FLNP

JOINT INSTITUTE FOR NUCLEAR RESEARCH

Directions of Scientific Research at the Advanced Pulsed Neutron Source at FLNP JINR

Volume I

Joint Institute for Nuclear Research

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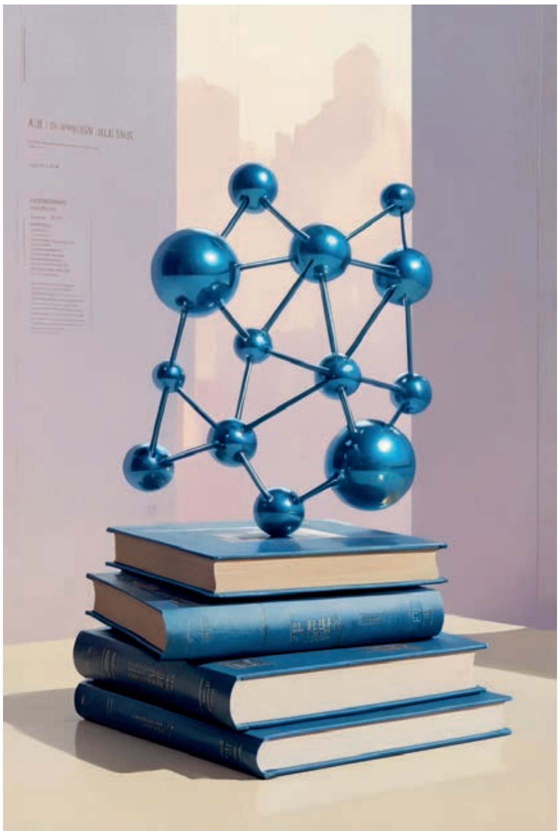


The development and formation of modern civilization are inextricably linked with the development and use of new materials and technologies. Current challenges in solving scientific and technological problems facing humanity require the development and improvement of methods for conducting research and diagnostics of new materials, verification of model objects and scientific theories, development and creation of advanced experimental facilities. New achievements in the fields of energy engineering, materials science, quantum technologies, drug development, major breakthroughs in chemistry, biology, geophysics, and engineering sciences are impossible without conducting research into the internal structure and dynamics of a wide range of materials and biological objects. Understanding the internal structure at the atomic level, studying the mesoscopic and microscopic organization of matter in combination with computer simulations allow us to gain a deeper understanding of the nature of phenomena at the macroscopic level and make it possible to synthesize functional materials with specified properties. Neutron and synchrotron scattering methods, the use of free-electron lasers, NMR spectroscopy, scanning and transmission electron microscopy, ultrasound, optical and a number of other complementary techniques make it possible to adequately respond to emerging scientific challenges.

The relevance of the neutron as a tool for studying various properties of materials at a level ranging from the atomic nuclei to entire objects is determined by its properties: electrical neutrality, the existence of a magnetic moment, and a long lifetime. Non-destructive neutron research methods help to determine ways of creating new drugs, shed light on the causes of diseases, develop quantum materials, search for new high-temperature superconductors, contribute to the creation of more capacious and durable chemical current sources, new functional materials, improve the properties of structural steels and alloys, develop new methods of additive technologies, allow us to see how components inside mechanisms work in real time, reveal the secrets of history when studying cultural heritage objects and much more. Neutron methods are unique in experiments that require determination of the internal structure and dynamics of materials with light nuclei, magnetic structures, textures and internal stresses in bulk specimens, as well as the spatial distribution of components within massive objects and mechanisms.

In addition to using the neutron as a tool, the neutron itself is no less interesting as an object of research. Our fundamental knowledge of nature would be further refined by understanding the properties of the neutron, its lifetime in a free state, the existence of an electric dipole moment. The study of neutrons can contribute to understanding the Universe at an early stage of its evolution, in particular, to answer the question of why there is more matter than antimatter, etc.

Despite all the advantages of neutron research methods related to the depth of neutron penetration, magnetic properties, sensitivity to isotopic composition, and, consequently, the possibility of varying the scattering contrast, the main disadvantage still remains the relatively low luminosity of beamline instruments. As a result, there is a limitation on the minimum size of samples under study, time resolution, duration and accuracy of experiments. This problem can only be solved by increasing the flux of neutrons of required energies on the sample and improving the efficiency of detection, data collection and analysis. This can be achieved by combining the high brilliance of the neutron source with the optimization of all units of neutron scattering instruments, including neutron moderators, modern elements of neutron optics, an increase in the solid angle and efficiency of detecting elements, and the use of advanced data acquisition and processing systems. Higher neutron flux density on the sample and better statistics in experiments in less time will make it possible to reduce the size of new synthesized samples for research, increase the accuracy of measurements and see more subtle processes in complex systems. At pulsed neutron sources, the use of time-of-flight techniques in real time with generated extreme conditions on samples under study provides additional opportunities for studying internal processes and dynamics.

In all leading countries of the world with a well-developed research infrastructure for investigations at beamline facilities in condensed matter physics and nuclear physics, in addition to the construction and use of steady-state powerful research reactors (ILL HFR — France, HFIR — USA, FRM-II — Germany, OPAL — Australia, PIK — Russia, CARR — China and others), which generate continuous neutron beams with high time-averaged intensity, pulsed neutron sources are constructed, which produce periodic neutron pulses with a high peak flux density, making it possible to effectively apply time-of-flight techniques in experiments using almost the entire spectrum of neutrons from the source [Aksenov, Balagurov, 2016]. Such sources are built on the basis of accelerators or pulsed reactors of periodic operation. Examples of pulsed neutron sources are IBR-2 (JINR, Russia), SNS (USA), J-PARC (Japan), ESS (European Union, Sweden), CSNS (China), ISIS (UK). In addition to the construction of new high-intensity neutron sources, modernization programs have been announced and are being developed to upgrade the existing ones: ISIS-II, SNS STS, a second target at CSNS. World experience shows that it takes about 20-25 years to develop and build such a large-scale scientific facility. The IBR-2 pulse reactor, which was commissioned in 1983 and underwent a deep modernization in 2012, taking into account the annual work programs and operating power, has, according to preliminary estimates, an expected service life until the 2040s-2050s, depending on the operating modes.

In this regard, in order to replace the IBR-2 reactor, which is the only high-flux pulsed research neutron source in the JINR Member States, there is an urgent need to develop and build a new advanced high-intensity pulsed neutron source with a cutting-edge instrumentation base for collective access to equipment for researchers from the JINR Member States, Associate Members and Partner Countries.

Life sciences. Health and medicine.

