetic properties investigated by the longitudinal magneto-optic Kerr effect and magnetic force microscopy. The thickness is in the range 110-125 nm and roughness is about 3-5 nm. The coercive force of mirrors is 150-200 Oe. The remanent magnetization is 720 Oe.

The mirrors are placed parallel face to face to each other but their remanent magnetizations are perpendicular. The external magnetic field of 10-30 Oe is perpendicular to mirrors surfaces. So that the magnetizations and the external field are perpendicular to each other. In this system the mirrors are perpendicular “polarizer” and “analyzer” correspondingly which detect the neutron beam spin polarization precession in the external field. The neutron reflection experiment is made at the Spectrometer of polarized neutrons REMUR of the high flux pulsed IBR-2M reactor of the Joint institute for Nuclear research.

It is shown the reflectivity of unpolarized neutrons in such system is strongly depends on the magnitude and direction of the external magnetic field. The reflection becomes nonreciprocal when the mirrors are magnetized perpendicularly to each other.

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On the stability of magnetic fluids under excess of surfactants

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Magnetic fluids (MF) or ferrofluids are colloidal suspensions of magnetic nanoparticles coated with surface-active agents (surfactants) to prevent aggregation under various conditions. The characteristic size (~10 nm) of magnetic nanoparticles in a colloidal system corresponds to a single-domain state, thus determining a superparamagnetic behavior of the system, a specific property, which is very useful for different technological and biomedical applications of ferrofluids [1,2].

Aggregation stability of ferrofluids is significantly determined by the interaction of surfactants with the solvent. The concentration of surfactant molecules in solution is one of the important factors affecting on the stability of MFs, especially in the case when magnetic liquid systems contain some excess of stabilizer molecules. The optimal amount of surfactant in the MFs at which ferrofluids shows the most possible stability as colloidal liquid system is selected in practice. The present work was carried out within the framework of systematic investigations of the influence of surfactant excess on the structure of the different types MFs [3-7].

The method of small-angle neutron scattering (SANS) is one of the most informative in the structural studies of multicomponent nanosystems and particularly magnetic fluid [8]. The structural parameters of the classical magnetic fluids based on decalin at different excess of oleic and myristic acids in MFs volume (up to 20 vol.%) were determined by SANS as well as the structure parameters of polar ferrofluid stabilized by oleic and dodecylbenzenesulfonic acids were obtained. On the basis of further comparison of behavior oleic and myristic acids in the MFs and their solvents in decalin it was analyzing the changes in the interaction between the free (non-adsorbed) surfactant molecules in the presence of magnetic nanoparticles. In the case of polar MF the interparticle interaction in the system was considered by analyzing the effective structure factor.

However, ferrofluids are stable in respect of the formation of large aggregates of the magnetic nanoparticles in the studied range of the surfactant concentration. Comparison of the results with previously reported data for similar MFs based on benzene [3-5] is carried out in the work as well.

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Истоки современной кристаллографии

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Общепризнанными историческими событиями, положившими начало рентгеноструктурному анализу и современной кристаллографии, стали дифракционные эксперименты М. фон Лауэ и вывод отца и сына Брэггов уравнения дифракции рентгеновских лучей на кристаллической решетке. Однако, справедливости ради, следует начать отсчет эпохи современной кристаллографии с Федоровских пространственных групп, без которых современная кристаллография немыслима. Наряду с именами Федорова, Лауэ и Бреггов необходимо напомнить о вкладе в современную кристаллографию русского профессора Г.В. Вульфа. Об условиях, в которых создавалась современная кристаллография, о процессе создания навой ветви науки, о людях-творцах будет идти речь в докладе. Доклад посвящается Году кристаллографии, каким объявлен 2014 г. Организацией Объединенных Наций.

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Структура и магнетизм туннельных многослойных наносистем Fe/MgO/Fe

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Мультислойные наносистемы Fe/MgO/Fe, благодаря наблюдаемому в них эффекту туннельного магнетосопротивления (ГМС), представляют большой технологический и научный интерес, так как могут использоваться в качестве элементов устройств спинтроники. Гигантские изменения сопротивления при комнатной температуре под действием приложенного магнитного поля, делают исследования в области ТМС-систем одним из наиболее востребованных направлений в физике конденсированного состояния. В настоящем докладе сообщается об исследованиях зависимости магнитных свойств ГТМС системы Fe/MgO/Fe от толщины прослойки MgO.

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Кристаллическая структура и магнитные свойства двойных перовскитов

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Сложные магнитные перовскиты с общей формулой A2B'B''O6 (где A= La; Pr; Sr; Ba и т.д., а B' и B'' = W; Co; Mn; Fe; Mo и т.д.) обладают уникальными физическими свойствами: высокой степенью спиновой поляризации электронов проводимости, значительным туннельным магниторезистивным эффектом в слабых магнитных полях при комнатной температуре, высокими значениями температуры Кюри, что открывает широкие перспективы их практического применения в устройствах спиновой электроники (спинтроники) для создания спиновых клапанов и сенсоров магнитного поля. Величина влияния спинового эффекта таких материалов сильно зависит от степени поляризации и плотности состояний на уровне Ферми, на которую, в свою очередь, критическое влияние оказывают как валентное состояние, так и средний размер катионов B' и B''.

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Исследование магнитной структуры сверхрешеток Fe/Cr/Gd методами поляризационной нейтронной и резонансной рентгеновской магнитной рефлектометрии

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Известно, что при прямом обменном взаимодействии слоев Fe и Gd их магнитные моменты выстраиваются антипараллельно. В искусственной магнитной системе, состоящей из наноразмерных слоев Fe, Cr и Gd, можно управлять взаимной ориентацией магнитных моментов слоев Fe и Gd, изменяя толщину антиферромагнитного слоя Cr. В настоящей работе мы обсуждаем применение метода поляризационной нейтронной и резонансной рентгеновской магнитной рефлектометрии для определения магнитной структуры внутри тонких ферромагнитный слоев.

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ЭЛЕКТРОХИМИЧЕСКИЙ СИНТЕЗ НАНОСТРУКТУР СОСТАВА Ni/Fe

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Одним из аспектов развития нанотехнологий являются методы и механизмы синтеза наноструктур. Одним из наиболее продуктивных методов является метод шаблонного синтеза, в котором применяются пористые материалы в качестве матрицы (в нашем случае – трековые мембраны). Данный метод позволяет синтезировать наноразмерные объекты различной формы и размеров, которые можно очень точно контролировать.[1-4]
Для получения металлических нанотрубок и нанопроволок удобно использовать метод электрохимического осаждения. Осаждение материалов в поры происходит путем пропускания постоянного тока через раствор электролита, что позволяет получать композитные наноструктуры, главным достоинством этого метода является возможность контролировать скорость осаждения металлов в поры, путем изменения величины силы тока и приложенного напряжения, а так же времени осаждения. Регулируя эти параметры можно получить наноразмерные объекты с желаемой структурой.

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Neutron and optical investigations of multi-component crystalline Y3Al5O12:Ce3+/Lu2O3 and Lu3Al5O12:Ce3+/Lu2O3 luminophors

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The peculiarities of crystal structure and spectral-luminescent properties of compound oxide Y3Al5O12:Ce3+/Lu2O3 and Lu3Al5O12:Ce3+/Lu2O3 systems are investigated by neutron diffraction and optical spectroscopy methods. The influence of injected oxide on structural and luminescent properties of these systems is discussed. This influence is complex and depends not just on formation of stable defective garnet structure and Ce3+ ion diffusion from matrix to oxide, but also on interaction between oxide and matrix that progresses with new phases formation.

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Complementary Vibrational Analysis of Bromanilic Acid : 2,3,5,6-Tetramethylpyrazine Co-Crystal

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Organic electronic materials including semiconductors, dielectrics and conducting polymers are emerging family of materials with applications similar to their inorganic counterparts, but of much greater potential ease of integration with silicon and other inorganic matrices. One of the most promising organic ferroelectric materials are two-component crystals formed by hydrogen donor and acceptor molecules. The family of bromanilic and chloranilic acid complexes reveals very promising properties which are extensively studied since last decade.
Here, we present the complementary studies of bromanilic acid complex with tetramethylpyrazine synthesized at our laboratory. The crystal structure was solved with single-crystal X-Ray diffraction giving basis for theoretical topological analysis. The optical vibrational spectra were recorded in the middle- (FT-IR; FT-RS) and low-frequency (FT-FIR) range. The low-energy transfer range was explored by time-domain Terahertz spectroscopy. Finally, the Inelastic Neutron Scattering (INS) studies were performed revealing the closer insight into the vibrational proton-dynamics.
The complex experimental studies have been deeply supported and interpreted by applying theoretical solid-state computations. The high-quality plane-wave density functional theory computations (DFT) were performed in periodic boundary conditions at the generalized gradient approximation (GGA) level. The lattice-dynamics was probed with linear-response computations, providing both optical and neutron vibrational spectra. In addition to the zone-center computations, the phonon-dispersion relations were calculated across the high-symmetry points throughout the reciprocal space. The theoretical results stay in excellent agreement with the experimental data allowing for full understanding of the structural and vibrational properties of the title system.

