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Poster abstract	Remarks

1. Incorporation of water into citrate shell of Au nanoparticles: neutron reflectometry study

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The assemblies of optically active gold nanoparticles (AuNp) on a functionalized silicon planar substrate were considered in terms of the interface depth density distribution obtained by atomic-force microscopy, X-ray diffraction/reflectometry and neutron reflectometry. Aqueous suspensions of AuNp coated with trisodium citrate were synthesized in light (H_2O) water and mixture of light and heavy (H_2O/D_2O) water using the modified Turkevich protocol [1]. The objective of the work was to verify sensitivity of neutron scattering methods (in particular, neutron reflectometry) to the potential isotope H/D substitution in the stabilizing organic shell around particles in colloidal solutions [2].

First, the isotope effect was studied with respect to the changes in the structural properties of metal particles (size, shape, crystalline morphology) in solutions by electron microscopy including high-resolution transmission electron microscopy from dried systems. Then, neutron reflectometry was applied to the layered nanoparticles anchored on a silicon wafer via 3-aminopropyltriethoxysilane molecules to reveal the presence of deuterated water molecules in the shell presumably formed by citrate molecules around the metallic core [3].

Further, two layers of nanoparticles were sequentially deposited using an additional cross-linking agent. First layer was made of nanoparticles being synthesized in light water while the second one in light/heavy water mixture. The isotope difference in layers observed in the neutron reflectometry experiment was related to water molecules incorporation into the organic shell around nanoparticles. The results are discussed with respect to the possibilities in resolving the structure of complex multilayer assemblies [4].

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

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

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

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

The crystal and magnetic structure of nanostructured manganite $La_{0.53}Sr_{0.47}MnO_3$ has been studied by means of a neutron diffraction method on diffractometer for investigation microsamples DN-12 of high-flux pulsed reactor IBR-2 (FLNP, JINR, Dubna) in wide temperature range 15K - 320K. The sample of polycrystalline ferrite spinel $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ was chosen and performed neutron powder diffraction measurements at ambient and high pressures up to 4.7 GPa temperatures using DN-12 diffractometer of high-flux pulsed reactor IBR-2 using the sapphire anvil high-pressure cell. In additional, for studies the role of structural parameters across the paramagnetic-ferrimagnetic phase transition we had investigate structure and magnetic moments evolution in temperature range 300 - 425 K.

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

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

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3. Nanoporous materials for magnetic and biomedical applications

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Periodic nanoporous silica (PNS) with its perfect regular structure, biocompatibility, thermal stability and durability, and high specific surface is very promising material from the application point of view.

We have prepared series of nanocomposites, where PNS (of two different kind of symmetries) serves as a matrix in which nanoparticles of Gd_2O_3 or Fe_2O_3 are embedded. Such materials have already exhibited extraordinary large magnetocaloric effect [1,2,3,4] and applicability as contrast agents for MRI [5], while their utilization for targeted drug delivery is currently being examined. In this, the detailed information on the structure of as prepared nanocomposites is essential for understanding and tailoring their properties.

We have examined our PNS by means of small angle neutron scattering (SANS) and we proposed theoretical model assuming general features of the inner structure of the composite. By fitting the model to experimental data we are able to obtain information on matrix (size, shape and mutual distance of pores) as well as on size distribution and concentration of nanoparticles embedded in the pores. Hence, the combination of SANS experiments along with our model application appears to be suitable and effective tool for the revelation of inner structure of these kinds of nanocomposites.

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4. Neutron reflectometry modeling of structure in thin films of polystyrene-fullerene nanocomposites

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Thin polymer films have numerous technological applications in various industrial and biomedical sectors related to protective and functional coatings, non-fouling biosurfaces, biocompatibility of medical implants, separations, advanced membranes, microfluidics, sensors, devices, adhesion, lubrication and friction modification[1]. In many cases, the films can be of complex composition with different types of polymers with complex architecture and other components such as nanoparticles. Polymers in thin films and nanocomposite structures can exhibit unusual physical properties due to the geometric constraints imposed by the presence of surfaces and interfaces. Polystyrene-fullerene films present a suitable model system for investigation of these properties. Neutron reflectometry has proved to be an effective method for studying PS/C_{60}, allowing evaluating the structural peculiarities of nanoparticles ordering in the polymer matrix [2].

