Report on the concluding theme “Investigations of Condensed Matter by Modern Neutron Scattering Methods” and proposal for opening of the new theme “Investigations of Functional Materials and Nanosystems by Neutron Scattering Methods”

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The main results obtained during the realization of the theme 04-4-1121-2015/2020 “Investigations of Condensed Matter by Modern Neutron Scattering Methods” during the period of 2018-2020 are reviewed. The theme was realized mostly on the basis of the Department of Neutron Scattering Investigations of Condensed Matter of FLNP JINR. The primary scientific goal of the theme was the study of structure, dynamics and microscopic properties of novel materials and nanosystems in research topics which are actual for development of modern scientific concepts in the fields of condensed matter physics, materials science, chemistry, geophysics, engineering sciences, biology and pharmacology, or prospective for development of modern technologies in the fields of energetics, electronics, pharmacology and medicine, by means of neutron scattering and complementary methods. The central goal of the methodical and technical works was the development of the spectrometers complex of the modernized IBR-2 reactor. Most of the research activities were realized at the spectrometer complex of the IBR-2, while some additional scientific experiments were performed in other national and international research centers in a tough collaboration with JINR Member States. Another important activity in the framework of the theme was the realization of the User Programme at the IBR-2 spectrometer complex.

The most important scientific results include:

- Determination of the structural, magnetic and electronic P-T phase diagram of magnetite Fe_3O_4;
- Analysis of the structural phase transitions in giant magnetostrictive Fe-xGa alloys (x = 27.2 – 28 at. %) induced by isothermal annealing;
- Determination of the structural organization of iron oxide nanoparticles in SBA-15 nanoporous silica;

- Determination of the structural features of star-shaped poly(2-ethyl-2-oxazoline) and poly(2-isopropyl-2-oxazoline) with central thiacalix[4]arene fragments;
- Analysis of the non-uniform external magnetic field effects on the adsorption of magnetic nanoparticles from ferrofluids on a flat interface;
- In-operando analysis of the effects of non-electroactive additive (tetrabutyl ammonium perchlorate, TBAP) in a lithium-containing electrolyte on the formation of a solid-electrolyte interphase (SEI) on the electrode surface in model electrochemical interfaces of 'liquid electrolyte/solid electrode' type;
- Determination of the structural organization of C_{70} fullerene in polystyrene nanocomposite thin films;
- Determination of the structural features of the complexation processes between fullerenes and antitumor pharmacological ingredients;
- Analysis of the properties of magnetic and superconducting states in layered Nb(70nm)/$Ni_{0.65}Cu_{0.35}$(6.5 nm) nanostructures;
- Analysis of the vibrational spectra of Trans-1,3-cyclohexanediol, Cis-1,3-cyclohexanediol, Trans-1,2- cyclohexanediol and Cis-1,2-cyclohexanediol compounds with a general chemical formula $C_6H_{12}O_2$;
- Determination of residual stresses in steels and magnesium alloys under applied load;
- Analysis of the preferred crystallographic orientation of minerals in eclogites;
- Analysis of the internal organization of cultural and natural heritage objects by means of neutron radiography and tomography.

The most important methodical results include:

- Upgrade of the neutron splitting system at the 10 channel of IBR-2;
- Development of the isotope identifying reflectometry at the REMUR reflectometer;
- Modernization of the electrochemical cells for neutron reflectometry experiments;
- Installation of the parabolic neutron focusing device (m = 5) at the NERA spectrometer;
- Installation of the new mirror neutron guide (m = 2) at the FSS diffractometer at the 13 beamline of IBR-2;
- Development of the elements of the neutron transportation system of the new small angle neutron scattering and imaging spectrometer to be installed at the 10A beamline;

- Development, installation and putting into operation of the neutron radiography and tomography spectrometer at the stationary reactor WWR-K (INP, Kazakhstan).

During the reported period of 2018-2020, the JINR staff members participated in the 04-4-1121-2015/2020 theme activities, have published 363 papers in referred scientific journals and made 347 reports at conferences. The obtained scientific results were honored by 4 JINR prizes.

