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CONDENSED MATTER PHYSICS

The main objectives of research in the framework of the theme involved the application of neutron scattering techniques and complementary methods to investigate the structure, dynamics and microscopic properties of nanosystems and novel materials, which are of great importance for the development of nanotechnologies in the fields of electronics, pharmacology, medicine, chemistry, modern condensed matter physics and interdisciplinary sciences. In the first half of 2011 during the physical start-up of the IBR-2 reactor, the experimental activities conducted by the personnel of the FLNP Department of Neutron Investigations of Condensed Matter (NICM) were carried out in neutron and synchrotron centers in Russia and abroad. These activities were performed in accordance with the Topical Plan for JINR Research and International Cooperation under the existing cooperation agreements and accepted beam time application proposals. In the second half of 2011 during the power start-up of the reactor the first instrument-development and experimental activities were started on the IBR-2 spectrometers. The activities on the IBR-2 reactor were carried out in accordance with the modernization program plan for the spectrometers. Most attention was given to the realization of the top priority projects (construction of the new DN-6 diffractometer for studying microsamples, multipurpose GRAINS reflectometer and modernization of the SKAT/EPSILON spectrometers for geophysical research).

Within the framework of investigations under the theme, the employees of the NICM Department maintained broad cooperation with many scientific organizations in Russia and abroad. The cooperation, as a rule, was documented by joint protocols or agreements. In Russia, especially active collaboration was with the thematically close organizations, such as RRC KI, PNPI, MSU, IMP, ISSP RAS, IC RAS, and others.

A list of the main scientific topics studied by the employees of the NICM Department includes:

- Investigation of structure and properties of novel crystal materials and nanosystems by neutron diffraction;
- Investigation of magnetic colloidal systems in bulk and at interfaces;
- Investigation of structure of carbon nanomaterials;
- Magnetism of layered nanostructures;
- Investigation of nano-scale structure and functional characteristics of biological, colloidal and polymeric nanodispersed materials;
- Investigation of nanostructure and properties of lipid membranes and lipid complexes;
- Investigation of atomic dynamics of nanosystems and materials by neutron inelastic scattering;
- Investigation of texture and properties of minerals and rocks;
- Analysis of internal stresses in bulky materials and factory-made goods.

1. Scientific results

1.1. Structure investigations of novel oxide materials

Using neutron diffraction the structural disorder effects have been studied in the samples of fine-grained HTSCs $YBa_2Cu_3O_y$ with various average grain sizes $\langle D \rangle$ in the range of 0.4–2 μm and the oxygen content $y = 6.93 \pm 0.03$, having approximately similar $T_c \approx 92$ K [1]. It has been found that with a decrease in the grain sizes (i.e. an increase in the degree of non-equilibrium in the synthesis conditions) the oxygen content in the O(5) site increases several times as compared to the

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equilibrium coarse-grained state (**Fig. 1**). The obtained results have made it possible to explain the unusual physical properties of fine-grained $YBa_2Cu_3O_y$, in particular, the effect of coexistence of high values of superconducting transition temperatures T_C and significantly low values of magnetization in strong magnetic fields at $T < T_C$. It has been shown that in the fine-grained $YBa_2Cu_3O_y$ samples with the optimum oxygen content the nano-scale structural inhomogeneity takes place leading to the changes in the fundamental superconducting parameters – magnetic penetration depth and coherence length.

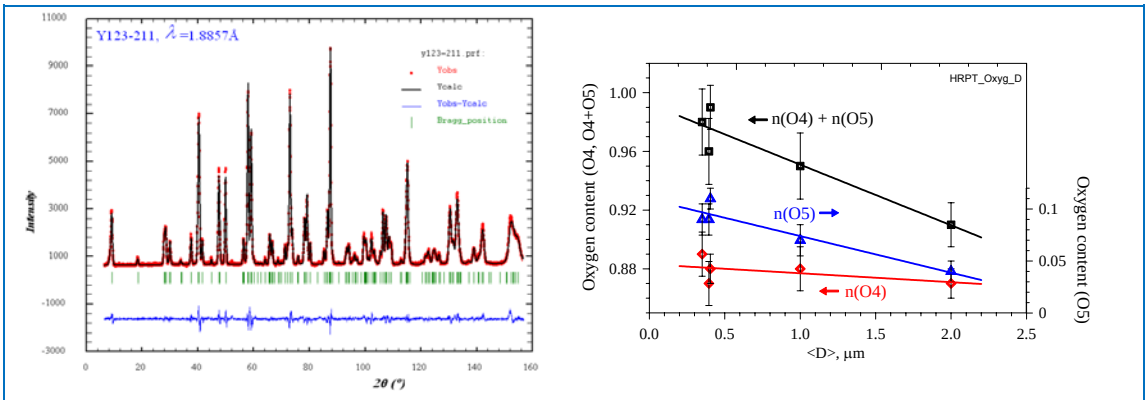

Fig. 1. Left: diffraction spectrum of $YBa_2Cu_3O_y$ sample (annealed at 930 °C with an average crystallite size <D> = 2 μm) obtained on HRPT (PSI, Switzerland) and treated by the Rietveld method. Right: site occupation factors for O(4) (left scale), O(5) (right scale) and their sum (left scale) as a function of the average crystallite size. Statistical errors of the points are indicated. Lines are drawn by the least squares method. Points for samples №1 and №1b are spaced ±0.005 μm apart on the *x*-axis for the sake of illustration.