Human health, treatment and prevention of diseases are among the most important social tasks that determine the quality of our lives. Their solution requires a deep understanding of the complex biological and molecular mechanisms responsible for the performance of various functions in living systems. These functions include the construction and maintenance of the structure of cellular elements; recording, storing and transmitting hereditary information; synthesis and utilization of chemical compounds; transmission and distribution of signals; energy production; motor skills. The main participants in these biological processes are proteins, lipids and nucleic acids. Due to their unique properties, neutrons can provide precise information about the position of hydrogen atoms and the geometry of hydrogen bonds, and determine molecular structures and their dynamics. This knowledge is crucial for understanding the behavior of proteins, enzymes, and cell membranes, which, in addition to a general understanding of the functioning of living organisms, contributes to increasing the efficiency of the development and use of drugs for the treatment and prevention of various diseases.

An increase in life expectancy also entails a change in the structure of diseases. Diseases such as diabetes, cancer, Parkinson's disease, high blood cholesterol and others are becoming more common. In addition, new multi-resistant strains of bacteria and viruses are emerging, which pose a growing threat to our collective health and safety. Neutron research methods, along with complementary methods, help to deepen our understanding of the mechanisms of disease development, contribute to the creation of effective pharmaceuticals, and facilitate the development of targeted drug delivery systems. Research into the causes of diseases using neutron methods, in particular, includes such areas as the study of Alzheimer's disease, which occurs as a result of damage to the membranes of neurons. Some examples of the application of neutron methods are the study of cholesterol transport and its effect on neurodegenerative diseases and heart diseases. Neutron methods contribute to the study of the structure and properties of lipid matrices of the skin. This knowledge makes it possible to advance in the treatment of dermatological diseases and develop methods for transdermal delivery of pharmaceutical and cosmetic products. Neutrons help to study the structural and mechanical properties of materials developed to create biocompatible implants. The use of neutrons occupies a special place in the treatment of malignant tumors using boron neutron capture therapy, as well as for the production of radionuclides that are widely used in medical diagnostics and radiation therapy.

The environment plays an important role in the quality of human life and health. Neutron methods for studying the elemental composition, structure and dynamics of matter are already actively used and find new directions for solving problems of ecology, quality of food products, their storage and processing, studying ways to minimize industrial waste and in solving problems of their disposal.

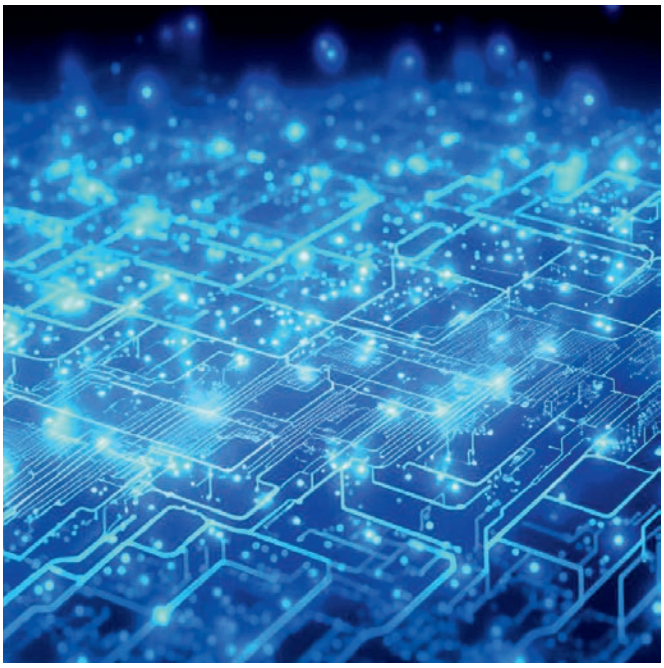
Energy

The production, storage and transport of energy is a critically important task for the development of our civilization. More and more research is being conducted in this direction using neutron methods. Neutrons provide ideal access to the structure, kinetics and dynamics of numerous materials and processes. Neutron methods are used to study and optimize the properties of structural materials and technological processes that play an important role in energy production, both in nuclear power reactors and in the creation of thermonuclear reactors of the future. The use of neutron scattering techniques has also made a considerable contribution to the study of the structure of high-temperature superconductors, the application of which can significantly reduce losses in energy transmission. The search for and investigation of compounds exhibiting superconductivity at room temperature is an ambitious task that can be accomplished at an advanced pulsed neutron source. The discovery and application of such superconducting materials will lead to a technical revolution in many areas of industry and a general restructuring of the economy.

One of the possible directions of development of modern "green" energy is the use of organic solar batteries. Light, flexible, translucent and potentially cheap batteries can become a widely used renewable energy source. Also, hydrogen energy is one of the most actively developing areas in the world for the energy industry of the future. Research programs on the development of hydrogen fuel cells or new materials for efficient and safe storage and transportation of hydrogen rely heavily on investigations using neutron scattering techniques.

The increasing use of mobile devices and electric vehicles requires the development of battery technologies based on high-capacity solid-state batteries. Due to the high penetrating power of neutrons, sensitivity to light atoms in the structure and the fact that the energy of thermal neutrons is comparable to typical excitation energies of the crystalline structure, neutron scattering methods are actively used in the study of materials for the energy industry. A large number of studies are already being conducted on lithium-ion batteries using neutron scattering methods in real-time charging and discharging. Investigations are underway of materials for components of commercial sodium-ion batteries, and undoubtedly, in order to increase the specific capacity, environmental friendliness, and durability of batteries there will be a further search and research into new, more efficient electrode materials, solid electrolytes, and other compounds.

Quantum materials in modern digital technologies



Digital technologies have penetrated many areas of our lives. Important areas related to storage, processing, protection and transmission of information are coming to the fore. Current topological integrated circuits no longer meet the needs of humankind, since there are physical limits to the performance of conventional computers because of limitations in the density of transistors on chips and the energy required for their operation. One of the ways in which this problem can be overcome is the use of quantum materials that have unusual magnetic and electrical properties and technologies for their production. They can be used to develop highly efficient electrical systems, faster and more accurate electronic devices, quantum computers with non-volatile memory, and neuromorphic computing networks. The use of spintronic devices increases energy efficiency, since spin-encoded information can be transmitted without the movement of electrons and, therefore, without loss of energy. Quantum computing has the potential to drive significant advances in the speed of data processing, opening up enormous opportunities for development and problem solving in many sectors of the economy.