Proposal for opening of the new theme "Investigations of Functional Materials and Nanosystems by Neutron Scattering Methods" for the period 2021-2025

Taking into account the successful realization of the theme 04-4-1121-2015/2020**,** directions of the 7 year plan of the strategic development of JINR in condensed matter physics and current trends in considered research fields, it is proposed to open the new theme "Investigations of Functional Materials and Nanosystems by Neutron Scattering Methods", leaders D.P.Kozlenko, V.L.Aksenov, A.M.Balagurov, for the period 2021-2025. The theme will be realized on the basis of the Department of Neutron Scattering Investigations of Condensed Matter of FLNP JINR.

The priority fundamental and applied research topics within the theme include:

- Condensed Matter Physics and Materials Science;
- Physics of Nanosystems and Nanoscale Phenomena;
- Physics of Complex Liquids and Polymers;
- Biophysics and Pharmacology;
- Applied Materials and Engineering Sciences.

The main scientific directions within these topics are:

- A study of structure and properties of novel inorganic and organic functional materials,
- A study of structural and magnetic properties of materials under extreme conditions,

- A study of characteristics of physical and chemical processes in functional materials in real time,
- Computer modeling of physical and chemical properties of novel crystalline and nanostructured materials;
- A study of structural and magnetic properties of layered nanostructures;
- A study of structural characteristics of carbon and silicon based nanomaterials,
- A study of molecular dynamics of functional materials;
- A study of structural characteristics of dispersed systems and complex liquids at bulk and interface states,
- Structural characterization of polymer materials;
- A study of structural characteristics and functional properties of biological materials,
- A study of structure and properties of lipid membranes and lipid complexes,
- A study of structural characteristics and properties of biohybrid complexes;
- A study of residual stresses and microstrains in constructional materials, industrial products and earth rocks,
- Neutron imaging of internal structure features of cultural and natural heritage objects, constructional materials, industrial products.
- A study of texture and physical properties of Earth's rocks, minerals, and constructional materials,
- A study of radiation damage effects in condensed matter.

A special attention will be paid to a modernization of the spectrometers complex of the IBR-2 reactor, development of new spectrometers, upgrade of existing ones and new experimental techniques:

- Development and creation of the elements of basic configuration of small angle neutron scattering and imaging spectrometer at the 10 beamline.
- Development of an Inelastic Neutron Scattering Spectrometer in Inverse Geometry at the IBR 2 Reactor, first stage (project within the teme).
- Upgrade of the neutron guide and modernization of the detector system of the DN-6 diffractometer for studies of microsamples under extreme conditions.

- Installation of new beam chopper of the multifunctional GRAINS reflectometer and development of electrochemical cells for neutron reflectometry experiments.
- Upgrade of the operational instruments of IBR-2 reactor (HRFD, RTD, DN-12, YuMO, FSD, REFLEX, REMUR, SKAT, EPSILON), aimed at improvement of their technical characteristics and extension of experimental capabilities.
- Development of test configuration of small angle spin echo neutron scattering spectrometer at 9 beamline.
- Modernization of the neutron radiography and tomography spectrometer.
- Modernization of the FSS diffractometer.
- Development of neutron scattering methods for condensed matter research, including those for in-operando monitoring and studies of electrochemical materials and interfaces.

The realization of the User Programme will be also high priority activity in the framework of the theme.

The planned research activities will be performed mostly using the spectrometers complex of modernized IBR-2 reactor. Additional experiments using neutron scattering and complementary methods will be performed at other research centers of Russia and Europe within collaboration agreements.

The financial budget of the theme is determined in the framework of the limits of the approved 7-year plan of the strategic development of JINR in condensed matter physics.

The collaboration within theme includes more than 100 research institutions from JINR Member States – Azerbaijan, Bulgaria, Belarus, Kazakhstan, Russia, Poland, Czech Republic, Slovak Republic, Romania, Moldova, Mongolia, Ukraine, Uzbekistan, Vietnam, Associated Member States – Egypt, Germany, Hungary, Republic of South Africa, Serbia, and Non-Member States – Latvia, France, Norway, Switzerland, Taiwan, United Kingdom, Japan.