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Исследование структурного перехода TlFeS2(Se2) при низких температурах методом порошковой дифракции нейтронов

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Кристаллические структуры TlFeS2 и TlFeSe2 исследовались методом нейтронной дифракции в температурном диапазоне 10-320 K. При комнатной температуре структуры в TlFeS2 и TlFeSe2 обладают моноклинной симметрией с пространственной группой C2/m. В TlFeS2 при температуре T ~ 200 K наблюдается антиферромагнитная фаза. Фазовый переход в TlFeSe2 возникает при температуре T ~ 290 K. Получены зависимости параметров и объема элементарной ячейки от температуры, рассчитаны коэффициенты температурного расширения и коэффициенты линейных расширений для каждого из параметров.

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Spectroscopic and crystallographic investigations of nitro derivatives of ortho-hydroxy acetophenones

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The report will present the complex investigations of the phase transition and intramolecular hydrogen bonding in nitro derivatives of ortho-hydroxy acetophenones. The phase transition was investigated by diffraction of neutron scattering, roentgenographic, calorimetric and spectroscopic methods. The assignments of vibrational spectra recorded in matrix condition, as well as IR, Raman and INS methods of 5-chloro-3-nitro-2-hydroxyacetophenone and 5-methyl-3-nitro-2-hydroxyacetophenone were accomplished. Quantum-mechanical calculations of two possible processes – isomerization of hydroxyl group and rotation of nitro group were carried out. In conclusion, the nature of the phase transition will be analysed.

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Spectrometer NERA: results of modernization and proposals for further development

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The main objectives of the modernization program of the NERA spectrometer (replacement of the 100-m neutron guide) were realized and after modernization of the IBR-2 core the spectrometer was commissioned in September, 2012. A new type of cold neutron source operating at the temperature of 30K was installed in the sector of six horizontal channels. The cold source in complex with water moderator allows one to effectively use incident neutrons in wide range of the wavelengths. Unfortunately the transmission of the new bent Ni-mirror guide limits the wavelength of thermal neutrons to about λ = 0.8 Å; as a result the neutron energy transfer for INS spectra is practicably limited to 127 meV (1000 cm-1). The gain factor (2012/2005) for the water moderator regarding the average thermal neutron flux at the sample position is 1.2, which is not high. Commissioning of the cold moderator significantly changed the spectral distribution of incident neutrons. The gain factor cold moderator / water moderator in the range of wavelength 2 Å < λ < 7 Å increases from 1 to 7, what provides much better conditions for measurements of neutron powder diffraction (NPD), low energy part of the inelastic neutron scattering (INS) spectra (up to 20 meV) and quasielastic neutron scattering (QENS) spectra in a high resolution mode with near back-scattering crystal analyzers.
Up to now, the neutron flux density at the sample position is about 106n*cm-2*s-1; the solid angle for INS ~ 0.2 sr; the solid angle for QNS ~ 0.05 sr;
It can be stated that the spectrometer NERA is much inferior for luminosity existing world analogues and planned spectrometers of this type (for example, the solid angle of LAGRANGE is about 2.5 sr).
In this paper the proposals for further modernization spectrometer NERA (increasing luminosity and resolution enhancement) are discussed.

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The magnetic and neutron diffraction studies of La1-xSrxMnO3 nanoparticles prepared via molten salt synthesis

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The ferromagnetic La1-xSrxMnO3 nanoparticles (x = 0.22 - 0.47) have been prepared from the flux of sodium nitrite at ≈ 500 °C. The advantage of this fast and facile method is the high yield of ≈ 50 nm particles without a very fine fraction that is common for an alternative preparation using sol-gel precursors. The single perovskite phase of the synthesized crystallites is confirmed by XRD patterns and their exact chemical composition is determined by XRF spectroscopy. The transmission electron microscopy shows that the manganite grains do not form typical sintering bridges and are easily separated by application of ultrasound. Compared to bulk material, there is some reduction of the perovskite cell volume detected by XRD, which becomes more pronounced for larger strontium contents. The nanoparticles exhibit also rather low magnetization and decreased Curie temperature. A detailed neutron diffraction analysis has been performed for the as-prepared and post-annealed samples of the x = 0.37 composition, as well as for a comparable sol-gel product. The results suggest that the anomalous behavior of the molten salt synthesized nanoparticles might originate in the overdoped outer shell resulting from the oxygen chemisorption at the surface of particles and from an increased Sr concentration in the shell compared to the interior. This overdoping is a source of compressive surface stress that drives the x = 0.37 ground state towards a mixture of FM and A-type AFM ordering.

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Small-angle scattering from multiphase systems: Investigation of the crossover between Porod and fractal regimes

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Small-angle scattering (SAS) intensities observed experimentally are often characterized by the presence of successive power-law regimes with various scattering exponents whose values vary from -4 to -1. The existing models explaining the crossover positions (that is, the points where the power-law scattering exponent changes) involve only one contrast parameter, which depends solely on the ratio of the fractal sizes. Here, a model that describes SAS from a multiphase system with a few contrast parameters is described, and it is shown that the crossover position depends on the scattering length density of each phase. The Stuhrmann contrast variation method is generalized and applied to experimental curves in the vicinity of the crossover point beyond the Guinier region. The contrast variation is applied not to the intensity itself but to the model parameters, which can be found by fitting the experimental data with the suggested interpolation formula. The model supplements the existing two-phase models and gives the simple condition of their inapplicability: if the crossover point depends on the contrast then a two-phase model is not relevant. The developed analysis allows one to answer the qualitative question of whether one fractal ‘absorbs’ another one or they are both immersed in a surrounding homogeneous medium like a solvent or solid matrix. The models can be applied to experimental SAS data where the absolute value of the scattering exponent of the first power-law regime is higher than of the subsequent second power-law regime, that is, the scattering curve is ‘convex’ near the crossover point.

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Alcohols, anesthesia, membranes, neutrons, excimers and MD simulations

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Normal alcohols (CnOH, n is the number of carbons in alkyl chain) with n<14 are general anesthetics. Lipid theories of anesthesia suggest the bilayer of biomembranes as their primary target: Bilayer structural perturbations induced by anesthetics affect membrane protein conformations and result in protein functional changes. In the bilayer, the OH group of CnOH is located on the level of phospholipid polar groups and the CnOH alkyl chain extends into the bilayer hydrophobic interior. At a constant CnOH concentration in the bilayer, the mismatch between shorter alcohol and longer lipid hydrocarbon chains should result in a decrease in the bilayer thickness; this decrease should diminish with the alcohol chain length increase up to the lipid chains length. Simultaneously, other physical properties of the bilayer must be affected. The aim of our investigations was therefore to study bilayer thickness as a function of CnOH chain length n to test this hypothesis. The bilayer thickness was obtained from small-angle neutron scattering (SANS) on unilamellar phospholipid vesicles (ULVs). Bilayer structural perturbations were also followed by dipyrenylphosphatidylcholine excimer fluorescence probes (diPYmPC, m=4 or 10, pyrene moieties are attached to the m-th carbons of both acyl chains) using multilamellar phospholipid vesicles (MLVs). The experimental data were compared with coarse-grained molecular dynamics (MD) simulations.

Samples were prepared from dioleoylphosphatidylcholine (DOPC) with small amounts (4 wt %) of dioleoylphosphatidylserine (DOPS) and dipymPC (<0.07 mol %). DOPC, DOPS, diPYmPC and CnOHs were mixed in $CHCl_3$+CH_3OH, the solvent was then removed by evaporation under a stream of pure gaseous N_2 and subsequent oil pump evacuation. Solid mixtures were dispersed in D_2O + H_2O by vortexing and brief sonication and MLVs thus prepared were extruded through 50 nm pores in 2 stacked carbohydrate filters to obtain ULVs. The SANS spectra were measured on PAXE spectrometer in LLB Saclay with sample to detector distance 1.3 m and 5.05 m, λ=0.6 nm at 25°C. The fluorescence spectra between 360 and 650 nm were recorded using FluoroMax-4 (HORIBA Jobin Yvon) fluorimeter with excitation at 345 nm, and excitation and emission bandwidths were 3 and 1 nm, respectively. The temperature was regulated to within ±0.01°C by a Peltier thermocouple drive. All MD simulations were carried out with the GROMACS molecular dynamics package, using the MARTINI coarse-grained force field.

