Poster session
Programme Advisory Committee
for Condensed Matter Physics
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Poster abstract	Remarks
1. Crystal and magnetic structure of ordered iron oxides $PbFe_{0.5}Sb_{0.5}O_3$: neutron diffraction data **B.K. Argymbek[1], S.E. Kichanov[1], D.P. Kozlenko[1], V. Chlan[2], E.V. Lukin[1], B.N. Savenko[1]** [1] *Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia* [2] *Faculty of Mathematics and Physics, Charles University in Prague, Prague, Czech Republic* argymbek92@mail.ru; (496-21)-6-21-12 Among the objects of the study of modern condensed matter physics, a special place is occupied by compounds and materials based on iron oxides with a structural type of perovskite. These materials have a wide range of crystal and magnetic properties depending on the degree of doping, temperature or high pressures. One of the interesting properties of the oxides $PbFe_{0.5}Sb_{0.5}O_3$ are the order and disorder of the magnetic and paramagnetic ions in the crystal lattice. This fact strongly affects the magnetic properties that determine the unique magnetic structures: from ferromagnetic to disproportionate. My report presents the results of studies of crystal and magnetic structures of iron oxides with a structural type of perovskite $PbFe_{0.5}Sb_{0.5}O_3$ over a wide temperature range using a neutron diffraction at the DN-6 diffractometer of the IBR-2 high-flux reactor in JINR, FLNP. The crystal structure of ordered perovskite $PbFe_{0.5}Sb_{0.5}O_3$ is described by tetragonal symmetry I4/m, in which iron and tin atoms alternate with each other. At low temperature, the appearance of magnetic reflexes is observed, which correspond to the antiferromagnetic ordering with the propagation vector k = [½, ½, 0]. The structural mechanisms of the formation of this magnetic state are discussed.	
2. Impact of delayed neutrons on reflectometry experiments at IBR-2 reactor **V.V. Sadilov[1,2], V.I. Bodnarchuk[1], A.V. Nagornyi[1,3], A.I. Ioffe[4]** [1] *Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia* [2] *State University of Dubna, Department of fundamental microphysics problems, Dubna* [3] *Taras Shevchenko National University of Kyiv, City of Kyiv, Ukraine* [4] *Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science, Garching, Germany* sadilov@jinr.ru; +7-962-9596573 The impact of background neutrons on scattering experiments is extremely important for the correct operation of instruments at the IBR-2 reactor. Understanding of contribution of such neutrons will provide to increase accuracy of neutron experiments. Current work is devoted to analyze the effect of the delayed neutrons background at the IBR-2 reactor on reflectometry measurements. The model of TOF-reflectometer such as REFLEX-P [1] at VITESS software package [2] simulates the operation of a pulsed source, with characteristics corresponds to the IBR-2 reactor [3]. Simulation give us unexpected result that pushes to conduct a further study of the causes of such result. **References:** 1. http://flnph.jinr.ru/en/facilities/ibr-2/instruments/reflex 2. https://www.helmholtz-berlin.de/forschung/oe/em/transport-phenomena/neutronmethods/vitess 3. Pepelyshev Yu.N., et. al. Model of the IBR-2M Pulsed Reactor Dynamics for Investigating Transition Processes in a Wide Range of Power Variation // Annals of Nuclear Energy. 2015. V. 85. P. 488–493.	

3. Structure analysis of anionic surfactant – poly (ethylene glycol) micellar aggregates by neutron scattering

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The physicochemical properties of anionic surfactant micellar systems such as sodium oleate (SO) and dodecylbenzene sulphonic acid (DBSA) directly influence on the ferrofluids structural organization and should be considered in the synthesis protocol [1].

At the same time, modification of systems with a neutral polymer poly (ethylene glycol) (PEG) leads not only to improvements in the biocompatibility of ferrofluids, but also to a reorganization of their structure [2].

In present work, we study structural and interaction parameters of SO and DBSA micellar systems under the effect of the addition of PEG. Small-angle neutron scattering (SANS) allowed us to determine the micelle parameters for various compositions of solutions [2,3]. It was shown that different ratio of substance concentration and polymer molecular mass leads to quantitative and qualitative changes of studied parameters.