In this work we model the neutron reflectometry experiments on a thin film of polymer-fullerene nanocomposite. Several physically based models of structural organization of the nanoparticles in polymer matrix are considered – a uniform distribution, a dense substrate layer, a layer on the surface of a polymer. The calculations show that it is possible to apply neutron reflectometry for clarifying the structural organization of nanoparticles in the nanocomposites with the mass concentration of fullerenes exceeding 1%.

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5. Effect of electrochemical cell parameters on the neutron reflectivity experiment

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Nowadays, Li-ion batteries are widely used in different electrical devices such as phones or, even, cars. Lithium is thought to be a good material that can potentially enable the development of batteries possessing extraordinary high specific energy (e.g. lithium-metal-polymer, lithium-air or lithium-sulfur batteries). The development of high-capacity rechargeable and safe metallic lithium negative electrodes for next-generation batteries requires an in-depth understanding of reasons for nonuniform lithium plating and formation of solid electrolyte interface (SEI) during the lithium-metal battery charge. It drives the interest for the tools, enabling efficient monitoring of electrochemical interfaces, where lithium electrodeposition occurs [1,2,3].

The neutron reflectometry (NR) is one of the methods for 'in operando' study of SEI and lithium dendrites formation. The special electrochemical cell is required for such type of experiments [3]. However, there are several requirements to liquid electrolyte and solid electrodes in order to conduct a successful NR experiment.

The aim of this work is to choose optimal parameters of metal electrode and electrolyte for further NR 'in operando' research of lithium electrodeposition. For this purpose NR curves were calculated for various types and thicknesses of metal electrode as well as liquid electrolytes (deuterated/protonated). Thus, the obtained calculations provide a possibility to enhance the sensitivity of the NR technique to interface changes, occurring upon lithium plating.

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6. Fullerenes for medical purposes. From active bioagent (water-soluble) to drug-delivery system with prolonged and selective activity

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Fullerenes due to pleiotropic activity are promising agent for different medical applications. They are used as a separate active component and as a carrier of medications in targeted delivery and/or prolonged therapy. The fullerenes water solutions, which were prepared by extraction from C60/NMP, characterized by the unique small cluster sizes (~ 10 nm) and the acceptable middle size cluster for nanomedicine (~60 nm) of fullerenes that lead to improved biocompatibility of fullerenes. We assume that fullerene interacts with NMP via a charge transfer mechanism. Stabilization of fullerenes in water solutions due H-bonding between water and NMP. The evidence of the type of the molecular interaction we found from the quantum-chemical calculation's results in the density functional theory with long-range separated hybrid functional and subsequent analysis: wave functions, PES, the charge transfer transition density matrix from time dependent DFT calculations of 100 excited states($f>0.001$).

Based on the aqueous dispersions of fullerene, it was designed a number of drug delivery system as fullerenes-polyphenols, fullerenes-alkaloids, polysaccharides-fullerenes. We presented crucial information about each active component of the drug-delivery systems, below in this narrative.

Oxyresveratrol is a polyphenols compound, well-known representative of stilbene, found in the roots, leaves, stem and fruit of many widely distributed plants. It possesses antitumor activity. As a bioactive compound oxyresveratrol has demonstrated strong antioxidant activity, effectively scavenge free radicals. Oxyresveratrol exhibited a wider effective dosage range as an intracellular antioxidant for reducing oxidative stress. The molecules of oxyresveratrol aggregates under the influence of additive fullerene as a result of supramolecular self-organization.

Berberine is alkaloids found in such plants as Berberis. It can reduce the growth and spread of various different types of cancer, and a inhibit cell proliferation and to be cytotoxic towards cancer cells. Nevertheless, the bioavailability of Berberine is low. In this reason, we proposed the fullerenes like a berberine's carrier to improve his bioavailability and selectivity.

Pectins, as a compound, are linear polysaccharides composed primarily of D-galactoronic acids. Pectin has the anti-adhesive apoptosis-promoting, apoptosis -inducing properties and can increase apoptotic responses of tumor cells to chemotherapy. Pectin can increase the bioavailability of the drug in oncology treatment because of similar structure of pectin to glucose, and the increased cancer cellular uptake of glucose on compare to healthy cell. So, if we will proved the existence of pectin's shell around fullerenes in water solutions we can say that we create the carrier-drug systems for active targeting with high selectivity and a wide set of bioactivity.

Small-angle neutron scattering, dynamic light scattering, and UV-Vis spectroscopy investigated the undermentioned systems. In addition, a computer model of carrier-drug interaction was proposed based on quantum chemical calculations.