In multiferroic $BiFeO_3$ a structural phase transition from the rhombohedral *R*3*c* (ferroelectric) phase to the orthorhombic *Pbam* (antiferroelectric*)* phase has been revealed at high pressures *P* ~ 3 GPa (**Fig. 2**). As a result of this structural phase transition the character of the antiferromagnetic order of Fe magnetic moments changes from a noncollinear (propagation vector $k = (\delta,\delta,0)$, δ~0.004)

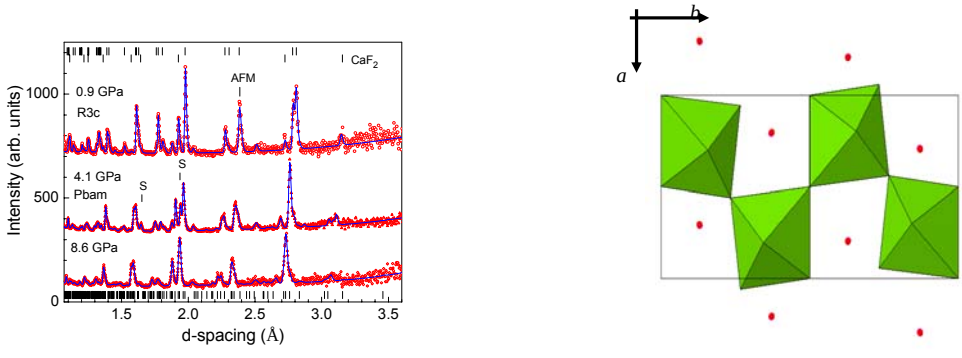

Fig. 2. Left: Neutron diffraction spectra of $BiFeO_3$ obtained at various pressures on the Pearl/HiPR diffractometer (ISIS, RAL, UK) and treated by the Rietveld method. Right: crystal structure of the orthorhombic antiferroelectric high-pressure phase of $BiFeO_3$.

to a collinear one ($\delta \sim 0.0$) [2]. On the basis of the obtained experimental data the predictions of the theory describing the magnetoelectric coupling effect in $BiFeO_3$ have been tested.

The crystal structure of crystal phosphors $Y_3Al_5O_{12}:Ce^{3+}/Lu_2O_3(Lu_2O_3:Ce)$ produced by the colloid-chemical method and the influence of the way of introduction of Lu_2O_3 into the system on the structure and spectral-luminescent properties of the samples have been studied at room temperature using the neutron diffraction technique. The study has demonstrated that in the spectra of the samples obtained under the most nonequilibrium conditions a Stokes shift and high intensity of photoluminescence are observed, which is caused by the disorder of their crystal structure due to the formation of stable associate-defects.

1.2. Investigations of magnetic fluids and nanoparticles

In the framework of the research of nanoparticles for biomedical applications the powders of magnetic nanoparticles coated with block-copolymers (based on substituted pyrrols for increasing biocompatibility) have been studied by means of small-angle neutron scattering [3]. It has been found that the structure of the formed precipitate depends strongly on the type of the stabilizing shell in the initial magnetic fluid (**Fig. 3**).

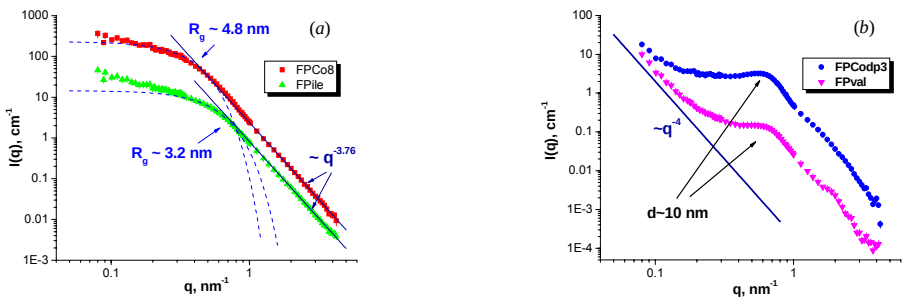

Fig. 3. SANS curves of magnetic particles coated with the polymers based on substituted polypyrrols (obtained in BNC, Budapest). Water-based magnetic fluids stabilized with DBSA (*a*) and LA (*b*) are used as a source of nanoparticles. The solid lines show the Porod law. The dashed lines in (*a*) denote the Guinier approximation with the indication of the respective radii of gyration. The arrows in (*b*) point to the peaks corresponding to the quasi-crystalline order in the aggregation complexes with the correlation length $d \sim 10$ nm. For the sake of illustration the curves for the samples FPile and FPval are divided by 5.

For the systems initially stabilized with dodecylbenzenesulphonic acid (DBSA) the scattering in the final samples comes from separate polydisperse particles with irregular surface. For the systems with the initial stabilization by means of lauric acid (LA) the experimental curves are additionally modulated by the scattering from a quasi-crystalline structure with the characteristic correlation length of 10 nm. The differences in the structural organization of the studied powders are explained by a different rate of the polymeric coating of magnetic nanoparticles, which is determined by the adsorption properties of surfactants in the magnetic fluids in respect to particle surface. The study has been performed in cooperation with the Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences (Hungary), National Institute for Research and Development of Isotopic and Molecular Technologies (Romania), Center for Fundamental and Advanced Technical Research of the Romanian Academy, Timisoara Branch (Romania) and the Faculty of Physics of the National Taras Shevchenko University of Kyiv.

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The water-based magnetic fluids with cobalt ferrite particles (volume concentration of 0.2%) have been investigated using the μSR-method. As compared to the earlier obtained results, the muon spin relaxation rate is much higher in the ferrofluid with magnetite particles with the volume concentration of 4% than in water, in contrast to the recent studies with the samples with cobalt ferrite particles, where this effect was not observed. This may be connected with the sensitivity threshold of the method for small concentrations of magnetic substance in the sample.

The investigation of biogenic ferrihydrite nanoparticles produced by bacteria *Klebsiella oxytoca* has been continued. The ultrasound-treated diluted samples of water suspensions of biogenic nanoparticles have been studied by the SAXS technique. It has been found that the nanoparticles have an elongated shape with the radius of gyration of 6.73±0.16 nm. The results obtained with the ultrasound-treated samples are close to the structural parameters determined earlier (using SAXS, high-resolution electron microscopy and magnetic granulometry) with the concentrated samples. This fact allows us to suggest that the ultrasound treatment does not affect the physical and chemical properties of the particles and only helps to minimize the effect of aggregation.