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4. Neutron activation analysis as a tool for tracing the accumulation of silver nanoparticles in tissues of female mice and their offspring

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The silver accumulation in different tissues of female mice and their offspring after prolonged oral administration of silver nanoparticles to the females during pregnancy and lactation was investigated. Silver content in different organs (blood, liver, brain, kidney and lungs) was determined by means of neutron activation analysis. According to the obtained data silver nanoparticles are able to reach and cross the placental barrier and blood-to-brain barrier in both mice female and their offspring. In mice female the highest silver concentration was determined in lungs, followed by brain, liver, kidney and blood. In offspring silver bioaccumulation changed in the following order lungs> brain> blood> liver>kidney. The average specific mass content of silver which crossed the blood-brain barrier was 373±75 ng (for female) and 385±57 ng (for offspring). The obtained results are important for studies in developmental and reproductive toxicity of nanomaterials.

5. Assessment of the geochemical and ecological conditions in surface sediments of the Varzob river

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The aim of the present study consists in getting more information concerning the geochemistry of the Varzob river unconsolidated sediments as reflecting the diversity of the South-Hissar range as well as evaluation of the anthropogenic contamination. The content of eight major, rock forming elements -Na, Mg, Al, K, Ca, Ti, Mn and Fe and 27 trace elements- Sc, V, Cr, Co, Ni, Zn, As, Br, Rb, Sr, Zr, Sb, Cs, Ba, La, Ce, Nd, Sm, Eu, Gd, Tb, Yb, Hf, Ta, W, Th, and U was determined by Instrumental Neutron Activation Analysis. A special attention was given to potential contaminants - V, Cr, Mn, Co, Ni, Zn, As, Sb and Ba whose concentrations were used to calculate environmental contamination proxies i.e. contamination factor, geo-accumulation, Pollution load index. At the same time, the content of Cr, Ni, Sc, Zr, REE, Th and U were used to establish the nature and origin of recent sediments. The high values of some pollution indices in the upper part of the Varzob River (Ziddi, Maykhura, Varzob 1) indicate on the anthropogenic origin of some elements, such as As, Sb and Mn. A geochemical anomaly was observed in the surface sediments of the river, associated with the Odjuk pegmatite rocks, characterized by high content of Th and U and accessory minerals such as samarskite, gadolinite, etc. Also a significant concentration of thorium and uranium were found in the Takob tributary.

In the Varzob River and its upper tributaries high concentrations of W, As and Sb were determined, that can be associated with coal mining in the Ziddy deposit and storage on the banks of the Maykhura tributaries as well as tungsten deposit in Maykhura.

6. Investigation of internal structure and atomic dynamics of pharmaceutical compounds under the influence of high pressure

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Due to the wide variety of phenomena realized in organic crystals at high pressure: polymorphic phase transitions, amorphization, etc., studies of pressure-induced changes in the crystal structure and atomic dynamics of complex molecular crystals is an urgent task in condensed matter physics [1,2]. In addition, structural studies of molecular crystals are important for optimization the of pharmaceutical production process, where, under additional mechanical influences (grinding or tabletting), irreversible polymorphic phase transitions or its amorphization can develop in the initial material, which entails significant changes in the physicochemical and pharmaceutical properties material. [3].

The use of high-pressure diffraction, NMR and Raman spectroscopy to study pharmacological components makes possible investigation of their structure and physical properties in the most complete way, which is necessary to understanding the nature and mechanisms of physical phenomena observed in them [4].

Therefore, the main objective of this study was detail investigation of physical properties and dynamics of the group of pharmaceutical compounds by means of different methods: neutron and X-ray diffractometry, solid-state nuclear magnetic resonance (NMR) and Raman spectroscopy.

Investigation of internal structure and atomic dynamics of pharmacological components: anti-inflammatory drug meloxicam $C_{14}H_{13}N_3O_4S_2$, hypolipidemic agent rosuvastatin calcium $[C_{22}H_{28}FN_3O_6S]_2$ Ca and antiulcerous component ranitidine hydrochloride $C_{13}H_{22}N_4O_3S{\times}HCl$ were carried out.