The extruded ULVs are polydisperse hollow spheres with a single bilayer separating the inside and outside aqueous compartments. The measured normalized SANS intensity I(q) as a function of the scattering vector q can be described by $I(q)=N\int T(q')\int G(R)I(R,q\ q')dRdq'$, where N is the number density of particles, T(q) is the resolution function, I(R,q) the structure factor of the ULV with radius R, and G(R) the Schulz function describing the ULVs polydispersity. The bilayer is divided into three strips corresponding to two polar headgroup regions and the bilayer center spanning hydrocarbon region. The scattering length densities of polar and hydrophobic regions were calculated using the known scattering lengths and component volumes of DOPC, DOPS and CnOH measured by densitometry. From SANS data, we evaluated by fitting the bilayer thickness, D, and the lateral area of the unit cell consisting of a phospholipid molecule and a particular fraction of the alcohol at the bilayer–aqueous phase interface, AUC, as a function of CnOH:DOPC molar ratio

and as a function of CnOH chain length n at fixed CnOH:DOPC=0.4 molar ratio. As we predicted, the thickness D is decreased due to CnOH and lipid chain length mistmatch; this effect is larger at higher CnOH concentrations and diminishes with the CnOH chain length n. The interface area AUC increases due to CnOH intercalation between lipid molecules. From the data, we have also calculated the molecular interface area of CnOH, ACnOH, in bilayers. Anomalously small values of ACnOH were obtained for n<12 – smaller than the chain cross-section area 20 Å2 in solid rotator phases of n alkanes.

To characterize the structural changes induced in the bilayers by long aliphatic alcohols, we have simulated a fully hydrated DOPC bilayer incorporating CnOHs at different concentrations and with variable chain lengths n = 8, 12, 16. For different alcohol concentrations and alcohol chain lengths, we have computed the area per lipid, the alcohol partial interfacial area, the bilayer thickness parameter and the uniaxial order parameter S for the bonds of the lipid tails. All computational results give an accurate description of the alcohol effects at the molecular level, being in good agreement with the experimental data. The anomaly ACnOH is caused by the lipid headgroup, which interfacial area is larger or equal comparing to the sum of hydrocarbon chains cross-section areas, so that a small alcohol OH group is located underneath at the lipid glycerol fragment.

The ratio η=Iexc/Imon calculated for emission intensities of diPYmPC excimer probes at 375.5 and 475 nm for monomer (Imon) and excimer (Iexc) correspondingly was used as a measure of structural perturbation of bilayers induced by CnOHs. At constant CnOH:DOPC molar ratios of 0.25 and 0.4, the value of η increases with the CnOH chain length from n=8 up to n=14-16 and than decreases nearly to the control value (MLVs without CnOH) for both dipy4PC and dipy10PC excimer probes.

Additionally, the lateral pressure profile along the bilayer normal has been calculated using MD simulations for different bilayers to capture the effects of alcohol localization in the membrane. Although the effects of alcohols on structural and thermodynamic properties of the bilayers are rather small, the bilayer lateral pressure profile changes significantly, especially in the center of the bilayer.

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Simulations of Neutron Beam at 6a Horizontal Channel of IBR-2 Research Reactor by Monte-Carlo method

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Neutron beam calculations are indispensable when designing and modernizing of neutron scattering instruments is necessary. Among all methods available, Monte-Carlo simulations are employed very often. They don't rely on empirical knowledge of beam characteristics but rather on the high computational power of the modern computers. A large number of neutrons are "created" virtually at the place of source (moderator) and their trajectories simulated until they reach the guide end to deduce the characteristics of the beam with a good statistics. We have chosen McStas software suit for such a study.

The study is devoted especially to simulation of neutron beam after passing through the mirror guide of horizontal channel 6a of research reactor IBR-2 at JINR, Dubna. Previous studies of the same neutron beam did not yield a conclusive explanation of the discrepancy between the expected and measured neutron intensities. These include integral intensities as well as resultant wavelength distribution. New simulations did not solve the problem, but brought more knowledge by investigating the situation of neutron guide with focusing geometry. The position of the guide opening relative to the cold moderator was accounted more precisely during these simulations as well. It was shown that widening of the guide entry of up to 30% leads to increase of the overall neutron intensity at the guide end connected with an increase of the long wavelength neutrons. Further increase of the width of the guide entry however leads to decrease of the shorter wavelength neutrons, drop of the overall intensity and occurrence of high inhomogeneity in space distribution of the resultant beam at the end of the guide.

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Transformation of wormlike surfactant micelles to spherical microemulsion droplets studied by small-angle neutron scattering

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Surfactant molecules can self-assemble and form long wormlike (cylindrical) micelles. Surfactant molecules are bound by weak non-covalent interactions within the micelle, therefore viscoelastic micellar solutions are highly responsive to external stimuli, e.g. the addition of hydrocarbons. In the present work we investigate the transition of wormlike micelles into microemulsion droplets induced by hydrocarbon.

At very small hydrocarbon concentrations, the solutions have viscoelastic properties due to the presence of entangled wormlike micelles, what is confirmed by SANS data, which show that aggregates with local cylindrical shape are present in the solution. Solubilization of hydrocarbon inside the micelles has only minor effect on their persistence length.

At slightly higher hydrocarbon concentrations, a mixture of cylinders and spheres is present in the solution, what indicates to the appearance of small spherical microemulsion droplets. As the hydrocarbon concentration is increased, the volume fraction and radius of spheres increases [1].

At high hydrocarbon concentrations, cylindrical micelles are fully disrupted and only microemulsion droplets are present in the solution.

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3D laboratory measurements of P and S-wave velocities in biotite gneiss and their correlation with the velocity calculation based on neutron diffraction texture analysis

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The study demonstrates that calculated 3D velocity distributions based on neutron diffraction texture measurements provide a powerful tool for the interpretation of the directional dependence (anisotropy) of experimentally determined P- and S-wave velocities. Neutron texture measurements were performed on a spherical sample of biotite gneiss at the time-of-flight texture diffractometer at JINR (Dubna, Russia). Quantitative texture analysis of the predominant minerals biotite (23.4 vol.-%), plagioclase (36.9 vol.-%) and quartz (39.6 vol.-%) was done by combining the neutron diffraction measurements and the WIMV method. The sample exhibits strong crystallographic preferred orientation (CPO) of biotite and only weak CPOs of plagioclase and quartz. 3D velocity calculation based on texture measurements confirms that the texture of the aligned biotite minerals controls significantly the intrinsic anisotropy of the bulk rock, due to the extreme single crystal elastic anisotropy of biotite. The calculated 3D velocity distributions for the spherical sample were compared with P- and S-wave velocities measured in 132 directions on the sample sphere. Measurements were done at the Institute of Geology AS CR in Prague, using an improved and modified equipment. Both, the experimentally-derived and texture-based velocity surfaces of the bulk rock compare reasonably well with respect to symmetry of P- and S-wave velocities distributions, to the position of P-wave velocity maxima and minima and their relation to the foliation plane.