1.3. Investigations of carbon nanomaterials

The complex investigations of the solution C_{60}/N-methyl-2-pyrrolidone (NMP) and its mixtures with the solvents of various polarities have been carried out using small-angle neutron scattering, UV-Vis spectroscopy and mass-spectrometry [4]. It has been shown that the main contribution to the temporal solvatochromism in C_{60}/NMP (change in the absorption spectrum with the solution age) is determined by the variation of donor-acceptor complexes between fullerene and solvent molecules with time. Nevertheless, the formation of fullerene clusters in the given system with time is reflected indirectly in solvatochromism and other effects. In particular, it influences the content of residual NMP in the precipitate obtained by the evaporation of the solution at different stages of its evolution after the preparation.

The comparison of the reaction of the system C_{60}/NMP on the addition of toluene (low-polarity solvent) and water (high-polarity solvent) has been made employing the fact that NMP is fully miscible with the solvents of both types. It has been found that a partial dissolution of the initial clusters (size up to 500 nm) takes place at the volume fraction of the additive above 40 %. In particular, the effect manifests itself in a sharp increase of small-angle neutron scattering, which points to the appearance of the clusters with sizes in the interval of 10-100 nm (**Fig. 4**).

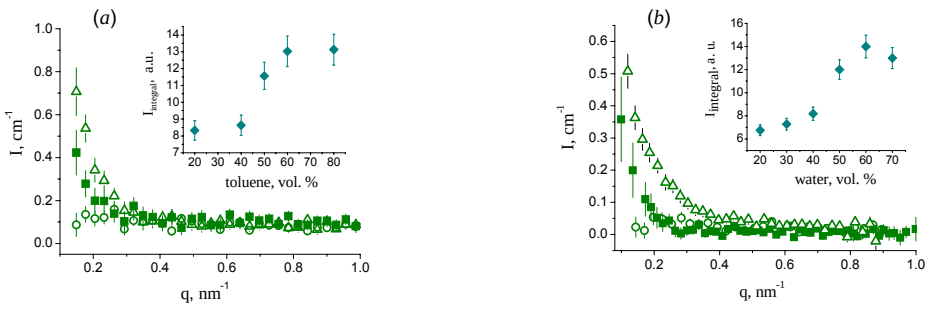

Fig.4. Experimental SANS curves on the systems C_{60}/NMP/toluene (*a*) and C_{60}/NMP/water (*b*) at different contents of the third component in the solution (measurements at BNC, Budapest). The curves are reduced to one fullerene concentration. The insets show dependences of the integral scattered intensity (calculated over a *q*-interval of 0.1-0.5 nm^{-1}) on the volume fraction of the third component in the mixture.

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It has been shown that the point of reorganization does not depend on the solvent type, so the observed solvatochromic effects (change in the absorption spectra when varying the solvent content) again depend indirectly on the reorganization of the cluster state. A thorough investigation and a comparison of all possible solvatochromic effects observed on the addition of the solvents of two types have been carried out. It has been demonstrated that along with the shifts of the characteristic peaks in equilibrium solutions, their appearance and disappearance exhibit a complicated dependence on a number of factors including the volume fraction of the added solvent, the sequence of the mixture preparation and the age of the initial solution C_{60}/NMP.

The theoretical description of the kinetics of the cluster growth in C_{60}/NMP has been proposed. The developed model takes into account the processes of fullerene dissolution, the formation of C_{60} complexes with the molecules of the solute (NMP), as well as a slow growth of clusters from new complexes. For 'freely' dissolved C_{60} molecules the solution is under saturation, so there is no cluster formation. The model corresponds to the experimental observations: the cluster formation is possible over a wide concentration range; there are no free C_{60} molecules at the final stages of the system evolution; a wide distribution of large clusters is realized. The various regimes of the system behavior for different ranges of the model parameter values have been considered. A method for estimating these parameters based on the comparison with the experimental data on the extraction of C_{60} monomers into hexane from the C_{60}/NMP solution has been proposed. The study has been carried out in cooperation with the Faculty of Physics of the National Taras Shevchenko University of Kyiv and the Institute of Surface Chemistry of the National Academy of Sciences (Ukraine), the Faculty of Chemistry of MSU (Russia), the Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences (Hungary).

The theoretical and experimental studies of the kinetics of vitrification continued [5]. The dependences of thermodynamic parameters of glasses on the cooling and heating rates have been investigated. It has been shown that within the framework of the model developed in the approach, the Prigogine-Defay ratio (P) can be greater than unity (which is consistent with the experiment). The estimated values of P for typical glass-forming substances have been determined. The calculations have been made and the polystyrene heat capacity (C_p) curves have been obtained using fast differential scanning calorimetry. The study has been performed in cooperation with the University of Rostock (Germany).

The structure (level of 1÷100 nm) of aqueous dispersions of detonation nanodiamonds (DND) obtained in different conditions has been studied by means of small-angle neutron scattering [6]. As in the previous research a strong clusterization in the solutions has been observed. The characteristic cluster size (from 40 nm and higher) depends on the modification of the dispersions. At the same time, the cluster fractal dimension lies within 2.3-2.4 for different systems, which is indicative of some common clusterization mechanism. Using the contrast variation the existence of non-diamond component in the composition of colloidal particles in the dispersions has been testified, which correlates with the presence of the graphene layer on the crystallite surface. The study has been carried out in cooperation with the Institute of Geology, Karelian Research Center of RAS (Petrozavodsk, Russia), the Research Center in Geesthacht of the Helmholtz Association (Germany), the Fraunhofer Institute for Non-Destructive Testing (Dresden, Germany).