At pressure P>4 GPa, several changes in the Raman spectra of meloxicam were observed, which can indicate a pressure-induced phase transformation. Near the polymorphic transition pressure, the changes in the part of Raman spectra were obtained. In additional, the new Raman lines were detected at pressure P>10 GPa. These changes can indicate another polymorphic phase transition in the meloxicam. Around this phase transformation, the noticeable anomalies in the pressure behaviour of different vibration frequencies of the meloxicam were found.

At high pressure a gradual broadening of Raman lines of rosuvastatin calcium is followed by their disappearance up on further compression. Such a behavior corresponds to a gradual phase transition to the amorphous phase of rosuvastatin was observed.

The pressure dependence of vibrational modes of ranitidine hydrochloride measured at high pressures up to 9.8 GPa and room temperature were shown. The changes in a pressure behavior of the Raman lines were observed at pressures 2.2 and 6 GPa. Those changes can indicate the polymorphic phase transitions ranitidine hydrochloride under pressure.

The structural mechanisms of the phase transition in presented pharmaceutical compounds were discussed.

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7. Optimization of neutron reflectometry experiments for planar interfaces on example of electrochemical interfaces

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

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

This work is aimed to find the method for optimization initial parameters of samples to increase the sensitivity of the NR experiment, i.e. finding maximum ratio between initial and final NR curves of the sample. Some examples of interfaces modeling and selection the best configuration to study small changes at the interface [3] are presented in the given work [2-4] on the example of electrochemical interfaces in Li-ion batteries, where, correctly formation of solid electrolyte interface (SEI) is substantial process for batteries working properties, safety and time of life.

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8. Raman spectroscopy of NETosis: search for spectral biomarker

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NETosis is one of the first protected mechanisms of the immune systems. Neutrophils extracellular traps (NETs) were first described in 2004 by Brinkmann and his colleagues who observed the release of web-like structures by neutrophils after stimulation with phorbolmyristate acetate (PMA). NETosis is the third type of phagocytic antimicrobial protection along with phagocytosis and degranulation. Daily neutrophils fight to protect our body, however, they have some negative influence that may destroy our immune system. Among them are various autoimmune diseases (Systemic lupus erythematosus), preeclampsia, ulcerative colitis, thrombosis, etc.

Raman spectroscopy is a powerful and sensitive diagnostic tool in life sciences based on vibrational spectroscopy that can detect a specific chemical fingerprint of molecules. Furthermore, it is non-invasive technique, suitable for chemically selective cell imaging and one can avoid many problems associated with the fluorescence microscopy, like photobleaching and photoinduced damage of living organisms due to the presence of exogenous tags. Thereby, study of NETosis by Raman spectroscopy method looks as an attractive and proper technique.

The main aim of this study was to reveal a possible spectral biomarker in neutrophil activation by measuring and comparing the Raman spectra of activated (biologically and chemically) and non-activated neutrophil granulocytes, which will be more detailed in the report.

9. Research and synthesis of magnetic nanoparticles of the “core-shell” type

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One of the promising areas of nanotechnology development is the medical field of application of nanostructures. Nanomedicine is a rapidly developing area in the last decade, including methods for the prevention, diagnosis and treatment of a wide range of diseases using various types of nanostructures. The control of the shape, size, and chemical composition of nanostructures allows to set their physical properties at the synthesis stage and opens up new possibilities for bioprocessing. A rather interesting possibility of using nanostructures is the targeted delivery of useful goods (drugs or proteins) using a magnetic field. In this method, a drug or protein is attached by functional groups to a magnetic nanostructure and introduced into the circulatory system, after which it is transported to a problem area through a magnetic field. One of the most promising materials for creating magnetic nanostructures is iron oxide or an alloy of iron with nickel due to its greater saturation magnetization compared to this value for pure ferromagnetic metals Co, Ni, and Fe.