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Low temperature phase transition in [Ni(NH3)4](ReO4)2 studied by infrared spectroscopy and neutron scattering

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The hexaamminenickel(II) perrhenate belongs to the so called Werner type coordination compounds which still remains as an interesting object for investigations. They attract attention because of their rich polymorphism connected with changes in crystal structure and dynamics of complex cation and anion.
The titled compound was investigated by DSC method. One reversible phase transition at Tc = 187.8 K (on heating) was detected [1]. The X-ray powder diffraction pattern registered at room temperature was indexed in monoclinic system (space group No. 14 P21/n) with the following lattice parameters: a=11.98 Å, b=12.34 Å, c=7.80 Å and ⍁=90.48°. Diffraction pattern registered below phase transition temperature suggests that change of crystal structure take place.
The middle and far infrared spectra taken with the aid of vacuum fourier-transform spectrometer Bruker Vertex 70v in the temperature range of 300 – 9 K on cooling and heating (temperature step 10 and 25 K, respectively) show characteristic changes in the vicinity of phase transformation. The splitting of bands at 1615 cm-1 and 1410 cm-1 connected with ligands NH3 vibrations is clearly observed. The changes observed in the 3000-4000 cm-1 wavenumber region during cooling can be attributed to hydrogen bond formation. The activation energy for NH3 reorientations determined from temperature dependency of FWHM band at 1615 cm-1 in the high temperature phase is small and is typical for amminacomplexes.
The incoherent inelastic/quasielastic neutron scattering spectra as well as neutron powder diffraction patterns were measured simultaneously using the time-of-flight method on a NERA spectrometer [2] at the high flux pulsed reactor IBR-2M in Dubna (Russia) at temperatures of T = 40, 155, 215 and 293 K. Additional reflexes visible in the NPD pattern the in the low temperature phase suggests lowering of crystal symmetry.
The quasiealstic peak registered at 155, 215 and 293 K shows broadening. Taking into account the energy resolution of the NERA spectrometer, this implies that protons from NH3 ligands perform fast (correlation time 10-12 – 10-13 s) reorientational jumps around three fold symmetry axis above and below phase transition. This is typical behavior for the orientationally disordered crystals (ODIC). The QENS wings are not visible at 40 K. The IINS spectra obtained at 155, 215 and 293 K are very diffuse because of a large dynamical disorder connected with the fast molecular reorientations, especially of NH3 molecules. The IINS spectra are compared with infrared data and with DFT calculations performed for isolated [Ni(NH3)4]2+ cation.
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Neutron diffraction study of MgNi2D3

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Hydride and deuteride of a MgNi2 compound have been produced by high pressure synthesis, quenched and recovered to ambient pressure. The hydrogen (deuterium) content was 2.2(1)wt.%H (4.3(2)wt.%D), corresponding to H/MgNi2=3.2(1) (D/MgNi2=3.1(1)), as measured by hot extraction in vacuum. An X-ray diffraction investigation has shown that the samples had an orthorhombic crystal structure with the Fmmm(69) space group, a=4.55Å, b=4.69Å, c=8.80Å, with the metal atoms at positions Mg(4a) and Ni(8i). Neutron diffraction has shown the D atoms to be located at the 4b and 8f positions.

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Comparison of dynamical properties of [Ca(H2O)4](ClO4)2 and [Ca(NH3)6](ClO4)2 compounds studied by vibrational spectroscopies (IR and IINS)

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Tetraaquacalcium perchlorate [Ca(H2O)4](ClO4)2 and hexaamminecalcium perchlorate [Ca(NH3)6](ClO4)2, are a particularly interesting molecular materials, because of the occurrence of reorientational motions of the H2O and NH3 ligands, ClO4- anions and entire [Ca(H2O)4]2+ and [Ca(NH3)6]2+ complex cations.
The vibrational spectra of the [Ca(H2O)4](ClO4)2 and [Ca(NH3)6](ClO4)2, are investigated by means of infrared and inelastic neutron scattering spectroscopies together with density functional theory calculations.
At room temperature tetraaquacalcium perchlorate crystallizes in a triclinic crystal system, within the space group No. 2 = P-1, with two molecules in the unit cell. The following unit cell constants: a = 5.578(5) Å, b = 7.813(5) Å, c = 11.761(5) Å, alfa = 100.740(5)°, beta = 89.658(5)°, gamma = 91.069(5)° were determined by us [1].
Fourier transform middle infrared spectroscopy and inelastic/quasielastic incoherent neutron scattering data for [Ca(H2O)4](ClO4)2 in the temperature range of 14–295 K and 21–290 K, respectively, are reported. No significant changes (sudden splitting or changes in bands width) of the FT-MIR spectra at the phase transitions range can be seen, which suggests that the phase transitions are probably not connected with a change of the symmetry. The lack of broadening of the infrared bands connected with vibrations of ClO4- and [Ca(H2O)4]2+ ions suggests that neither the ligands nor the complex cation do not perform fast (picoseconds time scale, characteristic for infrared spectroscopy) stochastic reorientational motions in the low and intermediate temperature phases. The G(v) spectra obtained at 180, 225 and 290 K are very diffuse. This is due to a large dynamical disorder connected with the fast molecular reorientations, especially with the disorder of the hydrogen atoms. The G(v) spectrum obtained for the low temperature phase at temperature 100 K shows some separate peaks characteristic for an ordered phase. However, a marked broadening of all these bands indicates some kind of the orientational disorder present down to the low temperatures.
At room temperature hexaamminecalcium perchlorate crystallizes in the cubic system (Fm-3m space group, No = 225) with unit cell parameter: a = 11.685 Å and four molecules per unit cell [2]. The results of inelastic and quasi-elastic incoherent neutron scattering with simultaneous neutron powder diffraction and of Fourier transform far and middle infrared spectroscopy measurements carried out for [Ca(NH3)6](ClO4)2 between 20–220 K and 8.5–295 K, respectively, are reported. The far and middle infrared spectrum on cooling the substance indicates splitting of some degenerated vibrational modes, which suggests lowering of the crystal structure at the phase transition temperature TC = 122.0 K, revealed by us earlier using differential scanning calorimetry. In turn, lack of simultaneous abrupt narrowing of some broad infrared bands suggests an existence of fast molecular reorientational motions, which do not change their character in the wide temperature range. On the other hand, the quasi-elastic neutron scattering peak registered at 110 K and also at higher temperatures, shows distinct broadening, which is typical for dynamically, orientationally disordered crystals (ODIC). The G(v) spectra obtained for the low temperature phase at temperature 20 K show some sharp and separate peaks characteristic for an ordered phase. However, a marked broadening of all these bands indicates the existence of NH3 orientational disorder present even at lowest temperatures. The G(v) spectra obtained at 110, 131 and 220 K are very diffuse, because of a large dynamical disorder connected with the fast molecular reorientations, especially of NH3 molecules. All these facts suggest that the discovered phase transition is associated with a change of the crystal structure without a sudden change of the NH3 reorientational dynamics.
We performed quantum chemical calculations of normal modes using two approaches: periodic boundary conditions (CASTEP code [3]) and isolated molecule (Gaussian 09 package, Revision B.01 [4]) .
We have obtained good agreement between calculated and experimental data (IR and IINS spectra).

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КИНЕТИКА ФАЗОВЫХ ПРЕВРАЩЕНИЙ В ТОНКИХ ПЛЕНКАХ CuIn5Se8

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Методом кинематической электронографии исследованы процессы фазообразования и фазовых переходов в тонких слоях CuIn5Se8, позволяющий производить непрерывную съемку объекта при различных условиях термообработки. Показано, что полученные пленки как испарением синтезированного соединения так и при термического напыления двойных соединений составов Cu2Se и In2Se3 в соотношении 1:5 образуются аморфные пленки. Установлены кинетические параметры кристаллизации аморфных пленок составов CuIn5Se8. Определены мерность роста кристалликов и значения энергий активаций зародышеобразования и дальнейшего их роста.

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High Pressure Effect on Crystal Structure of Antiferroelectric NaNbO3

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Among the materials that exhibit spontaneous electric polarization, sodium niobate can undergo many different structural phase transitions with a change in the thermodynamic parameters and at an external electric field. Both ferroelectric and antiferroelectric phases can be formed under certain conditions, as a result of which the structure and physical properties of this compound are of great interest. In addition, ferroelectric materials based on sodium niobate are promising for electronic and optical devices and piezoelectric sensors as an environmentally safe alternative to lead containing ferroelectrics.
To obtain the baric dependences of the structural parameters of NaNbO3 and in wide pressure ranges, neutron diffraction have been performed at high pressures up to 4 GPa at room temperature. The neutron diffraction experiments were performed on a DN-12 spectrometer of the IBR-2 pulsed high_flux reactor (Frank Laboratory of Neutron Physics, JINR, Dubna) using high_pressure cells with sapphire anvils. The diffraction spectra were measured at the scattering angle $2\theta = 90^{\circ}$. The characteristic time of measuring one spectrum was 10 h.
At the ambient conditions, the NaNbO3 structure is tetragonal with the space group Pbcm (antiferroelectric phase), in this phase cell parameters are a = 5.534(7) Å, b = 5.587(3) Å and c = 15.594(6) Å. At high pressure P = 2 GPa and room temperature structural phase transition from the orthorombic antiferroelectric phase to the new high pressure phase have been observed. The symmetry of crystal structure of nigh pressure phase of NaNbO3 and pressure dependences of the lattice parameters, unit cell volume, and interatomic bond lengths have been obtained. It is seems that we found suppression of antiferroelectric phase in NaNbO3 at high pressure.
The work has been supported by grant RFBR No. 14-02-00948-a.