1.4. Investigations of magnetic layered nanostructures

The phenomenon of neutron magnetic resonance in neutron reflection from a 0.5μm-thick permalloy film (80%Ni+20%Fe) has been studied [7]. A static magnetic field of 20 Oe and an oscillating magnetic field of 10 Oe perpendicular to it were applied to the film in its plane. At a

frequency of the oscillating magnetic field of 26.2 MHz the intensity of the specularly reflected neutron beam decreased and off-specular reflection appeared (**Fig. 5**).

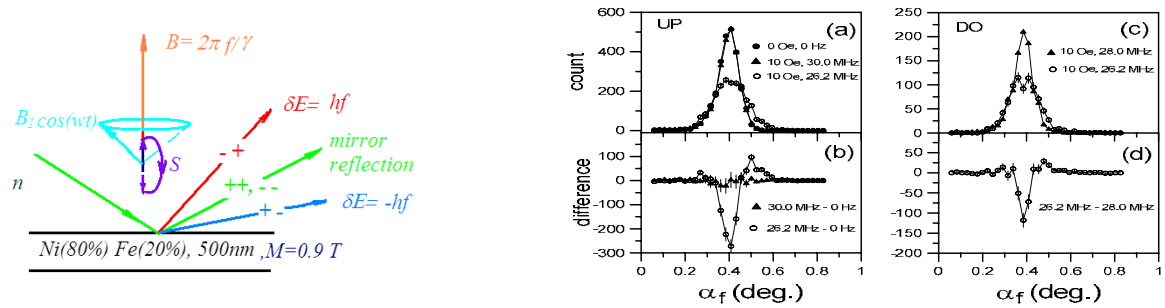

Fig. 5. Left: the layout of the experiment on the observation of neutron magnetic resonance. Right: the intensity of reflected neutrons depending on the scattering angle without an oscillating magnetic field and with an oscillating magnetic field of different frequency and corresponding difference spectra showing the appearance of off-specular reflection for spin-up neutrons (left) and spin-down neutrons (right) under the applied oscillating magnetic field with a resonance frequency (26.2 MHz).

Resonance, as is well-known, occurs when the frequency of an oscillating magnetic field coincides with the frequency of precession of the neutron magnetic moment (neutron spin) around the magnetic induction vector. The induction value of 0.899 T corresponds to the frequency of 26.2 MHz. The magnetometric measurements have demonstrated that this induction value corresponds to the saturation induction, which exists in domains. Thus, it has also been shown that by means of neutron scattering it is possible to simultaneously measure the average value of the induction vector determined by the angular distribution of its direction in domains and the saturation induction.

It has been demonstrated that in non-coplanar layered magnetic structures used for the development of principally new elements of nanoelectronics in the presence of absorption or scattering of neutrons there exists a left-right asymmetry of nonpolarized neutron transmission [8]. This phenomenon is an indication of the structure with rough interfaces and can be used for determination of the degree of its imperfection.

1.5. Investigations of biological nanosystems, lipid membranes and lipid complexes

The ultrastructure of the inner mitochondrial membrane and the formation of supercomplexes of oxidative phosphorylation enzymes in it, as well as the influence of the tonicity of the incubation medium have been studied [9]. The search for supercomplexes and the conditions of their formation from oxidative phosphorylation enzymes (ATP-synthetase, respiratory chain enzymes, nucleotide translocator) has been conducted using the double inhibitor titration (DIT) technique. The formation of enzyme complexes in mitochondria has been detected.

Aqueous suspensions of multilamellar vesicles (MLVs) of the membranes based on ceramide-6 modeling the lipid component in the mucous membranes of the oral cavity of mammals have been investigated by means of X-ray diffraction at the DIKSI station of the Kurchatov Center for Synchrotron Radiation and Nanotechnology, National Research Center «Kurchatov Institute» (**Fig. 6**). In the previous experiments it has been found that in the Cer6/Chol/PA/CholS/PL systems at a temperature of 80 °C the inverse hexagonal phase H_{II} is observed simultaneously with the lamellar liquid crystal phase. To determine the effect of the hydrocarbon chain length on the parameter of the inverse hexagonal phase H_{II}, the MLVs of the Cer6/Chol/FA/CholS/PL membrane have been studied with the same component ratio (28/23/15/8/26, w/w) but with different fatty acids: FA=PA (C16:0), AA (C20:0),

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BA (C22:0), LA (C24:0) and CA (C26:0). Water solutions of the MLVs of the Cer6/Chol/FA/CholS/PL membranes in the medium with pH=5.8 (deionized water) and 8.4 (20 mM Tris-base + 100 mM NaCl) have been measured in the temperature range of 20 - 90 °C.

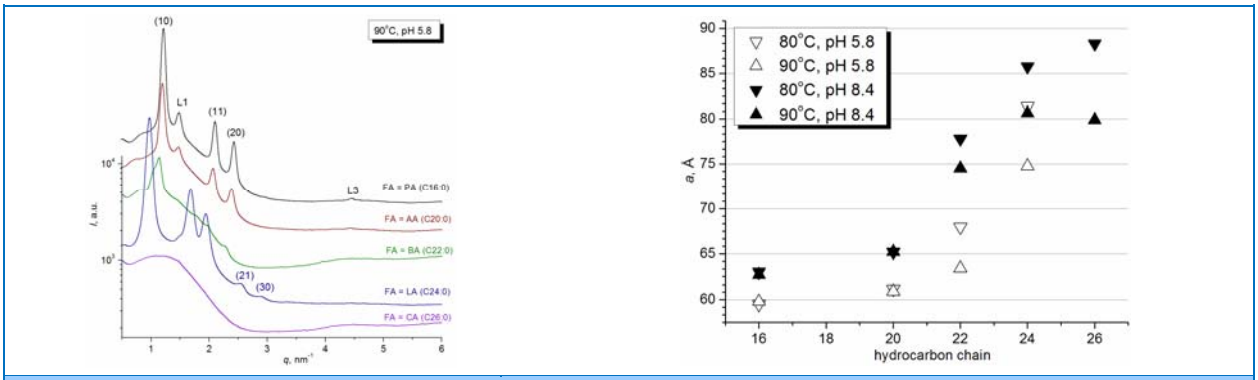

Fig. 6. Left: diffraction spectra of the CER6/Chol/FA/CholS/PL2 membranes with the component ratio 28/23/15/8/26 at 90 °C and pH 5.8. Right: lattice parameter a of the inverse hexagonal phase H_{II} of membranes Cer6/Chol/FA/CholS/PL = 28/23/15/8/26 (w/w) at 80 and 90 °C and pH 5.8 and 8.4 depending on the length of the hydrocarbon chain of the fatty acid FA.