The use of magnetic nanostructures in medicine can not only efficiently deliver biologically active molecules through various body barriers that they are not able to overcome on their own (skin, blood-brain), but also significantly change the nature of the drug. Nanostructures of magnetic metals (iron, cobalt and nickel) are rarely used in pure form for therapeutic purposes. Usually they are encapsulated or placed in bioinert matrices (various organic compounds or polymers, including those of natural origin) in order to reduce the possible toxic effects of the magnetic phase, increase its physico-chemical stability and create the possibility of immobilization of the surface of such capsules or matrices of drugs. Coating magnetic metals with a carbon shell or noble metals such as gold and silver increases their effectiveness in medical applications.

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10. Microelements in shells and soft tissues of mussels collected along the South African coast

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The samples of mussels, which were collected from the different sites along the South-African coast were irradiated at the REGATA facility of the IBR-2 reactor. The sample were collected from West coast of South Africa: Port Nolloth, Saldanha Bay, Waterfront and Hout Bay, South and East coast: Plettenberg Bay, Port Elizabeth and Durban. The mussels from Saldanha Bay were collected from two sites: Strandloper and Bokriver, which are considered polluted stations.

The coastal stations were devided by relative pollution levels based on the concentration of such elements as Zn, As, Se and Br in soft tissues and shells of mussels and compared with the Saldanha Bay. The station of Port Nolloth with the lowest levels of majority of elements in mussels can be considered as relative pristine station in biomonitoring studies.

Such elements as Ti, Cr, V, Sc, Th etc., which can be used as markers of terrigenous matter reached high values at the almost all stations along African coast, but the maximal content of these elements was determined in samples from Durban. High content of Fe can be associated with resuspended terrigenous particles accumulated by molluscs during and after storm seasons. High concentrations of Na and Ca in shells of mussels in Durban (and particularly Port Elizabeth) can be explained by high salinity and content of suspended particles of rocks and dissolved elements in the coastal waters than in other stations.

Elements, which are considered as markers of anthropogenic pollution (Zn, As, Se and Br), reached higher or close level of values in the mussels from the Hout Bay and Waterfront stations in the Cape Town area. These elements are not influence by size of shells (age of molluscs) and are determined by their concentrations in the surrounding waters. For example, the soft tissues of small shellfish from Hout Bay, Waterfront (Cape Town) and Strandloper (Saldanha Bay) contained higher amounts of Zn than the larger shellfish from Port Nolloth and Durban that could indicate on anthropogenic pollution.

The positive correlation for Zn (0.78) and Mn (0.82) between shells and soft tissues among all stations was found. This feature exists because of the greater concentration of these elements in the gonadal tissues of female mussels before the spawning season [1].

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11. Biomonitoring using moss bag technique of trace elements atmospheric deposition on the territory of recreational zones of Moscow

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For the first time active moss biomonitoring was applied in park zones of Moscow, which perform a recreational role, in order to assess trace elements atmospheric deposition. Moss *Sphagnum girgensohnii* was chosen as a bioindicator. Moss bags were exposed on the territory of seven parks in Moscow (at three sites in each park): Tsaritsyno, Izmailovo, Elk Island, Sokolniki, Ostankino, Kuzminki-Lublino and Victory Park from June to September 2018. The content of 29 chemical elements (Na, Mg, Al, Cl, K, Ca, Sc, V, Mn, Fe, Co, Zn, As, Br, Rb, Sr, Mo, Sb, Cs, Ba, La, Sm, Tb, Hf, Ta, W, Au, Th, U) in moss samples was determined by instrumental neutron activation analysis. The concentrations of Cu, Pb and Cd were determined additionally by atomic absorption spectrometry.

Obtained results showed increase of concentrations of elements Al, Sc, Pb, Cu, Zn, Sr, Sb, V, Fe, La, Co, U, Th, etc. in different degree, depending on the site of exposure. Some of these elements can be associated with oil combustion, emissions from traffic, deterioration of tires, brakes, etc., while another elements may originate from re-suspension of soil and road dust [1,2]. In all samples of *Sphagnum girgensohnii* decrease of concentrations of physiologically active elements K, Cl and the alkali elements Rb and Cs was observed, which can be associated with the damage of the moss cell membrane under the impact of air pollutants and ion-exchange process [1]. Moss bag technique can be used in combination with existing methods of air control in Moscow as simple and cost-effective tool for air pollution monitoring.