An important component in the study of magnetic structures is the use of neutron scattering methods with their high sensitivity to the magnetic properties of materials. For example, topologically stabilized spin vortices, the so-called skyrmions, have already been studied using neutron methods. Due to the unique sensitivity to the magnetic properties of materials, the use of neutron methods is extremely effective in determining the static and dynamic properties of a wide range of materials. With the help of neutrons, the effect of giant magnetoresistance was discovered, which has found wide application in data storage devices and various miniature magnetic sensors. Such a highly sensitive magnetic sensor is the key to magnetoencephalography, which can detect small magnetic field with high spatial resolution and is widely used along with superconducting materials in medicine, namely in magnetic resonance imaging. Experiments using neutrons open up new possibilities in the study of thin-film heterostructures, including superconductors and ferromagnets, magnetic nanoparticles, topological insulators, as well as new quantum states of matter that will make it possible to develop new electronic devices in the future. The development and construction of the advanced high-flux pulsed neutron source with state-of-the-art instrumentation will significantly contribute to overcoming a number of limitations in the study of magnetic materials.

Structural materials and Earth sciences

The development of our civilization is impossible to imagine without the development, synthesis, research and application of new materials. Throughout its existence, humanity has revolutionarily changed the course of history with their use. In today's world, materials play an increasingly important role in both technological breakthroughs and everyday life. The quality of life in our society is in many cases linked to the availability of objects and devices made from new materials. Knowledge of their crystal structure and the nature of their defects provides insight into the chemical and physical properties of materials, as well as the ability to develop materials with predetermined physical properties and predictable behavior. The development of advanced materials that support new technologies depends on the ability to manipulate their properties at the atomic level. Neutron research techniques are among the key methods for achieving these results. The large depth of neutron penetration into the material makes it possible to carry out non-destructive studies of the internal structure, properties and processes in bulk massive materials and complex systems with high accuracy. Especially valuable is the possibility of investigations under external influences on the studied material, which are close to natural or operating conditions, including extreme ones or with an aggressive external environment: high pressure, magnetic and electric fields, high and low temperatures, during oxidation/reduction reactions, various chemical processes, etc. These possibilities are of great importance in engineering and Earth science research. Rapid characterization of materials is essential for optimizing the process of their synthesis, diagnostics, and subsequent application. Neutron research methods shorten the cycle of development and testing of new materials, which allows them to be introduced into practice more quickly. The creation of the new advanced pulsed research neutron source can significantly speed up the processes of diagnostics and analysis of materials. At the same time, most functional materials are of fundamental scientific interest. Their study is an additional channel for interaction between applied and fundamental research.

Aerospace and automotive industries, mechanical engineering and construction, shipbuilding and reactor construction, medicine and pharmaceuticals, renewable energy sources, communications and information technology, food and chemical industries — practically in all areas where new materials are required and where their development and characterization are carried out, neutron research methods are used. Materials science deals with a wide range of compositions and structures: from well-known and widely used metals, steels, alloys, glasses, cements, ceramics, polymers, etc. to materials that have emerged and attracted attention in recent decades, such as high-entropy alloys and giant magnetostriction alloys, superduplex steels, bulk metallic glasses, metal-organic frameworks, nano- and biomaterials, metamaterials, etc. Their processing employs both classical methods of thermomechanical processing, welding, etc., and new processes, such as intensive plastic deformation or additive technologies.

A separate area in which neutron research methods are actively used is Earth sciences, where the objects of study are the composition, structure and dynamics of the Earth. To develop methods for predicting earthquakes and volcanic eruptions, to study changes in the relief of the Earth's surface and the ocean floor, to solve applied problems, for example, for justifying the choice of sites for the construction of deep storage facilities for radioactive waste, for oil and gas production, information is needed on the deformations and stress state of rocks, the anisotropy of properties. Obtaining this information is possible due to the high penetrating power of thermal neutrons. For example, neutron textural analysis makes it possible to study the crystallographic textures of relatively large coarse-grained rock samples with high accuracy and provides information about the preferential spatial orientation of the crystal lattices of grains throughout the entire mineral ensemble. Neutron radiography and tomography are used to obtain three-dimensional models of the internal structure of rocks. Owing to this method, it became possible, for example, to separate mineral and metal components in meteorites of mixed composition, build their distributions according to the occupied volumes and average sizes of the components, and determine their morphological features.

Non-destructive investigations of cultural heritage objects

The application of neutron methods for studying cultural heritage objects has a number of key advantages and is of increasing interest in archaeology, as well as in the restoration and conservation of historical artifacts, such as paintings, elements of weapons, sculptures, cooking wares, ceramics, etc. Neutron methods are already used on a regular basis to study various objects from state museums and private collections. The discovery of ancient artifacts and works of art usually raises many questions related to the correct determination of the historical and cultural periods of their creation, places and methods of production, the technologies and techniques used, and also requires the development of recommendations on the choice of methods and conditions for restoration and their preservation for future generations.

Neutron methods are non-invasive, non-destructive and ideal for obtaining structural information about historical artifacts, determining their composition, the presence of changes caused by environmental conditions, detecting inclusions, structure, reconstructing manufacturing technology, and place of origin.

Neutron diffraction and tomography help to quantitatively determine the phase components, their proportions in a sample and the features of the crystal structures of certain phases in coins, weapons, statues, etc. Neutron measurements combine chemical and structural sensitivities related to phase composition and texture, revealing historical production technologies. A key advantage of neutron techniques is the ability to probe the internal composition and structure through coatings and corrosion layers, which reduces the need for potentially hazardous cleaning and preparation of samples for restoration. Neutron tomography makes it possible to obtain three-dimensional models of the internal parts of artifacts without opening or destroying them, even when studying massive objects of cultural heritage.

Why are neutrons used?

Neutron scattering methods in the study of condensed matter make it possible to study the internal structure and dynamics of matter over a wide range of correlation lengths and energies. The absence of interactions with electrons allows neutrons to easily penetrate deep into the material being studied, including through the walls of devices that maintain the required external conditions, including extreme ones: high pressure, tensile and compressive loads, high and cryogenic temperatures, magnetic and electric fields, etc. Non-destructive neutron research methods at pulsed neutron sources provide an additional opportunity to effectively apply the time-of-flight technique, including in real-time studies of chemical processes, phase transitions and dynamics.

– Neutrons easily penetrate most materials, allowing the study of bulk samples or scanning of small areas deep within a massive sample. This also makes it possible to study samples exposed to extreme conditions generated by external devices (e.g. cryogenic temperature and/or high pressure).

– Since neutrons are scattered by atomic nuclei, it is possible to determine which element and isotope is present. Isotopic contrast—sensitivity and selectivity to different isotopes of chemical elements, for example, hydrogen and deuterium—allows one to distinguish certain groups of atoms in mixtures, complex biological and other hydrogen-containing materials, including in the presence of heavy elements.

– The wavelength of thermal and cold neutrons is comparable to the interplanar spacing in a substance, therefore neutron methods are widely used in studying the structure of materials in a wide range of distances from the atomic level to hundreds of nanometers and above.

– The energies of thermal and cold neutrons are comparable to the energies of elementary excitations in condensed matter. Using neutron scattering methods, it is possible to determine both the collective and individual dynamics of atoms, excitations and elementary vibrations of molecules and the crystal lattice.