It has been found that the parameter of the phase H_{II} ,*a*, increases proportionally to the length of the hydrocarbon chain of the fatty acid, the increase in the medium acidity from pH 5.8 to 8.4 results in the increase of the *a* parameter for all membranes with individual fatty acids.

Abbreviations: SM – sphingomyelin, DPPE – dipalmitoylphosphatidylethanolamine, DPPC – dipalmitoylphosphatidylcholine, PL = DPPE/DPPC/SM = 1/2/1 (m/m), Cer6 – ceramide-6, PA – palmitic acid (C16:0), AA – arachic acid (C20:0), BA – behenic acid (C22:0), LA – lignoceric acid (C24:0), CA – cerotic acid (C26:0), FA – fatty acid, Chol – cholesterol, CholS – cholesterol sulphate.

1.6. Investigations of polymer and colloidal nanosystems

The localization of the terminal groups in organosilicon dendrimers with fluorocarbon substituents at the silicon atoms in the surface layer of the molecular structure has been studied. It has been shown that there is no polydispersity in the sizes in the samples under study and identity in the scattering amplitude density distribution. The analysis of the dependence of the invariants on the contrast has demonstrated that in a wide range of contrasts the dependence has no strongly pronounced square-law character, which in its turn proves that fluorocarbon terminal groups are localized not only at the peripheral part of the macromolecule. With the application of the Monte-Carlo method and the search for a global minimum for initial determination of the structure with low resolution using the data on the small-angle X-ray scattering from the solutions of organosilicon dendrimers *G7.5(F)*, the calculation of the model of localization of fluorocarbon terminal groups of organosilicon dendrimers has been performed.

Structural peculiarities of an ensemble of nanoparticles from a ferrofluid, which are distributed in a silicone rubber polymer matrix have been investigated depending on the preparation conditions by small-angle neutron scattering [10]. It has been found that in the absence of an external field the organization of particles (geometry and cluster sizes) is entirely determined by dipole forces between the particles. Clusters with a closed magnetic flux (rings of particles, other structures with opposite magnetic moments of particles) are the most stable, because the condition of the free-energy minimum (total energy of magnetic and van der Waals interactions between particles) is fulfilled for

them. An external field orients the magnetic moments of particles thus inhibiting the growth of clusters with a closed magnetic flux. The competition between the orienting action of an external field and the opposite tendency of dipole fields of particles results in the weakening of the initial short-range magnetic order. As the field, which to a great extent aligns the moments, reaches some critical value B ~ 1 kG, linear clusters (like the chains of particles stretched along the field) start to prevail, which has been repeatedly observed in the magnetization of ferrofluids.

1.7. Atomic and molecular dynamics

The phonon spectra of lanthanum cobaltite $LaCoO_3$ have been studied in the temperature range of 4-120 K using the inelastic neutron scattering technique [11]. First-principles quantum-chemical calculations of the phonon spectrum have been performed to analyze the experimental data. Good agreement has been obtained for the calculated and experimental values of the frequencies of the phonon modes. The behavior of the phonon state density in the spin transition region has been studied (**Fig. 7**).

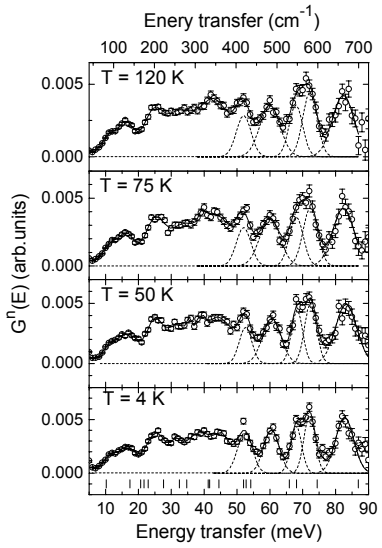

Fig. 7. Inelastic neutron scattering spectra of $LaCoO_3$ obtained at the initial neutron energy E_0 = 110 MeV at different temperatures. The vertical lines below correspond to the energy values of phonon modes calculated using the density functional theory.

The anomalies in the temperature dependences of the frequencies of the optical phonon modes have been revealed in the spin transition region.

The crystal structure and vibrational spectra of various isomers of dimethylpyridine $NC_5H_3(CH_3)_2$ have been studied by means of neutron diffraction and inelastic neutron scattering. In the vibrational spectra the lattice modes have been revealed, as well as the torsional and bending vibrations of the methyl groups connected with the pyridine ring in various positions. First-principles quantum-chemical calculations for isolated molecules, dimers and trimers linked by C-H…N interactions have been performed to analyze the vibrational spectra (**Fig. 8**).

On the basis of the experimental data obtained at the DIN-2PI spectrometer the frequency spectra of uranium mononitride (UN) (nuclear fuel for reactors) have been determined and used for calculating its thermodynamic parameters. The obtained temperature dependences of heat capacity, enthalpy and entropy of UN in the temperature range from 293 to 1400 K have been compared with the macroscopic experimental data. Good agreement between the calculations and the experiment has been observed [12].