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12. Investigation of atomic ordering processes in the surface layer of Fe-27Ga alloy

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Recently some atomic ordering processes in the Fe-Ga alloys were successfully studied by neutron diffraction method, see for example [1]. Neutron diffraction allows to obtain volume averaged information about the crystal structure of bulk samples. Usually, experiments on the structure study of alloys are performed on conventional X-ray diffractometers due to their wide availability. However, X-ray radiation from conventional sources (X-Ray tubes) is characterized by small penetrating depth in such Fe-based compounds. It allows us to explore only a small surface layer - about 4-6 μm. Noticed, that some XRD studies of Fe-Ga alloys (see work [2,3]) show the presence in them a certain type of atomic ordering which has never been observed by neutron diffraction experiments.

In this work, we have studied in detail a bulk sample of Fe-27Ga alloy by neutron and conventional XRD (CuKα irradiation). The results of the neutron diffraction experiment showed that the sample is characterized by the ordered $D0_3$ phase only. For the XRD study of the sample, the surface of the ingot was specially prepared. Firstly, it was mechanically cleaned by abrasive material and then it was etched in dilute nitric acid. The XRD experiments have shown that most part of the surface layer (i.e. 4-6 μm thickness) of the sample (~90% by mass) is characterized by the ordered $D0_3$ phase, and the remaining part (~10% by mass) consists the less ordered B2 phase. Further investigation of this sample showed increasing the partially ordered phase B2 when the sample was stored in the air for a long time.

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13. C_{60} and C_{60}-arginine aqueous solutions: *in vitro* toxicity and structural study

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A unique geometry of C_{60} fullerene molecules together with their physical and chemical properties opens up wide possibilities for their applications in various industrial and biomedical areas. At present, many fullerene derivatives are of interest with respect to their biological properties, including their antioxidant, antitumor, antiviral, antimicrobial, neuroprotective and membranotropic activities. A new approach for the prevention and treatment of allergic diseases is based on the use of fullerenes. In this connection, fullerene complexes with amino acids are being increasingly studied, which simultaneously increase both the biocompatibility of fullerenes and the stability of colloidal solutions.

Small-angle X-ray and neutron scattering was applied for the structural characterization of aggregates in water dispersions of fullerene C_{60} prepared by dialysis method and its conjugate with amino acid arginine [1]. Two-level aggregation, difference in the aggregate size for the systems under study, as well as a fraction of C_{60}-Arg primary aggregates that are not collected into secondary associates were observed. Two compounds are also compared with respect to their toxic properties. Experiments on the cytotoxicity of these systems on the A549, HepG2 and HeLa cells showed no toxic effects of the dispersions. Low toxicity in combination with the nanosize of the conjugate associates can be further used in the development of anti-allergic therapeutic drugs based on fullerene-amino acid compounds. One can hope that the next studies based on the contrast variation technique with the hydrogen/deuterium substitution (their potentials are proved by the current studies) will clarify the inner structure of the aggregates in details.

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14. Revealing the structure of composite nanodiamond – graphene oxide aqueous dispersions by small-angle scattering