7. Neutron Scattering Study of Nano-sized Niobium Carbide Powders

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Today, investigation of nonstoichiometry and small particle size impact on a structure of material and therefore on its' properties is a topic of particular interest due to changes in the properties of solids with a decrease in the size of crystallites. However, this field has not been well studied due to high complexity of nanosized, strongly nonstoichiometric compounds production. Basically they are superhard cubic carbides and nitrides of transition metals.

In this work niobium carbide nanosized powders NbC_y with y = 0.77, 0.84 and 0.96 were investigated. NbC is an extremely hard material, commercially used in tool bits for cutting tools. There are several methods for the production of ultrafine particles of different solids. We used high-energy ball milling as it is a simple and effective method that can be exploited in industry. Initial coarse-grained powders were synthesized by high-temperature solid-phase vacuum sintering and than grinded in a planetary ball mill for 5, 10 and 15 hours.

The main method for simultaneous structure and microstructure study in terms of particle size and microstrains is the diffraction of short-wavelenght X-ray or neutron radiation. The experiment was held at High Resolution Fourier Diffractometer (HRFD, IBR 2, JINR, Dubna) with $\Delta d/d \approx 0.001$ that is almost constant in the whole range of d spacing available. To calculate the size of coherent scattering regions and the value of microstrains modified Williamson-Hall method was used.

The analysis of the diffraction reflections profiles revealed the presence of two fractions with different particle sizes. It also showed that microstrains in nanosized powders are strongly anisotropic. It was shown that the hardness of niobium carbide ultrafine powders increases as stoichiometry decreases. The value of microdeformations slightly increases during milling process; the lowest value is being yielded by the most nonstoichiometric sample $NbC_{0.77}$.

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8. Highly Sensitive SERS based on Silver Dendritic Nanostructures

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Surface – Enhanced Raman Scattering (SERS) is a technique developed to detect extremely small quantities of molecules by determining their characteristic Raman signal [1]. However, the adoption of SERS remains limited due to the difficulties in fabrication of effective and affordable nanostructured plasmonic platforms.

At the present time, there are many approaches to the development of various types of plasmonic platforms based on silver nanostructures in different shapes, but still, none of them gave a high sensitivity being affordable at the same time [2]. In the present study an effective and highly sensitive nanostructured plasmonic platform of two different types composed of silver nanoparticles and separate silver dendrites in matrix of silicon dioxide/p-Si templates [3] are provided to application for Surface– Enhanced Raman Scattering.

The SERS measurements have been performed with using DTNB as a model analyte. It has been shown that Ag – dendrites structures in contrast with Ag – nanoparticles templates enable the SERS enhancement signal with a single molecule detection sensitivity at the level of 10^{-15} M. The enhancement factor of silver dendrites nanostructures templates is found to be orders of magnitude larger than that of silver nanoparticles. Evolutions of SERS spectra shows the possibility of detection of ultra-low concentrations of the model DTNB analyte by applying localization silver – dendrites. The results were obtained by SERS technique with laser excitation at wavelength of 633 nm and 785 nm.

Thus, the SERS measurement results indicate the possibility of ultra-low analyte concentration detection, comparable to the concentrations of single molecules. The high sensitivity of the silver dendrites nanostructures is justified by the coexistence of electromagnetic and chemical contributions to the Raman signal amplification.

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9. The Structural Analysis of Particulate - Filled Polymer Nanocomposites by Small-Angle Neutron and X-Ray Scattering Methods

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Polymer nanocomposites are among the promising materials for use in space technology. The ability to create lightweight polymer nanocomposites with high strength and heat resistance, as well as the necessary electrical, optical and other characteristics, makes them suitable for use as both structural and functional materials of spacecraft. One of the main requirements for spacecraft materials is that they maintain their initial parameters during long-term operation in space [1].

Effects of gamma irradiation at different doses up to 500 kGy on HDPE+%ZrO_2 nanocomposite films have been investigated by by small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS).

Small-angle neutron scattering (SANS) measurements were performed at the time-of-flight YuMO spectrometer situated at IBR-2 pulsed reactor, JINR, Dubna, Russia [2]. The investigations by small angle X–ray (SAXS) method were performed on a pinhole camera Molecular Metrology SAXS System at the Institute of Macromolecular Chemistry CAS (Prague, Czech Republic) and on a Rigaku X-ray instrument with high-speed Cu rotating anode (SMAXS 3000 Point SAXS system, at MIPT, Dolgoprudniy, Russia) using a standard transmission configuration [3].