– The existence of a magnetic moment of the neutron makes it a unique tool for studying the magnetic properties of both bulk materials, and thin films and surfaces. Neutron methods are ideal for studying the microscopic magnetic structure and spin dynamics of matter.

– Neutron methods are non-destructive, so delicate materials such as biological objects or cultural heritage items can be studied without fear of damaging them.

– Neutron scattering techniques are complementary to synchrotron scattering, electron microscopy and other methods of structural diagnostics. Their use provides a clearer understanding of the overall picture of the structure and dynamics of condensed matter under study.

– At high flux density and irradiation time, neutrons are capable of activating a sufficient number of nuclei of a substance for analysis, and by registering emitted gamma-rays, its elemental composition can be determined with high accuracy.

– The neutron is an important object for studying its fundamental properties. The results of these studies lead to an understanding of the origin of the Universe and the physics of elementary particles, and open up additional possibilities for testing the Standard Model. This is facilitated by experiments with ultracold neutrons on measuring the lifetime of a free neutron and the electric dipole moment, neutron interferometry and searching for neutron-antineutron oscillations, measuring gravitational mass, etc. Each of them requires a high neutron flux to increase the accuracy of measurements.

Preliminary parameters of the advanced neutron source at JINR

The implementation of a scientific program on beamline instruments of the new pulsed neutron source at FLNP JINR, in addition to the analysis of scientific problems for which these instruments are developed, requires a more comprehensive consideration of parameters at which experiments are carried out. In particular, these are the expected parameters of the future neutron source, neutron fluxes at the sample position on beamline instruments, the efficiency of detection, data acquisition and processing. The neutron flux determines the luminosity of the experiment, and the pulse width influences the neutron energy resolution. For a number of experiments, an important characteristic is the background level between the source pulses and the background level of delayed neutrons uncorrelated with the pulse. Table 1 shows the basic characteristics of five operating neutron sources and two sources currently under construction (CSNS and ESS), from which it can be seen that the parameters vary within a fairly wide range.

Source	Country	Year of start-up	P, MW	Φ_0, ×10^{13}, n/cm^2/s	Δt_f, μs	Δt_0, thermal neutrons, μs	ν_0, Hz
IBR-2	Russia	1984	2	0.8	215	350	5
ISIS-I	UK	1985	0.2	0.07	1	20	50
LANSCE	USA	1985	0.1	0.05	1	20	20
SNS	USA	2006	1	1	1	20	60
J-SNS	Japan	2009	1	1	1	20	25
ISIS-II	UK	2009	0.05	0.02	1	60	10
CSNS	China	2018	0.14	0.07	1	20	25
ESS	Sweden	2026	5 (plan)	30	2860	~3000	14
New source at JINR	Russia	2040 (plan)	10	10	200	~300	10

Table 1. Basic characteristics of research pulsed neutron sources.

The scientific program of the new pulsed neutron source at JINR, as well as a suite of beamline instruments required for its implementation, should be largely determined by potential users of the instruments being developed. The number of experiments performed by scientists from organizations external to JINR on the advanced pulsed neutron source will be significantly higher than on the IBR-2 reactor. This is connected, among other things, with new possibilities opening up due to an increase in the neutron flux density on beamline instruments of the new source, both owing to the improvement of the instruments themselves (optimization of optical elements, multiple increase in the solid angle of detectors, development of more efficient electronics for data acquisition and analysis, automation of the operation of sample environment systems, etc.), and an increase in the brilliance of the source due to the optimization of neutron moderators.

User Access Policy on research instruments of the IBR-2 reactor

In FLNP JINR, access to the experimental research infrastructure of the IBR-2 reactor, and first of all, to its neutron scattering instruments is provided within the framework of the User Program. Researchers from any country are granted beam time for experiments on the basis of an external peer review of submitted beamtime proposals. Financial support is provided to researchers from organizations of the JINR Member States and Associate Members. Under regular reactor operation, more than 200 experiments are conducted annually, resulting in more than 80 publications per year. Figure 1 shows the distribution of the researchers who were granted beam time in 2021 by country of their affiliation and scientific areas in which they conducted experiments.

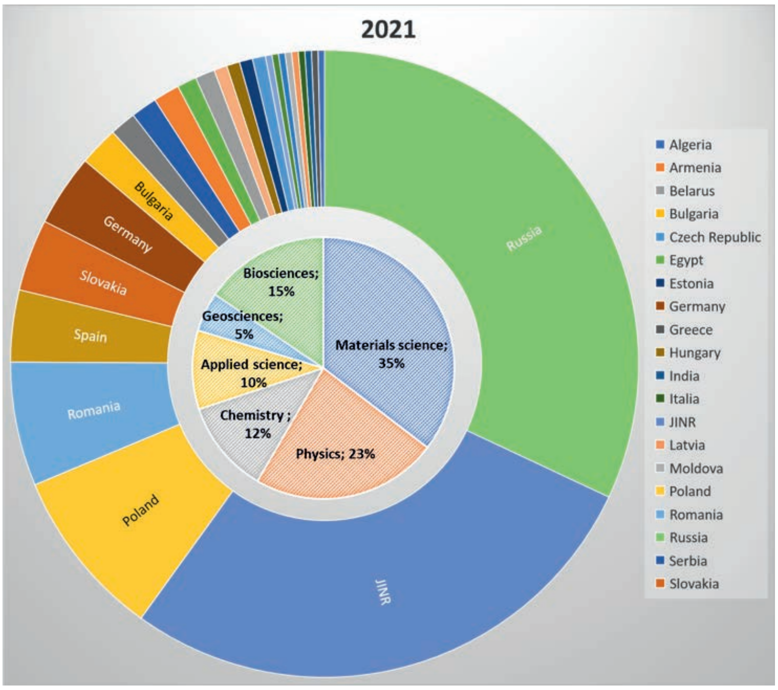


Fig. 1. Distribution of users of the IBR-2 reactor by country of their affiliation and scientific areas in which experiments were conducted.

Figure 2 illustrates the distribution of the number of submitted and accepted beamtime proposals by year of proposal submission.