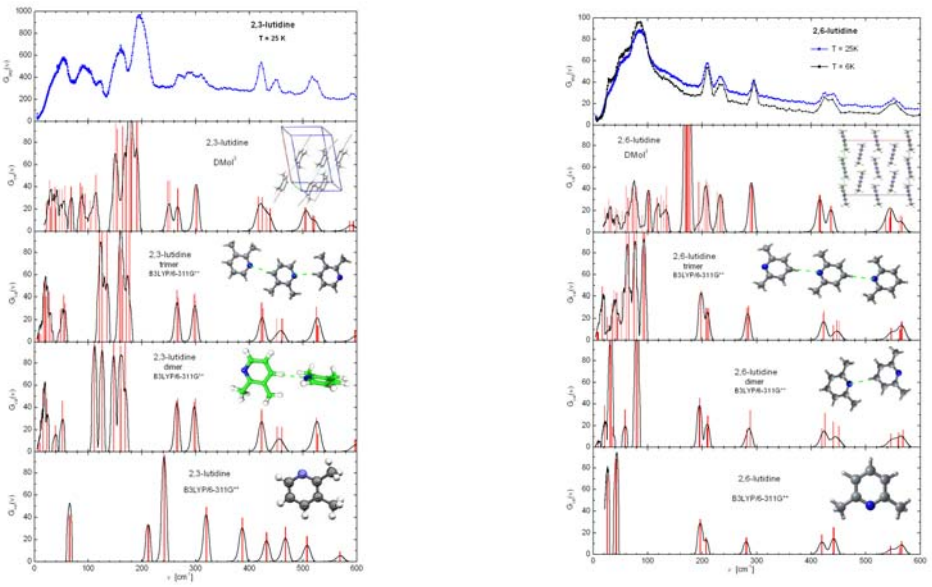

Fig. 8. The experimental and calculated spectra of inelastic incoherent neutron scattering for isomers of 2,3-dimethylpyridine and 2,6-dimethylpyridine obtained when studied isolated molecules, dimers and trimers linked by C-H…N interactions as well as their periodic arrangement in a crystal.

1.8. Applied research

Among traditional applied investigations in the Department of Neutron Investigations of Condensed Matter are the experimental studies of internal stresses and texture of rocks and minerals, determination of internal stresses in bulk materials and products, including engineering materials and components of machines and devices. For the most part, these investigations are carried out using neutron diffraction.

In cooperation with the University of Kiel (Germany) the comparison of the results of the neutron diffraction texture analysis and laboratory acoustic measurements with the seismic borehole logging data has been continued for the biotite gneiss samples from the research Outokumpu borehole (Finland) (**Fig. 9**).

It has been suggested that the reason for the increased seismic reflection zones on the contacts between biotite gneisses and pegmatic granites found at a depth of 1500 m is the preferred orientation of biotite grains in biotite gneisses and the microstructural peculiarities of the latter (foliation). Texture measurements at the modified SKAT diffractometer (FLNP) with a larger series of samples including those from the increased seismic reflection zones of the Outokumpu borehole will help to support this suggestion.

The experiments to study the microstructure of a single crystal turbine blade made of heat-resistant nickel alloy ZhS-32 have been carried out (**Fig. 10**). Single crystal turbine blades of various materials are used in the aircraft engines produced by the NPO “Saturn” (Rybinsk, Russia). The prototype of a turbine blade was studied at the FSD diffractometer of the IBR-2 reactor and the radiography station of the IR-8 reactor in NRC KI. A rather complex topology of the diffraction-peak regions and the presence of a "parasitic" single crystal grain outcropping at the blade surface with

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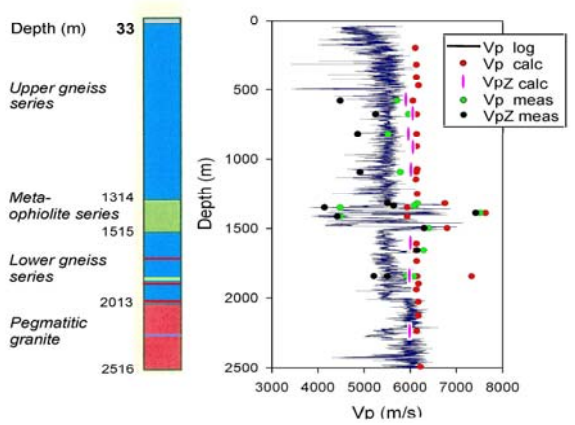


Fig. 9. The comparison of the results of the neutron diffraction texture analysis and laboratory acoustic measurements with the seismic borehole logging data for the biotite gneiss samples from the research Outokumpu borehole (Finland). The velocities of longitudinal elastic waves V_{pZ} along the borehole axis calculated using the neutron diffraction texture data are in satisfactory agreement with the velocities V_{plog} measured in the borehole.

different (compared to the basic matrix) orientation have been revealed. The obtained diffraction data are in good agreement with the results of neutron radiography and topography performed in NRC KI.

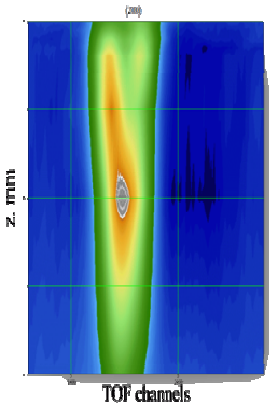
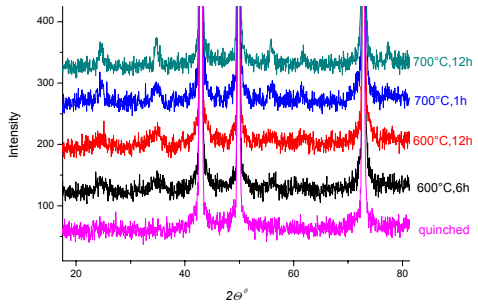


Fig. 10. Left: a turbine blade fixed on the goniometer of the FSD diffractometer for the experiment on the analysis of its microstructure. Right: 2D cross-section of the region of the diffraction peak (200) revealing its complex topology. In particular, the presence of a grain with different (compared to the basic matrix) orientation can be seen.