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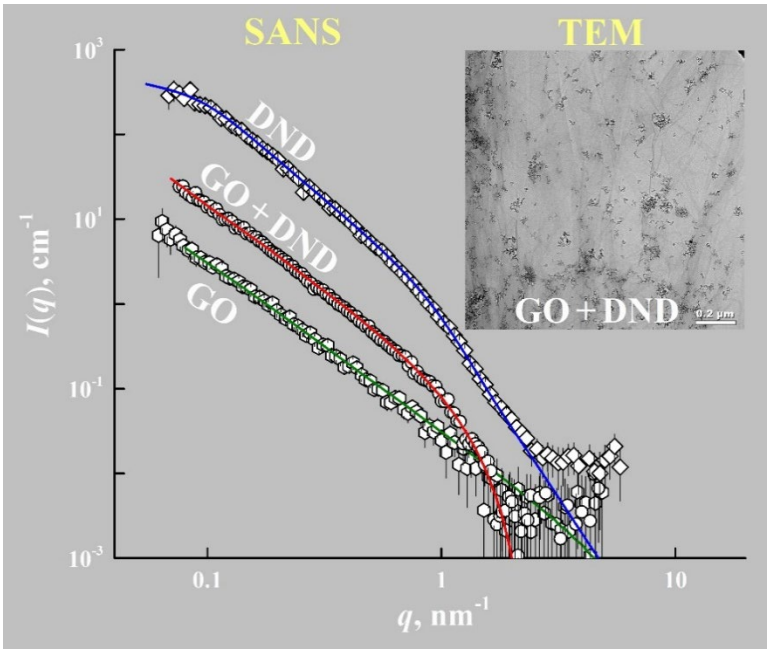
The work presents the results of studying the structure of binary liquid nanocarbon systems obtained by mixing hydrosol of detonation nanodiamond and aqueous dispersions of single layer graphene oxide flakes [1-2]. We studied size and space distribution of nanocarbon clusters formed upon interaction of the components in aqueous media by mutually complement methods of small-angle X-ray and neutron scattering. The formation of small secondary agglomerates of nanodiamond particles on the surface of graphene oxide flakes was concluded and supported by the data of transmission electron microscopy from dried samples. The observed effect can significantly modify the structure of nanocarbon composites formed of nanodiamond and graphene oxide. The structural features of binary dispersions detonation nanodiamond–graphene oxide should be taken into account at the preparation of the conductive composites of carbon nanoonions and reduced graphene oxide for energy storage systems.



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15. Polarized neutron reflectometry with secondary radiation registration

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One of the most actual problems of the physics of low-dimensional superconducting/ferromagnetic heterostructures is determination of the correlation between magnetic spatial profile and the spatial profiles of the elements at the interface between layers. Standard neutron reflectometry cannot be used to measure neutron interaction with separate element, in particular, magnetic field induction. A new method allows one to determine the elemental and magnetic profiles. The reflected neutron beam and secondary radiation are simultaneously recorded in this method. Charged particles and gamma-quants can be secondary radiation because of neutron capture reaction. Also scattered neutrons and spin-flip neutrons can be secondary radiation. At the REMUR reflectometer at the IBR-2 reactor, channels for secondary radiation registration were realized: spin flip neutrons, charged particles and gamma-quanta. Currently, a sufficiently large number of element isotopes are available for measurements. At measuring time t=1 day, resolution by the wave vector $\delta k/k$=0.1, λ=1.5 Å, cross section of the beam at a sample of 0.1 cm^2, layer thickness 5 nm and neutron flux density at the sample of $2 \cdot 10^4$ $cm^{-2}s^{-1}$ it's: a) for the charged particles registration channel, the minimum value of the cross section is σ_{min}=0.025 barn, the cross section $\sigma > \sigma_{min}$ has 22 isotopes; b) for the gamma-quanta registration channel, σ_{min}=0.3 barn, more than 100 isotopes have a cross section σ>0.3 barn; c) for the polarized neutrons registration channel, the minimum, perpendicular to the neutron polarization, component is 1 G. Further progress is possible. The first is increasing of neutron intensity to 5–10 times. The second is the reduction of the fast neutrons and gamma-quanta background from the reactor core by 5-10 times. Third is increasing of the solid angle visible to gamma-ray detector by 4 times or increasing of the detectors number to 4. Realization of these improvements at the REMUR reflectometer make available cross section 1 mbarn for an absorbing layer 5 nm or cross section 50 mbarn for 1 Å layer. The spatial resolution can reach 1 Å by using super-mirror neutron reflector at the structure. In the case of studying periodic structures, high spatial resolution can be achieved by reducing the period of the structure. At nowadays technological level, structures with period 1 nm are available, which gives a value of 1-2 Å for resolution.