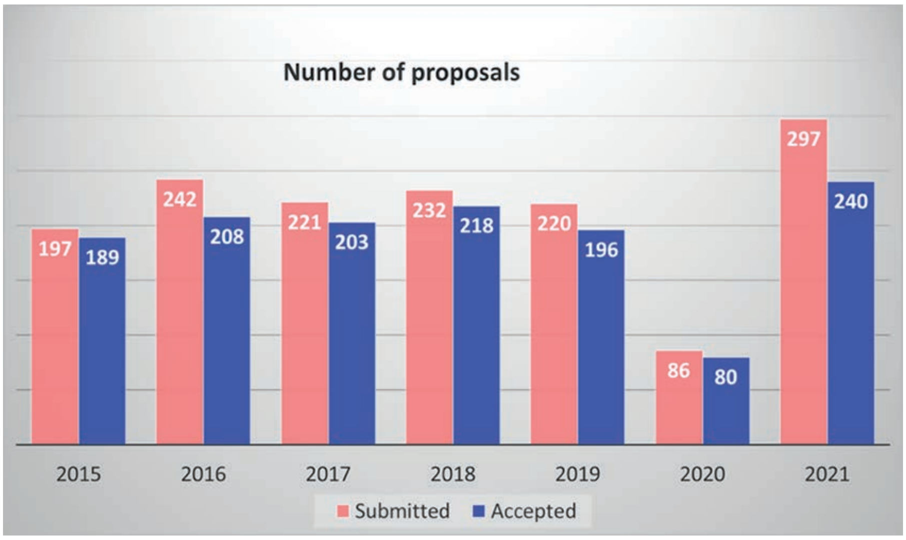


Fig. 2. Distribution of the number of submitted and accepted beamtime proposals by year of proposal submission.

Along with the experimental work carried out by FLNP scientists, attracting researchers from other organizations makes it possible to significantly expand the scientific program implemented on beamline instruments at the IBR-2 reactor and obtain more scientific results reflected in publishing activity (Figure 3).

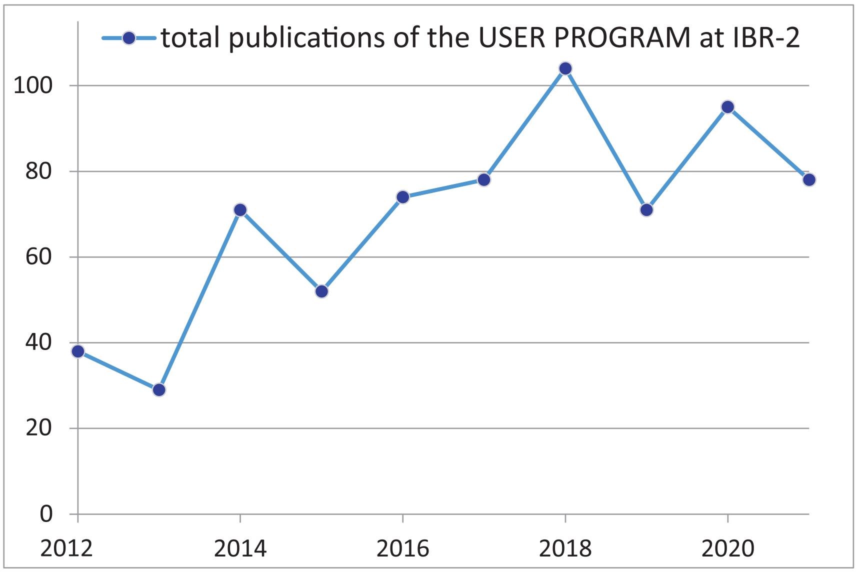


Fig. 3. Number of publications in scientific journals within the FLNP User Program at the IBR-2 reactor.

Taking into account a long and successful experience of IBR-2 operation and new opportunities that the advanced neutron source with its state-of-the-art beamline instruments can provide (for example, an increase in luminosity, more advanced sample environment systems, etc., as well as improved conditions for preparing and conducting experiments), we can expect an increase in the number of new users at beamline instruments from among organizations of the JINR Member States, Associate Members and Partner Countries.

Neutrons in Life Sciences

At present, there is an increased interest in life sciences, which will only grow in the near future for objective reasons. This is due, among other things, to the emergence of new technologies, the growth of computing power, the improvement of the instrumentation base and, as a consequence, the expansion of the range of tasks to be solved. Of great interest is the understanding of the structure and functioning of biological systems, the interaction of individual components of these systems at various space and time levels. The acquired knowledge is used in such areas as biotechnology, medicine, pharmacology, ecology, agriculture. By understanding the structure and mechanisms of functioning of living systems at nanoscale levels, we can regulate their work, correct defects and errors in existing ones, create our own systems with specified properties, that is, create new drugs, new materials, search for new energy sources, etc.

A significant part of information on the structure and dynamics of biological systems (at the level of macromolecules and their complexes) is obtained by such methods as X-ray and neutron scattering, nuclear magnetic resonance, mass spectrometry, electron paramagnetic resonance, fluorescence spectroscopy and electron microscopy. In this series, neutron scattering and spectroscopy techniques occupy a special place due to the unique properties of the interaction of neutrons with matter. These properties are of particular importance when studying biological objects. Neutrons are sensitive to light elements, which are the main elements in living systems: carbon, nitrogen, oxygen, phosphorus, sulfur and hydrogen. These elements are effectively detected by neutrons even in systems in which heavier elements are also present.

Biological objects consist of 50% hydrogen atoms, which are clearly "visible" using neutron methods, including the contrast variation technique. This makes it possible to isolate the scattering contribution of individual components within complex systems. This technique is extremely useful in structural studies of such multicomponent systems as biological membranes, protein complexes with nucleic acids (e.g., chromatin, aptamers with proteins), membrane proteins in a detergent medium, lipoproteins, multicomponent enzymatic complexes, and even entire organelles and cells.

A variety of neutron scattering and neutron spectroscopy techniques can provide both structural and dynamic information. Structural characteristics can be obtained in a wide range of sizes — from one angstrom to hundreds and thousands of angstroms. The spectrum of objects under study is extremely wide: small molecules (water, bioactive molecules, peptides, etc.), biopolymers (proteins, RNA, DNA), aggregates (micelles, model and biological membranes), multicomponent complexes (multi-subunit proteins, fibrils, protein-DNA-RNA, chromatin, lipoproteins), cellular organelles, unicellular organisms (bacteria, viruses), tissues and even multicellular organisms (e.g., plants) (Figure 1.1).

The dynamic properties of biological systems can be studied in wide time and space ranges — from picoseconds to microseconds on scales from 1 Å to hundreds of angstroms, and the resulting spatial information about the structure of living systems can be correlated with their dynamic behavior. Neutrons provide information on autocorrelation vibrations of hydrogen atoms, substrate binding to the catalytic center of an enzyme, conformational mobility of subunits in protein and other macromolecular complexes, diffusion and rotation of lipid molecules in membranes, formation of rafts in membranes, undulation vibrations in the membrane, the process of protein folding, dynamics of the hydration shell of macromolecules and the entire volume of water in cells. At the same time, as in structural studies, selective deuteration can be used to isolate the signal from individual components of the object under study.