The measurements of microstresses and the kinetics of Ni_3Ti-phase precipitation in the model FCC alloy H26X5T3 with 3 wt% of Ti have been carried out. The alloy samples quenched and annealed at different temperatures and for different periods of time have been studied. The analysis of the diffraction spectra has made it possible to reveal a clear correlation between the formation of the Ni_3Ti intermetallic phase and the time and temperature of annealing (**Fig. 11**). It is significant that with increasing temperature and time of annealing the intensity of the spread-out peaks of the Ni_3Ti phase grows and the peaks become narrower.

The measurements of the local structure in the cross sections of a number of samples of magnesium alloy MA21 (Mg-4.5%Al-1%Zn) have been carried out within the framework of the studies of properties of the materials produced by the intensive plastic deformation method using the equal channel angular extrusion (ECAE) technology. This deformation method is known as a technique for

Fig. 11. Neutron diffraction spectra of the H26X5T3 alloy quenched and annealed at different temperatures and for different periods of time. Apart from the peaks from the main FCC phase, we can see the diffraction peaks from the Ni_3Ti γ'-phase. As the temperature and time of annealing increase, the intensity of the peaks of the second phase grows and the peaks become narrower.



producing structures with submicrocrystalline and nanometer grain sizes. The measurements were conducted using synchrotron radiation diffraction on beam W2 in the DESY research center. The pole figures obtained from a set of experimental Laue patterns for the sample with an initial texture and samples with a structure formed as a result of one and two passes through the equipment by routes A and C are in qualitatively good agreement with the corresponding pole figures measured earlier by the neutron diffraction method for the same magnesium samples. It is planned to continue the measurements of the local structure for the samples subjected to a greater number of passes and for the samples deformed on route B_c during ECAE. It is also planned to improve the data processing procedure for quantitative comparison of the results from synchrotron and neutron texture experiments.

In cooperation with the Institute of Geology of the Academy of Sciences of the Czech Republic (Prague) the experiments have been conducted to explore the effect of various factors (volume content of mineral, its crystallographic texture, various types of texture) and to study the propagation of elastic waves in model inhomogeneous anisotropic media, specifically the composites of quasi-isotropic (epoxy resin) and anisotropic (powders of crystalline minerals) components. The simulation of the properties of «epoxy resin + mica + quartz» materials with various sizes of muscovite grains has been performed using the combination of geometric averaging and self-consistent approach suggested by Prof. Z. Mattis. In this study we used model axial textures of muscovite obtained by rotation around a crystallographic direction [100] and differing in a portion of chaotically oriented crystallites and texture maximum width. The model angular distributions of longitudinal wave velocities in the materials are in qualitatively good agreement with the results of ultrasonic measurements, however, to perform a quantitative analysis requires precise data on the shape of muscovite grains, which significantly affects the resulting elastic anisotropy.

In collaboration with the Tula State University the experiments on the registration of acoustic emission in the samples of iron-copper composites have been carried out in various modes of uniaxial compression (up to ≈ 260 MPa). During the experiments using the multichannel system Vallen AMSY-5 the basic characteristics of acoustic emission of the samples were determined and the acoustic emission sources were located. According to the neutron diffraction texture analysis data obtained at the SKAT diffractometer the texture of iron and copper components is weak (texture index is 1.03 and 1.14, respectively) and with growing degree of deformation up to 40 % the texture sharpness slightly increases (up to 1.13 and 1.17). The symmetry relation of pole figures for bcc iron and fcc copper follows the Kurdyumov-Sachs rules. As the degree of deformation increases, the size of coherently scattering regions in copper and iron decreases by a factor of 2-3, in the iron component of the composite the residual stresses of the first kind are in the range of 84-132 MPa, in the copper

component the residual stresses of the first kind are in the range of 84-87 MPa. The microdeformations in the iron component of the composite increase ≈ 6 times, in the copper component they grow 6 times at the degree of deformation of 7 %.

2. Instrument development

Since the power start-up of the modernized IBR-2 reactor the spectrometers YuMO, HRFD, REMUR, REFLEX, FSD, DN-12, DIN-2PI have been put into operation after the planned modernization. The first instrument-development and experimental work has been performed at these spectrometers.

Fig. 12. Sections of the mirror vacuum neutron guide installed on beam 6b.

The construction of the new diffractometer DN-6 (beam 6B at the IBR-2 reactor) for studying microsamples has continued. The beam chopper has been installed at its regular place. The manufacturing of mirrors for the tail part of the neutron guide has been completed. The assembling of the tail part of the neutron guide is planned to be completed by the end of 2011 (**Fig. 12**). The manufacturing of the mechanical units of the diffractometer is nearing completion. A gas PSD detector for the DN-6 diffractometer has been designed at the Spectrometers' Complex (SC) Department.

The work on the construction of the new multifunctional reflectometer GRAINS (beam 10 of the IBR-2 reactor) has continued. The background chopper of the drum type (horizontal aperture) has been manufactured and assembled at its regular place in the experimental reactor hall (**Fig. 13**).

Fig. 13. Left: background neutron chopper for the GRAINS reflectometer at its regular place in the IBR-2 experimental hall. Right: beam-forming system of the GRAINS reflectometer in the IBR-2 experimental hall.

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The beam-forming system (including automatic apertures, mirror deflector, mirror polarizer, leading magnetic system) has been assembled at its regular place. The autonomous vacuum system of the reflectometer has been manufactured. The first spin-flipper has been produced. The antivibration platform for the sample table has been purchased. The work on the manufacturing of the platform for the detector unit and of the liquid-containing cell for reflectometry measurements has started.

The modernization of the EPSILON, SKAT and NERA spectrometers has continued. The curved neutron guides for the EPSILON (7A-1) and SKAT (7A-2) spectrometers have been installed and adjusted. The manufacturing of vacuum, positioning and optical elements of the NERA spectrometer is nearing completion. New electronics and PC program control for the positioning system of the crystal analyzers of the NERA spectrometer have been created (in cooperation with the SC Department).