SANS experiments showed ZrO_2 nanoparticles mainly distributed in high-density polyethylene matrix as aggregates system [4]. Small angle neutron scattering (SANS) demonstrated in Guinier region that the internal structure of these aggregates could be characterized by the mass fractal dimensions of 2.1-2.5. Analysis of the SAXS data using Guinier's law revealed that the nanocomposites consisted of particles with a broad distribution of sizes from 41.8 nm to 104.5 nm. Analysis of the experimental data using Porod's law revealed that all the nanocomposite samples formed surface fractal aggregates behaviors.The SAXS results show that γ-irradiation of polyethylene leads to an increase in the content of its crystallites. A significant change was not observed even at irradiation doses of 500 kGy in the structure of the polymer composite.

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

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After discovery of a new allotropic form of carbon – fullerenes, much attention is paid to possibilities of their applications in various fields, including medicine, photoelectronics and optics [1-3]. Despite of a wide application of fullerene solutions, the processes of their aggregation are still not clear in both weakly polar solvents and their mixtures with polar solvents [4]. It is well-known, that the solubility of fullerenes decreases with increasing polarity of the solvent, and the arising clusterization process is critical and reversible [5]. An exception to this rule is the fullerene solutions in nitrogen-containing solvents, like pyridine or N-methyl-2-pyrrolidone (NMP).

NMP is a comparatively good solvent for fullerenes and it is also mixable with water. This solvent is suitable for fullerene transferee into aqueous media that is important for employing biological functionalized fullerenes in medical applications [6].

In the present work, the changes in the cluster state of fullerene C_{70} dissolved in NMP/toluene mixture after toluene addition have been studied. In order to measure the wide range of particle sizes, including sub-single-molecule region and respectively large clusters, the Small-Angle X-ray Scattering, Dynamic Light Scattering were used. The main task was to find out correlation between the fullerene clusterization state and a volume concentration of the second nonpolar solvent. It was observed a common dependence of the structure state of fullerene C_{70} on the polarity of the liquid medium; an increase in toluene content led to further dissolution of existing large agglomerates. The obtained data were analyzed in comparison with the previous results on the inverse colloidal system, C_{70} / toluene / N-methyl-2-pyrrolidone, and with semi-empirical calculations, UV-Vis spectroscopy measurements and experimental measurements on similar solutions based on fullerene C_{60}.

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11. Application of neutron radiography and tomography in studies of cultural heritage objects

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Cultural heritage sites, including archaeological objects, have special value due to their uniqueness and antiquity, being the main source of information about the past of mankind. Therefore, the involvement of modern methods of non-destructive testing for research is the most justified. One of the progressive methods of nondestructive control, for the study of structural features and internal macro-heterogeneity of archaeological objects, is the method of neutron radiography, which is to obtain neutron images of the research objects. The difference in neutron absorption cross sections for different elements allows visualization the internal distribution of inhomogeneities of the materials under study. A particular case of the neutron radiography method is neutron tomography, in which the volumetric model of the studied sample is reconstructed from a set of individual radiographic images obtained at different angular positions of the sample relative to the direction of the neutron beam [1].

It should be noted that, at the present time much attention is paid to the unique research of physical and chemical processes in archaeological remains, associated with the penetration of corrosion or various salts in the thickness of different materials, and the definition of different technologies for the production of human products [2].

The report is devoted to the presentation of the results of studies of archaeological objects, conducted at the facility of neutron radiography and tomography of high-flux pulsed reactor IBR-2 [3]. The possibilities of further application and prospects of these methods are also discussed.

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12. Carbon nanostructures for drug delivery systems

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Chemotherapy for cancer treatment presents many disadvantages such as low therapeutic efficiency and high non-productive drug distribution. With a view to overcoming these significant issues, novel drug delivery systems that exhibit excellent properties for the loading, release, tracking, and targeting of chemotherapeutic drugs, are drawing ever-increasing amounts of interest in cancer diagnosis and treatment. A number of drug delivery systems have been developed whose specific design aid in the targeted delivery of the anticancer agent [1].