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A modified approach to study anisotropy of elastic P and S-waves on spherical rock samples: based on acoustic and neutron diffraction measurements

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The acoustic measurements and neutron diffraction study have been performed on a biotite gneiss from the Outokumpu scientific drill hole. The calculation of the 3D velocity distribution of P- and S-wave velocities based on neutron diffraction texture measurements were used to improve the acoustic signal processing. The different numerical methods for recovering of 21 independent components of the tensor of elastic (stiffness) parameters from the measured elastic wave forms are presented.

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Neutron diffraction evidence of the stability of the γ-phase in the Ti-D and Zr-D systems

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Monohydride gamma-TiH and gamma-ZrH were proposed (and generally accepted now) to be metastable. Their formation was attributed to the mechanical stress in the lattice matrix at the eutectoid transformation beta - alpha + delta.
Now we have well-aged (about 20 years) TiH(D)x and ZrH(D)x samples. We attempted estimating the phase compositions of the bulk TiDx and ZrDx samples from the neutron diffraction measurements on DN-2 in order to compare the phase composition of the same sample after long aging and after heating to (or over) the eutectoid temperature.
We obtained a number of indirect experimental evidences that the gamma-phases have their stability regions in the equilibrium T-C diagrams.

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Texture characterization of mantle peridotites (Balmuccia, Italy) and its influence on seismic anisotropy

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In order to estimate the elastic anisotropy of the mantle peridotites, texture measurements were performed on a number of samples from the Balmiccia massif (Ivrea zone, Italy) and the elastic properties were calculated from the mineral textures. Emphasis is placed on the relating preferred mineral orientations to ultramafic rock compressional (Vp) wave velocities and their anisotropies, and using these relations to interpret seismic velocities. The ultramafic peridotites are mainly composed of olivine and ortho- and clinopyroxenes with varying volume fractions Neutron texture measurements were performed at the time-of-flight (TOF) texture diffractometer SKAT at Dubna, Russia. Using the orientation distribution function (ODF) as a parameter characterizing the lattice preferred orientation (LPO) of the constituent minerals, the seismic properties (3D velocity distribution of P- waves) of bulk samples were calculated from the corresponding properties of major minerals. It was shown that the elastic anisotropy of peridotites strongly depends on olivine crystallographic textures. Moreover, the comparison of recalculated olivine pole figures (100), (010) and (001) with the typical database of the olivine preferred orientations were important for meaningful interpretations of the conditions of texture formation and texture forming processes in the Earth's mantle. Comparison of textures of experimentally and naturally deformed olivines allowed us to determine that the texture formation process for the studied samples is the result of high temperature (1300-1600°C) deformation along the slip system (010)/[100] and corresponds to the depths of 100 km and deeper. The complete 3D P-wave distributions at confining pressures ranging from 0.1 to 400 MPa were measured at the Institute of Geology AS CR (Prague, Czech Republic) and the experimental patterns were compared with the patterns calculated from the elastic stiffness tensor of the samples The texture-derived (modelled) P-wave velocity distributions reflect the experimentally determined bulk rock anisotropy quite well. Known patterns of P-wave velocity distributions may help to reconstruct the kinematics of deformation processes during the upwelling of ultramafic rocks from mantle into the Earth's surface.

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The neutron TOF strain/stress diffractometer Epsilon-MDS for material sciences and geosciences

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The high resolution neutron time-of-flight diffractometer EPSILON-MDS for in situ strain / stress determination is located at beamline 7A-1 of the long pulse neutron source IBR-2M. The main features are the 2Θ=90° geometry of nine detector banks and more than 100 meter neutron flight path using curved mirror neutron guide. The instrument is designed for application on tasks in material sciences and geosciences, like the determination of residual and applied intracrystalline strain. Different gauge volumes can be investigated and strain scans can be carried out using a diaphragm system in the incident beam.
This diffractometer is equipped with an unaxial pressure device, which allows uniaxial deformation experiments up to 100 kN (150 MPa) with sample dimensions of 30 mm in diameter and 60 mm in length. An acoustic emission detection system for micro-crack analysis, a laser extensometer for macro strain detection and a Paris-Edinburgh cell VX4 with pressures up to 8 GPa allows in situ – experiments. This can be used for a wide spectrum of scientific applications in material sciences and geosciences.
Some applications of residual and applied strain investigations in geological materials will be presented.

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Neutron diffraction texture analysis: application to minerals and rocks

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Many materials, such as metals, ceramics, and rocks are polycrystals, formed by grains of different size, shape and orientation. Crystallographic texture is the preferred orientation of grains within the polycrystalline material. Specific textures are formed during crystallization, recrystallization, plastic deformation/twinning, phase transitions, etc. and they influence physical properties of polycrystals. There are several possibilities to measure grain preferred orientations experimentally; and one of them is to use diffraction methods. In particular, neutron diffraction is applied due to ability to measure bulk samples to be able to provide sufficient grain statistics to quantitatively study preferred orientations in often coarse-grained samples of minerals and rocks. The recently upgraded SKAT diffractometer (installed at the beamline 7 of the pulsed IBR-2 reactor, Frank Laboratory of Neutron Physics, JINR, Dubna) allows to measure samples of up to 125 cm^3 volume, possesses good d-resolution to be able to resolve diffraction peaks of multi-phase rocks formed by several low-symmetry minerals, and perfect angular resolution on the pole figure. Some examples of experiments performed on SKAT, data analysis and obtained scientific results are given.

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FLNP JINR User programme at IBR-2 reactor after modernization

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The realization of the User Programme at FLNP JINR after IBR-2 modernization has been started in 2012. The spectrometer complex of the IBR-2 pulsed reactor at present consists of 11 instruments available for scientific research: 6 diffractometers, 1 small angle neutron scattering spectrometer, 2 reflectometers, 2 inelastic neutron scattering spectrometers. There are also 4 new facilities under realization: Diffractometer for studies of microsamples (DN-6), Multi-functional reflectometer with polarized neutrons (GRAINS), the new Neutron Imaging Instrument at the Beamline 14 of IBR-2 for radiography as well as tomography studies and finally the Fourier spectrometer for stress measurements.
Present state and the plan of development of a User Programme at Frank Laboratory of Neutron Physics, JINR are presented.

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Study of detonation nanodiamond dispersions by small-angle neutron scattering

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A spatial transition of the carbon state in detonation nanodiamond (DND) from diamond inside the particle to a graphite-like state at the surface is proposed on the basis of small-angle neutron scattering (SANS) analysis. The SANS contrast variation from concentrated dispersions of DND fractal clusters in liquids (water, dimethylsulfoxide) reveals a shift in the mean scattering length density of DND as compared to pure diamond, which is related to the presence of a non-diamond component in the DND structure. At the same time, the diffusive character of the particle surface is deduced based on the deviation from the Porod law. The two observations are combined to conclude that the continuous radial density profile over the whole particle volume conforms to a simple power law. The profile naturally suggests that non-diamond states are concentrated mainly close to the particle surface.

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Дифрактометр RTD: текущий статус и перспективные направления исследований

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Предоставлены данные о текущем состоянии и характеристиках нейтроновода, детекторной системы, системы окружения образца и программного обеспечения дифрактометра RTD (Real-Time Diffractometer).
Даны заключения о направлениях и возможностях дальнейшего развития дифрактометра.

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Ti-D and Zr-D phase diagrams specified by neutron diffraction on DN-2 apparatus

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The phase diagrams of the Ti-H(D) and Zr-H(D) systems are known to include two interesting features, i.e., the β(bcc) <-> α(hcp)+δ(fcc) and γ(fco monohydride) -> α+δ transformations. Both processes occur at high rates characteristic of short-range hydrogen diffusion. However, there is a marked difference in generally accepted views on the thermodynamics of these transformations. The former eutectoid transformation is accepted in the equilibrium phase diagrams [1,2]. The latter one, peritectoid, is not represented in the equilibrium diagrams. This difference arose from inability of the authors of the first description of the γ-phase; [3] to produce samples containing more than about 5 % γ-phase. Therefore, they suggested that the γ-phase is metastable and originates due to mechanical stress of the crystal lattice after the eutectoid transformation. Now we disprove this idea. We show that the &gamma-phase; should be represented in the equilibrium diagrams on an equal footing with other stable phases.

We note several aspects for this statement.

First, we increased the amount of the monohydride &gamma-phase; in the TiH_x samples by an order of magnitude, up to 70-85 %. This was achieved due to a new synthesis technique [4]: heating to room temperature of the metastable &chi-TiH_x; phase quenched under pressure of about 60 kbar to liquid nitrogen. Our dilatometric and calorimetric measurements at normal pressure and respective thermodynamic estimates [4,5] demonstrated that the high-pressure behavior of titanium and zirconium monohydrides is essentially that of the equilibrium phases. They remain stable at normal pressure below the peritectoid temperatures, Tp^{TiH}=168°C (205°C for TiD) and $Tp^{ZrH(D)}$~330°C.