The sensitivity of the neutron scattering method can be significantly increased by using polarized neutrons. The neutron scattering length depends on the spin state of the nucleus by which the neutron is scattered and the neutron itself. This property can be used in the study of biological macromolecules. When a polarized neutron beam is scattered by a polarized sample containing hydrogen, the large incoherent cross section of hydrogen decreases sharply, while the coherent signal increases significantly. Polarization of biological macromolecules is a non-trivial task. However, for protein crystals, it is much easier to do, since protein crystals are usually quite small and require small and easy-to-use polarization devices. This makes it possible to study individual atoms within the protein [Zhao et al., 2013; Stuhrmann, 2023].

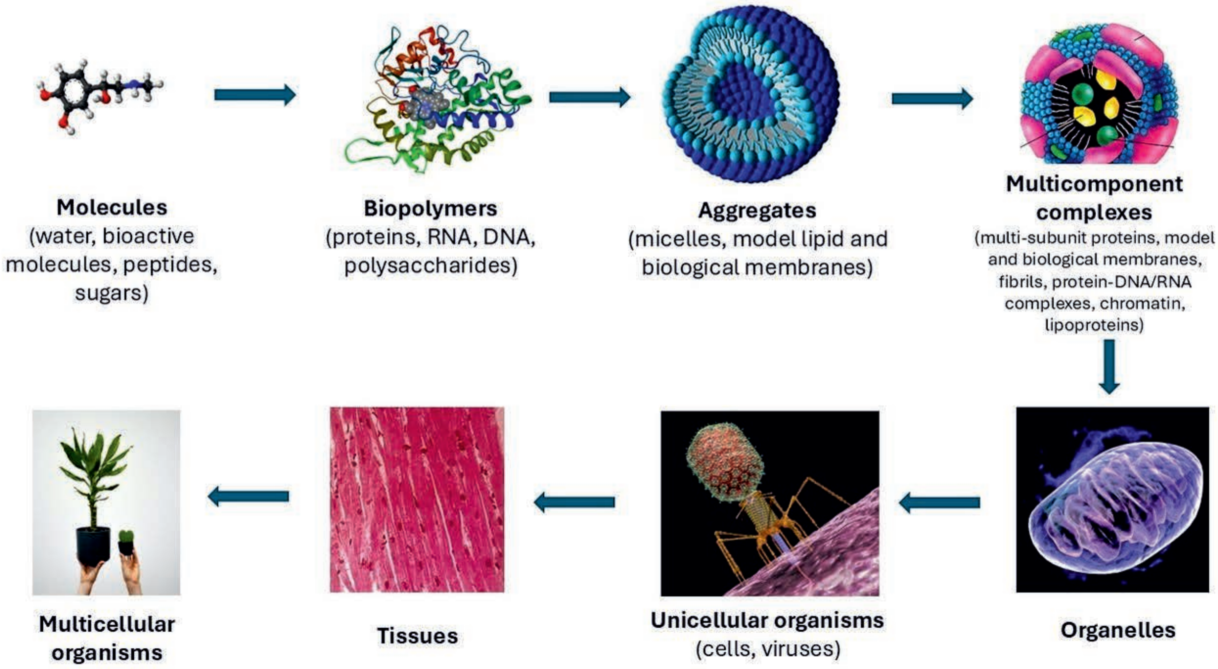


Fig. 1.1. A variety of biological objects studied by neutron methods.

In addition, it is worth noting that neutron scattering methods are non-destructive and deeply penetrating. Thus, they allow us to explore truly living systems in the process of their functioning and in conditions close to native ones. The high penetrating power of neutrons makes it possible to use and create a wide range of sample environment devices for regulating external conditions (for example, temperature, pressure, humidity, magnetic field, etc.).

1.1. HEALTH AND LONGEVITY

Due to their ability to obtain precise information about the position of hydrogen atoms and the geometry of hydrogen bonds, neutrons are widely used to determine the structure and dynamics of hydrogen-rich systems. These are primarily living systems, their complex structure and functioning mechanisms. Malfunctions and impairments that occur in cells at the biomolecular level (functioning of proteins, nucleic acids, membranes, etc.) lead to the development of diseases and sometimes even to the death of the organism. Studies of biomolecules and their interactions contribute not only to a fundamental understanding of the functioning of living systems,

but also to increasing the efficiency in the detection, treatment and prevention of diseases, as well as the development and use of new drugs.

Most diseases are associated with the functioning of proteins, which are the targets of most drugs currently used. This is due to the fact that proteins perform many functions in the body, including regulatory and enzymatic ones. Membrane proteins form a special class. In solution, they can exist only in the presence of stabilizing detergents, lipids, and polymers (Figure 1.2) [Yeh et al., 2020].

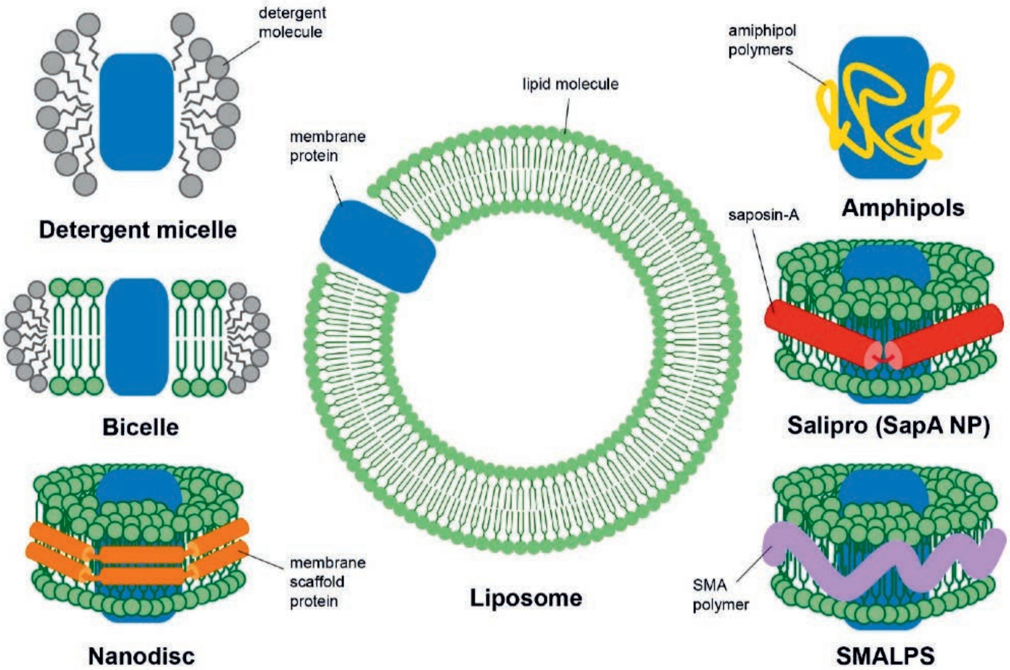


Fig. 1.2. Membrane protein stabilization systems. [Yeh et al., 2020]

Small-angle scattering and reflectometry methods are most often used to study membrane proteins in solution. The protein-lipid or protein-detergent system is heterogeneous. In addition to the signal from the protein of interest, the scattering curve also contains a signal from the detergent 'coat'. This signal must be eliminated because it interferes with the determination of the three-dimensional model of the protein. Neutrons are indispensable here, as they allow to 'shade the coat' by varying the contrast. To do this, one changes the ratio of light and heavy water in the solution, conduct selective deuteration of lipids, detergents, polymers [Maric et al., 2014; Naing et al., 2018; Midtgaard., 2018], as well as the target protein itself or its individual sections [Haertlein et al, 2016]. At the same time, it is possible to determine not only the three-dimensional shape of the membrane protein, but also to observe conformational changes in it in the presence of active molecules, since the object under study is in a solution close to physiological conditions [Josts et al., 2018].