The reconstruction of the head part of the HRFD neutron guide system has been completed. A new collimator-concentrator extracting a neutron beam to the Fourier chopper has been installed in the reactor ring corridor and in the ring corridor wall.

In cooperation with the specialists from the B.P.Konstantinov Petersburg Nuclear Physics Institute of RAS (Gatchina) and the FLNP SC Department the development of algorithms and creation of a pilot prototype of RTOF-analyzer of a new type for list mode registration of all events have continued.

At FSD a mirror furnace controlled by Eurotherm has been put into operation, an order has been placed for manufacturing a new diffractometer table. In cooperation with the employees of the SC Department the old control system for the FSD diffractometer on the basis of Sonix (OS-9) has been changed over to a new one on the basis of Sonix + software package (Windows/PC). At present, the adjustment work is in progress.

The complex modernization of the REFLEX reflectometer (including the start-up of the new control system and data acquisition and accumulation electronics, installation and debugging of the new experiment-control software) has been carried out.

The work on the analytical description of the operation of the spin-echo instrument with rotating magnetic fields has started. The purpose of the work is to determine maximum permissible field rotation frequencies inside a rotator and thicknesses of spin rotators. On the basis of the quantum-mechanical calculation a computer model of a polarized neutron beam passing sequentially through 4 spin rotators with rotating magnetic fields has been constructed. It has been demonstrated that the model adequately describes the state of polarization at the outlet of the rotator system. At present, the optimization of the computer model to reduce the counting time is in progress. The work was conducted in collaboration with the Jülich Research Centre (Germany)

At the small-angle neutron scattering spectrometer the measurements and simulation of neutron spectra from cryogenic and thermal moderators of the IBR-2 reactor have been carried out [13]. Numerical values of spectrum relations with the cold and grooved moderators have been obtained. The advantage of using a grooved moderator at the YuMO spectrometer has been demonstrated. Large losses in the thermal maximum region (more than 10 times for the maximum and 4 times for the working wavelength range) at the same reactor power (consequently, the background component remains unchanged) cannot be compensated by the gain at long wavelengths for the spectrometer having direct visibility of the moderator and using the time-of-flight technique. A degradation of the signal/background ratio becomes critical for the available geometry of the YuMO spectrometer in case of a cold moderator.

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A comparison has been made of the texture measurement results obtained with the texture diffractometer SKAT (FLNP JINR) and the neutron diffractometer HIPPO (Los Alamos, USA). It has been shown that SKAT in comparison with HIPPO has better resolution Δd/d, better angular resolution of pole figures (3-5 ° compared to 10 °, which is important for measurement of sharp crystallographic textures) and provides a possibility to measure samples of large volume. HIPPO has 10 times greater luminosity, which makes it possible to better determine the background and to measure texture of small-volume or weakly scattering samples. For the first time a modified Rietveld method realized in the MAUD program has been applied for analysis of data obtained at the texture diffractometer SKAT. An additional program SKAT2MAUD has been developed. It has been demonstrated that the application of the Rietveld method (MAUD program) simplifies the data treatment for polymineral rocks, and the possibility to use irregular coverage of pole figures allows one to reduce the experiment time by a factor of 4-10.

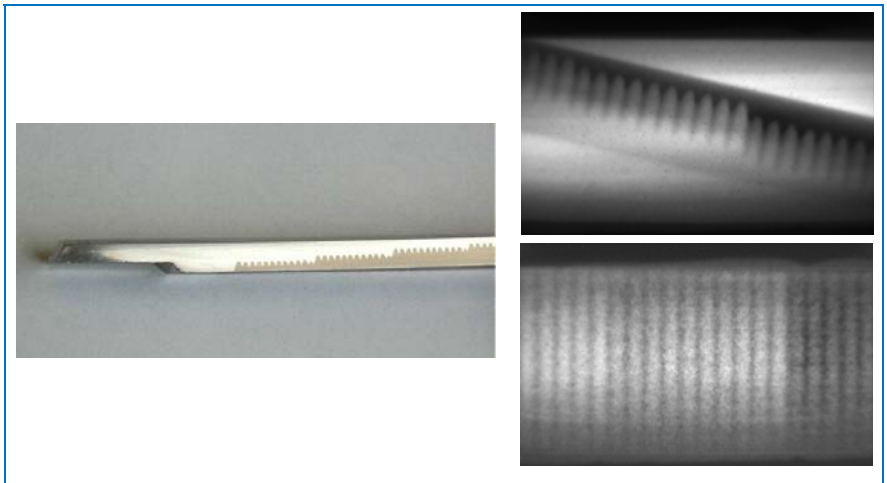

Fig. 14. Photo of bimetallic adapter of the high-power channel-type reactor (left) and neutron radiography images taken in two sample positions (right) obtained on beam 12 of the IBR-2 reactor.

On the DN-12 spectrometer the test experiments on neutron radiography using a CCD-chamber have been carried out. The obtained results (**Fig. 14**) show a high potential for the development of this method on the IBR-2 reactor. A satisfactory image quality can be obtained for a very short time of the order of 10 s.

On the REMUR spectrometer the experimental studies of the possibility to realize small-angle measurements with polarized neutrons using 2D PSD have been carried out. A magnetic mirror was a source of polarized neutrons. At a neutron wavelength of 7 Å the wave-vector transfer reached the minimum value of 2×10^{-3} $Å^{-1}$, and the integral intensity of a neutron flux at the sample position was 10^4 n/s. These parameters of the small-angle mode make it possible to study highly porous systems on the basis of vanadium and titan, which are accumulators of hydrogen and characterized by a large interval of linear pore sizes in the range of 1-1000 nm. It has been shown that on a spectrometer with a focused polarizer of neutrons the realization of wave-vector transfer measurements up to its maximum value of $3Å^{-1}$ is in principle possible, which will allow us to conduct investigations of inhomogeneities on a linear scale of 1 nm.

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