Second, we have chosen bulk samples for the present study. Compact medium allows minimizing the effect of surface oxidation and does not prevent hydrogen diffusion. The effect of the preparation technique of the powder samples on the monohydide phase is in progress now.

Further, we have chosen the time-of-flight neutron diffraction in order to use all advantages of this technique, that is, high radiation penetrability, neglect of the surface effect, fixed angle geometry with analysis and averaging over the detectors, higher statistics over grains and higher admissible grain size compared to X-rays. In addition to the opportunity of determination of the hydrogen concentration in the α-, δ- and γ-phases, further advantages of the neutron diffraction method appeared due to overlapping of the X-ray diffraction lines of the phases involved, ordering of the hydrogen sublattice of γ-monohydrides, and the occurrence of the intense superstructural hydrogen-induced peaks in the open ranges of the neutron diffraction pattern. This allowed use of DN-2, the high-flux apparatus of medium resolution.

At last, to establish the thermodynamic equilibrium, we studied well aged (for about 20 years) bulk TiD_x and ZrD_x samples of three compositions around the equiatomic one, x=D/Me=0.78÷1.35. The samples were prepared earlier from the high-purity ingots, now they were shaped as parallelepipeds of the 8x8x30 mm size.

The diffraction data demonstrate a large increase of the content of monohydrides in all samples upon aging, which proves their thermodynamic stability. Another fact found is that the phase diagrams may be well studied using neutron diffraction on real bulk samples.

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Small-angle neutron scattering on chondroitin sulfate solutions

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The linear polysaccharide chondroitin sulfate (CS) presents important biological functions, being the major component of the proteoglycans (that play an important role in the molecular organization and mechanical properties of connective tissues).
We have investigated by small-angle neutron scattering the morphology of chondroitin sulfate in aqueous solutions at LLB Saclay, PACE spectrometer and Frank Laboratory of Neutron Physics Dubna, YuMo spectometer.
The results suggest that we have a fractal distribution that does not change with the variation of volume ratio chondroitin sulfate : calcium. From data we can see that the differences are insignificant with increasing the temperature. When put $CaCl_2 2H_2O$ in polymer solution appear a correlation peak which disappear with increasing salt concentration.

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SMALL-ANGLE NEUTRON SCATTERING INVESTIGATION OF SPECIAL CEMENT MATRIX SAMPLES FOR CONDITIONING OF RADIOACTIVE WASTES

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The radioactive wastes are generated in a variety of physical and chemical forms and after the treatment must be immobilized in a form that is physically and chemically stable; the most known method being the cementation in hydraulic Portland cement [1]. In the case of cementation, the chemical nature and proportion of the precipitation products affect both the hydrolysis of the initial cement components and the reactions of metastable hydration constituents as well as the mechanical strength and the chemical resistance of the hardened cement system.

Solidification of radioactive wastes with hydraulic cement either with or without admixtures has been practiced for many years. Water from the waste reacts chemically with the cement to form hydrated silicate and aluminum compounds, which normally contribute towards the setting and hardening of the cement mixture [2]. In the Radioactive Waste Management Department (DMDR) from the IFIN-HH, Bucharest-Magurele, Romania, conditioning of the low and medium activity institutional radioactive waste is done by cementation in accordance with the limits for acceptance for final storage at the repository from Baiţa, Bihor County [3]. The precipitation products and their behavior during cementation are extremely hard to study because of the system complexity (phase composition and structure) and the lack of nondestructive analytical methods. The Portland cement paste remains fluid long enough to allow safe processing, and the set cement has adjustable properties. Chemically, after mixing with water, cement produces a reacting matrix with a porous microstructure [4]. Little is known so far on the chemical reactions taking place or, products that are formed as cement mixes with solid or liquid waste and water. But, knowing how the microstructure develops is therefore desirable in order to assess the compatibility of radioactive streams with cement and predict waste form performance during storage and disposal. In the present paper are investigated selected matrices of special cement compositions by means of SANS method. These samples are very important in the study of cement structure behavior by incorporating aluminum radioactive waste.

Keywords: cements, porosity, SANS, radioactive wastes

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Spatial distribution of diffracted neutron beam in perfect and strained Si crystal undergoing ultrasonic excitation

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The spatial distribution of neutron beam Bragg diffracted from Si single crystal undergoing on ultrasound excitation and bending have been measured. The values of ultrasound wave amplitude and uniform strain gradient were determined. For the perfect crystal, it was shown that at the same time as the acoustic wave amplitude is increased, the front-face peak position remains unchanged and its value grows linearly. For the strained crystal, the spatial distribution of diffracted neutrons inside the profile is analyzed as well as the mechanism of anomalous decrease of diffraction intensity, depending on acoustic wave's amplitude and on the value of the uniform strain gradient.

New types of Pendellösung fringes were observed. These effects observed at the first time, have a different nature in the case of a perfect and deformed crystal. It is supposed that in the perfect crystal this effect may be due to the appearance of the new "sound" extinction length, depending on the amplitude of the ultrasonic wave, thus, it leads to the new interference interactions between neutron wave and ultrasonic phonons. The influence of the crystal bending on the formation of the fringes in Bragg spatial profiles was studied. It is established that within the framework of the dynamical theory of the neutron scattering some asymptotic models valid for the case of Laue geometry can be applied in the case of Bragg geometry also. Good agreement between experimental data and the theory have been obtained.

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Интерференционные эффекты при дифракции нейтронов на упругих колебаниях совершенной и деформированной кристаллической решетки

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Исследовались интерференционные эффекты при рассеянии нейтронов на упругих колебаниях совершенной и искаженной кристаллической решетке. В работе приведены следующие экспериментальные данные, полученные впервые.

1) В условиях нейтрон - акустического резонанса в совершенном монокристалле кремния наблюдались биения интенсивности дифракции, контраст которых уменьшался с ростом частоты ультразвука (УЗ).

2) Приведены экспериментальные и теоретические результаты исследования распространения сферической нейтронной волны через толстый образец. Измерялись профили интенсивности дифракции внутри треугольника Бормана. При небольших амплитудах УЗ волны наблюдались пространственные биения пучка рассеянных нейтронов. Для объяснения полученных результатов использована модифицированная динамическая теория рассеяния нейтронов в присутствии УЗ возбуждений. С ростом амплитуды УЗ волны переход к кинематическому режиму рассеяния не наблюдался, несмотря на большие динамические напряжения кристаллической решетки. Это может быть связано с образованием сверхрешетки с периодом стоячей звуковой волны. При больших амплитудах УЗ волны осцилляции интенсивности разрушались. Происходила фокусировка, т.е. резкое сужение и рост интенсивности дифракции в центре пространственного профиля [1]

3) Наблюдалось УЗ разрушение экстинкционных биений Соменкова-Шильштейна уже при небольших амплитудах УЗ. Этот эффект аналогичен подавлению эффекта Бормана в условиях рентген - акустического резонанса [2].

4) В отличие от совершенного кристалла, где с ростом амплитуды ультразвуковой волны наблюдается рост интенсивности дифракции, в изогнутом кремнии интенсивность дифракции резко падает уже при небольших напряжениях на пьезопреобразователе. В деформированном (изогнутом) кристалле при частотах УЗ, превышающих резонансную частоту, наблюдается так называемый “ деформационный” Pendellosung, т.е. осциллирующая зависимость относительной величины спада интенсивности пучка нейтронов от градиента деформации, которая не обнаруживается при резонансных частотах. Экспериментальные результаты находятся в хорошем согласии с теоретическими расчетами.

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SMALL-ANGLE SCATTERING TECHNIQUES APPLIED FOR ME'S AND MRE'S INVESTIGATIONS

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Magnetic and magnetorheological elastomers (ME's and MRE's) make specific classes of smart substances responding in a complicated way to the changes of external conditions. These composites are soft elastomer matrices filled with nano- (ME's) or microparticles (MRE's) of ferromagnets, respectively. Both types of the materials are quite new, and the work on understanding their properties in dependence on the synthesis processes, composition, mechanical and magnetic fields, etc. is nowadays extensively progressing with regard to their nano- or microtechnology prospects.