The contrast variation technique is also successfully applied to more complex living systems: mitochondria [Murugova et al., 2011], outer segments of photoreceptor membranes [Feldman et al., 2019], thylakoid membranes [Nagy et al., 2011; Liberton et al., 2013] and even living bacteria [Liberton et al.., 2013]. At the same time, it is possible to carry out the deuteration of the studied systems at the stage of their synthesis or growth, using genetic engineering methods.

Among the most common diseases are cardiovascular diseases, cancer, obesity, diabetes, neurodegenerative diseases, HIV infection, and amyloidosis. A number of neutron methods, such as small-angle neutron scattering, reflectometry, and neutron diffraction, are successfully used to understand the molecular mechanisms of the development of these and other diseases: the kinetics of fibril formation [Eves et al., 2021], genetically determined changes in proteins involved in amyloidosis [Yee et al., 2019], the interaction of amyloid peptides with the lipid membrane [Ivankov et al., 2021; Martel et al., 2017], the interaction of capsid proteins with RNA and the membrane during the formation of viral particles (Figure 1.3) [Datta et al., 2011], etc.

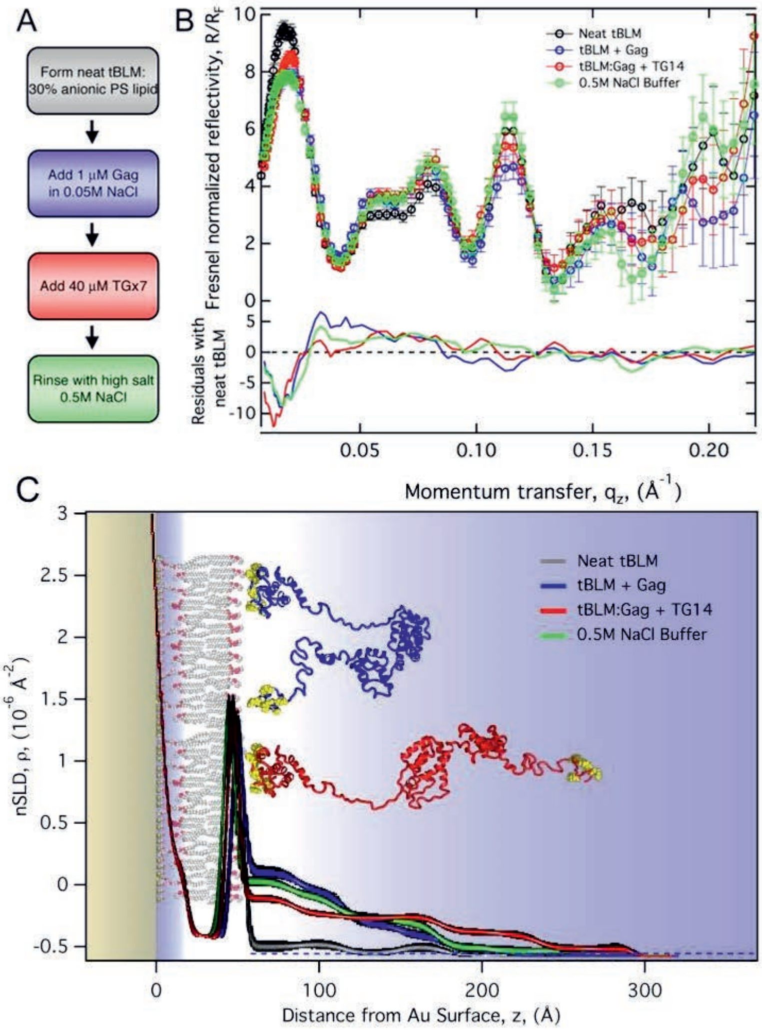


Fig. 1.3. Application of neutron reflectometry to study the conformation of the Gag capsid protein in interaction with the lipide membrane (tBLM) and DNA (TG) [Datta et al., 2011].

Neutron spectroscopy methods (inelastic, quasi-elastic and incoherent scattering) are used to study the dynamic properties of systems under normal conditions and their changes in pathologies. These techniques help to see how genetic mutations lead to a pathological increase in the mobility of certain regions of functional proteins [Takahashi et al., 2011; Matsuo et al, 2013]; how the dynamic properties of lipoproteins change in atherosclerosis [Peters et al., 2017; Cisse et al., 2021], how the mobility of peptide side groups affects the formation of amyloid fibrils and their toxicity [Bousset et al., 2014; Schirò et al., 2012; Tatsuhito et al., 2022]; how the dynamics of water in a cell depends on the type of cancer and the presence of anticancer agents [Martins et al., 2019].

1.2. MEDICINE AND PHARMACOLOGY

1.2.1. Development of new drugs

One of the main problems of medicine is the fight against pathogenic organisms (bacteria, fungi, viruses, etc.). The widespread use of antibiotics has led to the emergence of resistant bacterial species. Therefore, humanity is now looking for alternative antimicrobial agents. Among such agents are antimicrobial peptides, synthetic polymers, pluronics, bacteriophages, metal-based nanoparticles, complexes of polymers and antibiotics, etc. Composite materials with biocidal properties are also being developed, which can be used in the manufacture of medical equipment and instruments, prostheses, protective clothing, air and water filtration systems, which is very important for medical institutions. Neutron research methods are widely used to study the structural and dynamic properties of these materials both at the stage of their development and when studying their response to certain external conditions [Barbinta-Patrascu et al., 2021]. The interaction of antimicrobial agents with the biological membrane (e.g. destruction or formation of pores) [Ivankov, et al., 2021] and pathogen enzymes involved in its reproduction are also studied. Since the systems under study are often complex, the contrast variation technique is widely applicable.