Quite an interesting possibility of using nanostructures is the targeted delivery of useful goods (drugs or proteins) using a magnetic field. In this method, the drug or protein is attached by functional groups to the magnetic nanostructure and injected into the circulatory system, and then by means of a magnetic field is transported to the problem area. The presence of a magnetic core in nanostructures allows the creation of nanostructures with homogeneous switching fields, which guarantee the reproducibility of the results. One of the most promising materials for the creation of magnetic nanostructures is iron oxide or iron-nickel alloy.

Nanostructures of magnetic metals for therapeutic purposes are rarely used in pure form. Usually they are encapsulated or placed in bioinert matrices in order to reduce the possible toxic effects of the magnetic phase, increase its physical and chemical stability. In this work, cytotoxicity of synthesized nanostructures was investigated.

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13. NAU (New Activation Unit) – the new regulatory element in *D.melanogaster* genome

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Multicellular organisms consist of different cell types differing in structure and function. The path of development and active genes that will work at a certain point in time largely controlled by various genetic regulatory elements.

Radiation mutagenesis provides a unique opportunity to obtain mutant cells with the entire possible range of changes in the interactions between regulatory elements. The study of such mutants allows to discover new regulatory elements, and creation of molecular genetic constructions containing new elements in model systems allows to describe their properties, nature of interactions and gene control.

Identification and mechanisms of action description of regulatory elements are necessary to understand the structure of genome, gene systems and clusters, and in the long term allow to control the expression of certain genes at different points of cell life.

The experimental evidences of the presence of the new regulatory element NAU (New Activation Unit) in *D.melanogaster* genome have been obtained. NAU properties are being studied.

14. The influence of high pressure on the magnetic properties of intermetallic compounds YCo_5 and YCo_4Si

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$YCo_{5-x}M_x$ (M = Fe, Co, Ni) intermetallides are extensively studied, both from experimental and theoretical points of view. Such phenomena as high anisotropy, giant magnetoresistance, magnetocaloric effects, as well magnetoelastic lattice collapse are found in these compounds. That makes these compounds promising materials for magnetic refrigerators, permanent magnets, etc.

The RCo_5 and $YCo_{5-x}M_x$ compounds crystallize in $CaCu_5$-type structure with space group *P6/mmm*. In this lattice the cobalt atoms occupy 2c and 3g sites and form ferromagnetic ordering. These compounds are sensitive to changes in interatomic distances that can lead to significant changes in their magnetic properties and the simultaneous using of high-pressure chambers gives opportunity to control the changes of the interatomic distances.

In our work the results of the investigation of YCo_5 and YCo_4Si by the method of neutron diffraction at high pressures are presented. A lattice collapse is detected due to a change of cobalt ions spin states from the high spin to the low spin in YCo_5. The Curie temperature reducing with different baric coefficients for cobalt atoms in 2c and 3g positions is observed in YCo_4Si under pressure.

15. First experimental test of SESANS-TGF prototype and further improvements

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

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

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

In this work, the last results of experiments obtained on TGF-NSE prototype on 9-th channel of IBR-2 reactor are presented. Some technical problems and their solutions are discussed.

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16. Isotope-identifying neutron reflectometry at the pulsed neutron reactor IBR-2M

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The isotope-identifying neutron reflectometry is currently realized on the polarized neutron spectrometer REMUR at the pulsed neutron reactor IBR-2M (Dubna, Russia). This method is highly sensitive to the spatial distribution in the layered structure of various isotopes, magnetic elements and nuclei with spin. The realization of the standing or enhanced standing neutron wave modes [1] makes it possible to enhance the output signal at changing of the spatial distribution of isotopes. The method assumes simultaneous registration of neutrons and secondary radiation in the form of: γ-quanta; charged particles; fragments of nuclear fission. Also, as secondary radiation, the neutrons that change spin orientation in noncollinear medium are considered. Earlier, in [2], substantiation of isotope-identifying neutron reflectometry was carried out. This is especially important in the studies, for example, of proximity effects in ferromagnet-superconductor bilayers [3]. For registration of charged particles the ionization chamber was fabricated. A channel testing was performed using calibration structures containing ^{6}LiF and CoFe layers with a nominal thickness of 5 nm. It has been shown experimentally that the sensitivity of determining the spatial position of the ^{6}Li layer with thickness 5 nm is 0.09 nm/hour. At the same time, the sensitivity of 1 nm/10hours for a layer with thickness 5 nm is achieved with a minimal cross section of nuclei in the layer 0.05 barn. The spatial resolution of the measurements is 5 nm and can be increased to 0.5 nm by using a super-mirror neutron reflector.

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