In the literature one can find quite a big number of papers of the reinforcing effect of magnetic fillers, where the problem is approached from the magneto-mechanical side. With the data like that, the conclusions on the microscopic properties are deduced form investigations of the magneto-elastic response of the composites under some conditions. The treatment like that does not help, however, to understand the effects of the interactions between the filler particles and the polymer molecules surrounding them on the submicroscopic, and thus fundamental, length scales. Meanwhile, small angle scattering investigations are perfectly suited for that.

In the present paper we review our results on the microstructure properties of 2 types of elastomeric matrix filled with: (i) a ferrofluid; (ii) iron microparticles and nanoparticles otained by means of small-angle neutron and X-ray scattering (SANS and SAXS).

Keywords: magnetic elastomers, magnetoreologic elastomers, SANS, SAXS

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Study bilayer systems Ti/TiO2 deposited by magnetron sputtering

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Thin Ti films are widely used in microelectronics, in optics, in technology of corrosion preventing coating at present [1, 2]. For example, it is hard to overestimate their role in neutron optics. Polarizing neutron mirrors are made with a ferromagnetic metal layer (usually FeCo) with a low neutron optical contrast for one of the spin components, which is sputtered onto the substrate. The interaction potentials of a ferromagnetic layer for neutrons in the states with the spin projection “up” V+, i.e. parallel to, and “down” V-, i.e. opposite to the layer induction are V± =Vn±Vm, where Vn and Vm are the nuclear and magnetic potentials, accordingly. The composition of the ferromagnetic layer is chosen such that the potential of interaction for neutrons with spin “down” V- is close to 0. A non-magnetic oxide layer formed in air on the surface of neutron mirror sets up a barrier for neutrons with the spin “down” and significantly decreases the polarizing efficiency for cold and ultra-cold neutrons. The unfavourable effect of oxidation on the efficiency may be reduced to a considerable degree by depositing a thin Ti layer which, due to oxidation in air, forms an antireflection bilayer Ti/TiO2 [3]. The Ti/TiO2 bilayer of thickness 5-10 nm was shown to be efficient for suppression of the reflection of neutrons with the undesired spin. New polarizing coatings with antireflection bilayer may allow creating highly effective polarizing devices even for cold and ultra-cold neutrons.

We have investigated of the oxidation kinetics of Ti films with thickness 5-40 nm and the oxidation stability of the bilayer systems Ti/TiO2. Titanium films were deposited using magnetron sputtering of titanium on glass substrates. The samples were annealed in air at temperatures T=20÷300°C. The thickness and the roughness of Ti and oxide layers were determined by neutron (reflectometer NR-4M, PNPI, Gatchina, Russia and reflectometer REFLEX, JINR, Dubna, Russia) and X-ray reflectometry. The results have shown a high sensitivity of neutron reflectometry to the oxide layer thickness on the surface of Ti films [4-6].

The effective activation energy of oxidation was found to decrease with decreasing thickness of the Ti film deposited. Thinner titanium films were found to be oxidized to a greater depth; yet the metal layer was found to exist even in the thinnest (5 nm) samples. The latter was confirmed by the direct method of measuring the electrical resistance of the films [5, 6]. The kinetics of oxidation of thin Ti films is well described by a logarithmic function. The characteristic growth of the oxide layer at a fixed temperature is indicating the applicability of the known model of Cabrera-Mott [7] for the oxidation of thin Ti films.

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Fusion of DMPC ULVs in presence of the sulfoxides

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Fusion of the membranes plays an important role in physiological processes, such as exocytosis, secretion, formation of secondary lysosomes. In addition, directional cell fusion by various fusion agents in vitro is widely used to solve a number of problems in biomedicine and biotechnology. According to the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory the fusion process of lipid membranes is a result of van der Waals attractive forces and electrostatic repulsive forces. Additionally, the hydrophobic interactions make a significant contribution in balance of the intermebrane interaction at short distances and maintain neighboring vesicles in equilibrium at the distance of ~ 2 nm. Therefore, the reduction of the hydration repulsion leads to the membrane fusion. Indeed, the decreasing of water reduces the repulsion of bound lipid bilayers and induces the steric contact of membranes.
Dimethylsulphoxide (DMSO) is one of the fusion agents. The fusion of the membrane in presence of DMSO is a result of the pore formation, thereby increasing permeability of the membranes, and reduction of the membrane rigidity. However, it should be noted that the DMSO is toxic for living cells. Diethylsulfoxide (DESO) is less toxic than the DMSO and glycerol.
In current work the influence of the DMSO and DESO concentration on the structure of the unilamelar vesicles (ULVs) DMPC was investigation by SANS at IBR-2, Dubna. It was shown that fusion takes place at lower DESO molar concentration than the DMSO.
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COMPARATIVE STUDY OF SOME SOIL SAMPLES BY MEANS OF SMALL ANGLE NEUTRON SCATTERING METHOD

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Small angle neutron scattering investigation on several soil samples results are reported and analyzed.
The present study has been conducted on soil samples from plums orchard of didactical farm V. Adamachi pasture of Breazu (Iasi county, Romania) and Bicaz man-made lake area (Neamt county, in the middle basin of Bistrita river, Oriental Carpathians [470 North latitude, parallel and 260 East longitude meridian] [1].
Due to several factors, i.e. the climate conditions, geological composition, etc., the analyzed soil samples present specific and very different microstructure.

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Status of YuMO small angle neutron scattering spectrometer

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Status of YuMO small angle neutron scattering spectrometer
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Some problems concerning specific features of experimental realization at a small angle neutron scattering (SANS) spectrometer located at the 4-th beam-line of IBR-2 are discussed, including two detectors system, vanadium standard in front of each detector, high flux on a sample, central hole of detectors and geometry of beam line. The scheme of the experiment are described in detail. The main advantages of the existing spectrometer configuration are outlined.
Given the ongoing users policy and constantly increasing demand for this instrument, the emphasis was put on improving the overall functionality of the YUMO spectrometer [1-3]. The main specific characteristic of the YUMO spectrometer is based on its source, the pulse reactor. This allows utilizing a rather wide range of wave lengths (from 0.7Å to 10Å) by using flight-of-time method. The second feature is the two-detector system constructed in Dubna in 2000 and used for SANS experiments. We note that till 2000 such a system for SANS spectrometers has never been used before. Today there are several similar systems using the two-detector concept (e.g., RAL, ILL, Australian neutron reactor). The third feature of the YUMO spectrometer is the direct beam geometry. Such geometry allows obtaining flux comparable with that of the ILL reactor (as far as SANS instruments are concerned) [4]. One more important characteristic of the spectrometer is the usage of a special geometry of the ring-wire proportional He3 gas detectors, namely the central hole in the detectors. This allows implementing the so-called "direct beam detector" concept and which significantly decreases the background contribution. And finally, the YuMO spectrometer contains vanadium standards in front of each detector which periodically “chopper” the direct beam of the neutrons passing through the sample.
The report will focus on the recently realized major changes of the spectrometer as well as on its development related to implementation of the cold moderator. For the latter, some alternative ideas and suggestions will be discussed. It is also important to emphasize that further increase in the number of users on this instrument will require both qualitative and quantitative modifications of the current sample environment.
The perspective of YuMO spectrometer was discussed. In particular, the installation of new type of position sensitive detector (PSD) was considered. The new possibility for users after installation of PSD as well as corresponding changes in SAS programm was suggested.

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Structural factor analysis of small angle X-Ray and neutron scattering curves for apoferritin

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The problem of studying protein molecules in a solution by small-angle scattering is comparatively simple if the protein interaction is not taken into account and the solution is monodisperse. In this case it is possible to solve a structure of an object with a low resolution with the help of ATSAS program package[1].
In this work the comparative analysis of small-angle X-Ray and neutron scattering curves in small angle region for the set of concentrations of a protein apoferritin in a heavy water was done. Measurements were performed at spectrometer Rigaku, MIPT, Dolgoprudny; synchrotron BM-29, ESRF, Grenoble [2] and a small-angle neutron spectrometer YuMO [3,4].
However, the interaction between proteins has been detected even at low concentrations. By the approximation at zero concentration level and obtaining the form-factor the structural factor curve has been obtained. The type of interaction has been defined and the distances between the protein molecules in aggregates have been calculated. The results are being discussed.

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Comparative analysis of small angle X-Ray and neutron scattering curves in absolute units

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Small angle scattering curves analysis is known to be started with calculating invariants. One of the invariants is the intensity at zero value of modulus of a scattering vector q. It can be obtained by the approximation of the small angle scattering curve. Having been gotten the invariant can give additional information either about the concentration of objects being studied, the length scattering density contrast or about the objects volume.
In this work the comparative analysis of small-angle X-Ray and neutron scattering curves in absolute units has been conducted. Such an analysis allows one to estimate real data accuracy for installations: spectrometer Rigaku, MIPT, Dolgoprudny; synchrotron BM-29, ESRF, Grenoble [1] and a small-angle neutron spectrometer YuMO [2, 3].
The set of concentrations of a protein apoferritin in a heavy water has been studied. A vanadium (for neutrons) and water (for X-Ray) normalization has been done. Obtained data has been shown to be in a good agreement with each other. An accuracy of the concentration measurements made with the help of the Nanodrop installation has also been estimated. The small-angle scattering curves have been fitted by the ATSAS program package [4]. A number of parameters have been calculated. The results of the comparative analysis are being discussed.

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Small angle neutron scattering investigation of a concentrated CoFe2O4 ferrofluid sample

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In the present paper results on a new CoFe2O4/lauric acid/DDC-Na/H2O ferrofluid sample investigationed by means of small angle neutron scattering (SANS), high resolution transmission electron microscopy (HRTEM) and selected area electron diffraction (SAED) are presented.
High-resolution TEM (HRTEM) analysis was carried out on a LEO 912 AB OMEGA transmission electron microscope with an accelerating voltage of 120 kV (Advanced Technology Centre, Moscow).
SANS experiments were performed at the time-of-flight YuMO spectrometer in function at the high flux pulse IBR-2 reactor, JINR Dubna.

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Morphological and multifractal investigations on CoFe2O4/DBS-DBS/H2O ferrofluid sample

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In this paper we present preliminary investigations on the granularity properties and the multifractal characteristics of the CoFe2O4 nanoparticles coated with a double layer of dodecylbenzenesulphonic acid and dispersed in double distillated water. The microstructural investigation was carried out using transmission electron microscopy (TEM).
A statistical analysis of the particles diameters is made using the log-normal distribution confirming the diameter mean value previously obtained using the magnetic measurements. The 3-dimensionally reconstructed images show the characteristic morphology of the spatial dispersion of nanoparticles and nanoparticle conglomerates in the liquid suspension. A multifractal analysis of the two TEM images representing portions of the same sample using two different enlargements is made. The multifractal spectra of the studied images reveal universal multifractality.

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Effects of substitution in some bismuth and lead based oxides

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We will report on our recent results on several ABO3, AB2O5 and double perovskites A2BB'O6 containing p elements with lone pair electrons as Pb2+, Bi3+. These cations create irregular oxygen coordination environment of the cations and to stabilize them often requires the use of high pressure or specific soft chemistry.
Studied were the effects of substitution on the magnetoelectric coupling inf the perovskites (Bi1-yRy)1-xAxMnO3 (R = rare earth; A= Ca2+, Sr2+; x,y=0.5) [1], BiFexMn2-xO5 [2], La1-xBiXMn2O5 [3] and the like, the systems Y-Fe-Cr-O [4 and Cu3(Mn4-xFex)O12 (x = 0, 0.5, 1.0), PbLaFe2-xMnxO6 (0<x<1) etc. Ab-initio density functional theory calculations were performed to study the structure, magnetic and optical properties of multiferroic BiFeO3, also modified with La3+ and Mn3+ [5]. Synthesized and characterized were a new bismuth oxide - multiferroic BiFe2O5-δ [6] and RFeMnO5 (R = Tb, Yb) [7,8].

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Развитие нейтрон-дифракционного метода измерения напряжений в массивных образцах большой толщины

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Преимущество нейтронного метода стресс-дифрактометрии связано с высокой проникающей способности нейтронов в большинстве материалов. Это обстоятельство позволяет определять напряжения на глубинах порядка нескольких сантиметров (в стали). В то же время синхротронным методом, даже с использованием высокоэнергетичного излучения, напряжения можно определить на глубине порядка несколько миллиметров (в стали).

Нейтронные методы стресс-дифрактометрии начали развиваться примерно 20 лет назад. За это время был достигнут заметный прогресс в увеличении максимальной глубины проникновения возможной для измерения. Он был связан как с появлением новых, более интенсивных источников нейтронов, так и с использованием фокусирующих монохроматоров из изогнутых совершенных монокристаллов (обычно кремния) и позиционно-чувствительных детекторов, оптимизированных для стресс-дифрактометрии. В результате стало возможным измерить напряжения в стальных пластинах толщиной ~40мм, что соответствует длине пути нейтронов в материале lm~ 60мм. В то же время в атомной энергетике и судостроении имеется потребность в измерении остаточных напряжений в более толстых (~80мм) стальных деталях. Поэтому разработка способов измерения напряжений в стальных деталях толщиной более 40мм является актуальной задачей.

В 2011 году нами был предложен метод увеличения глубины проникновения нейтронов в сталях, основанный на использовании нейтронов с длинами волн соответствующих минимумам полного сечения нейтронов вблизи Брэгговских скачков. Используя нейтроны с длиной волны 2.39А и отражение 110 были измерены напряжения в сварных швах стальных пластин толщиной 50мм.

В развитие вышеуказанного метода был предложен метод измерения напряжений с использованием разных отражений и длин волн нейтронов для измерения разных компонент деформации. Пользуясь данным методом, было проведено измерение остаточных напряжений в сварном шве стальной пластины толщиной 70мм.

При измерении деформаций на больших глубинах в ферритной стали было обнаружено уширение дифракционных пиков с длиной пути нейтронов в материале. Уширение пиков приводит к уменьшению длины пути нейтронов, на которой можно измерить напряжения. Исследования показали, что уширение связано с многократным рефракционным малоугловым рассеянием нейтронов на границах магнитных домен. При приложении к образцу постоянных магнитов с индукцией 0.5Т уширение пиков уменьшается. Таким образом можно ожидать, что проводя измерения в достаточно сильном магнитном поле (>1.5Т) можно дополнительно увеличить длину пути нейтронов, на которой можно измерить напряжения.

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Structure of RecX protein complexes: molecular dynamics simulations and small angle neutron scattering

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Structure of the complexes of E.coli RecX protein with a single-stranded oligonucleotide and with RecA presynaptic filament were investigated by a combination of molecular modeling and SANS. The structures were crated based on the existing X-ray crystallography and electron microscopy data using molecular modeling and molecular dynamics simulations. As a result, we have put forward atomic-scale models of the two complexes of RecX protein which included their dynamics in the aqueous solution and details of the chain interactions and were experimentally verified by a low-resolution technique such as SANS. The models suggest a sandwich-like filament structure of RecX::ssDNA complex formed by pairs of RecX molecules bound to DNA chain, and RecX binding to the groove of RecA::ssDNA filaments at the stoichiometric ratio ca.1:4 that occurs mainly via Coulomb interactions between RecX and ssDNA.

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Shungite in light of neutron scattering

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The performed neutron scattering study turned out to be extremely effective and put the last point in proving the structure and chemical composition of shungite. The reduced graphene oxide (rGO) nature of the basic structural element, its size and chemical composition as well as five-six-layer stacking have received a direct experimental confirmation fully supporting the general concept on the shungite structure as a multi-level fractal structure of nanosize rGO fragments [3]. Both the linear size of individual rGO sheets and the sheet stacks are responsible for the obtained values of the coherent scattering region of 1.5-3 nm. The stacks of such dimension form globules of ~6 nm in size (the third level of structure) while the latter produce agglomerates of 20 nm and more (the forth level of structure) completing the fractal packing of shungite. The basic rGO fragments are hard reduced products of stable chemical composition described by 11:1:3 (C:O:H) atom content ratio due to which shungite deposits of Karelia present a natural pantry of highly important raw material for the modern graphene technologies.

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Методические преимущества реактора ИБР-2 как инструмента для получения фундаментальных знаний

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С 1986 г. на экспериментальных пучках ИБР-2 ведется деятельность в направлении максимального использования уникальных возможностей реактора. Рекордная импульсная мощность, рекордный диапазон скоростей нейтронов, использование холодного замедлителя, позволяющего получить высокое энергетическое разрешение при сохранении секундной экспозиции за счет многократного увеличения интенсивности нейтронов в области разрежения дифракционных пиков; возможность одновременной регистрации с секундной экспозицией спектров области больших и малых углов, включая область пропускания прямого пучка, - позволили получить и обобщить информацию фундаментального характера о таких процессах, как катализ, синтез, плавление, равновесные и неравновесные фазовые переходы в широком классе материалов [1-10]. Дальнейшее продвижение методики связано с идеей сокращения до 300 микросекунд временного интервала слежения за процессом в режиме набора спектров рассеяния за один импульс реактора [11] и уже протестировано экспериментально [12, 13].

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