One more method of combating pathogens (especially viral diseases) is vaccination. The structural characteristics of newly developed vaccines, the organization of components inside and their dynamic properties, as well as the interaction of these components with biological systems are studied using a wide range of neutron techniques — from small-angle scattering to spin-echo [Davies et al., 2021; Santamaria et al., 2022; Mamontov et al., 2021; Krueger et al., 2021].

The main target of drugs currently being developed are proteins. The first group of such drugs is aimed at improving and compensating for the functions of human proteins that, for some reason, do not work correctly. The second group of drugs affects functionally significant proteins of pathogenic microorganisms and blocks their work. Rational drug design requires information on the structure of proteins at the atomic level. The main tool for solving this problem at the moment is X-ray crystallography. However, in the case of X-rays, it is very difficult to determine the localization of hydrogen atoms in a protein molecule, since this element has a small number of electrons with which X-rays interact.

Hydrogen plays a central role in enzyme chemistry: it influences local electrostatic interactions and the formation of hydrogen bonds, thereby regulating the interaction of the enzyme with the ligand and substrate (i.e. potential drugs) and the rate of chemical reactions. Determining the positions of hydrogen atoms in a protein, the hydration of the protein, and the type of water molecules in its environment allows to decipher the mechanism of enzyme activity and regulate it: proton transfer; participation of water molecules in their transfer; participation of hydrogen and water in the position of the ligand in the active center of the enzyme; the process of protonation of chemical groups; the intermediate state of the ligand in the process of enzyme functioning. Difficulties arising in determining the positions of hydrogen in a protein molecule are solved using neutron crystallography. It should be noted that the problem of deciphering the structure of the protein and its related ligands is solved by combining neutron and X-ray diffraction with molecular dynamics methods [Ashkar et al., 2018].

In addition to detecting and localizing hydrogen in a protein, neutrons are indispensable in cases where it is necessary to bring the ambient temperature of the sample under study closer to physiological. In the case of X-ray diffraction, the crystal must be kept at liquid nitrogen temperatures to avoid protein destruction under the radiation of X-rays. Such freezing can affect the dynamics of the protein, its ligand, and their interaction. Neutrons, on the other hand, allow experiments to be conducted at room temperatures and avoid temperature-dependent artifacts in structural information (Figure 1.4) [Kovalevsky et al., 2018].

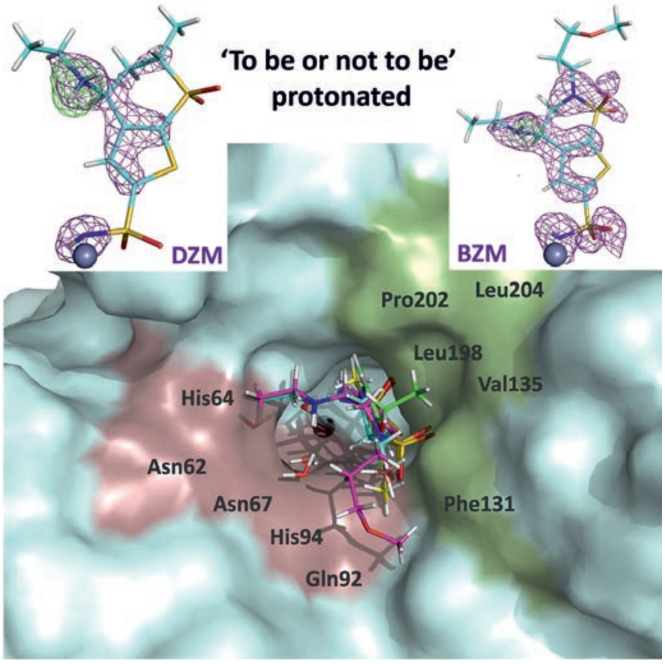


Fig. 1.4. Binding of drugs to the enzyme human carbonic anhydrase. The result was obtained using neutron diffraction [Kovalevsky et al., 2018].

The significant role of neutron scattering methods in the pharmaceutical industry in the development of new drugs is illustrated by examples of the use of neutron reflectometry, neutron spin echo and/or small-angle scattering, which are widely used in the study of the structure, dynamics, physicochemical stability, and functional properties of monoclonal antibodies [Wang et al., 2022b], a number of which have already received therapeutic approval for the treatment of various oncological diseases, migraines, and allergic reactions [Yearley et al., 2013].

As already noted, the unique sensitivity of thermal neutron scattering to light atoms, especially hydrogen, is used to determine their position in the structure of drugs and study their dynamics. For example, in [Kovalevsky et al., 2020], using neutron diffraction, complexes of HIV-1 protease, which plays a key role in the replication of the HIV virus, and clinical drugs for the treatment of HIV (Amprenavir and Darunavir) were studied, as well as changes in the position of hydrogen atoms and the protonation state with pH variations were determined. It was shown that the positions of hydrogen atoms in the catalytic site of the enzyme can change due to drug-resistant mutations or protonation of surface residues, which triggers proton transfer reactions between the catalytic aspartate residues and the hydroxyl group of Darunavir. The configuration of hydrogen bonds in the complexes suggests that Amprenavir and Darunavir are less bound to HIV-1 protease than could be assumed based on X-ray diffraction data.

The high demand for such types of research places special requirements for the parameters of the instruments on extracted beams of the new neutron source at FLNP. Since the maximum achievable sizes of crystals of biological molecules are usually small (tenths to hundredths of mm3), a high-flux neutron source is essential for conducting research aimed at establishing the biochemical mechanisms of drug functioning and developing new drugs.

1.2.2. Targeted drug delivery

With traditional methods of drug delivery (orally, by injection), the active substance enters the systemic bloodstream and spreads throughout the body. In most cases, only a small portion of the administered substance reaches its target. In this case, an increase in the concentration of the administered drug is required. At the same time, the drug may become toxic to other organs. This is especially important in cancer therapy, when drugs are used that kill not only cancer cells, but also healthy ones. Therefore, work is currently underway to develop targeted drug delivery. Drug carriers must have the following properties: biocompatibility; stability during transportation to the destination; transport and recognition ability; controlled release of the drug. All the described properties of transport systems can be studied using neutron diffraction. The main methods here are small-angle and inelastic neutron scattering.

At present, the main types of carriers being developed are liposomes, polyplexes, metal nanoparticles, microgels, micelles, graphene, fullerenes, pluronics, etc. Neutron scattering can be used to study these objects both at the stage of their synthesis [Draper et al., 2020; Shugare et al.] and at the stage of monitoring the structural and dynamic properties of these systems under various external conditions (temperature, pH, concentration of regulatory molecules, ultrasound, magnetic field, light, etc.) [Suner et al.]. Obviously, for objective reasons, research into drug carriers will not lose its relevance in the future.

1.2.3. Prosthetics and implants

As a result of diseases, accidents, and age-related changes, a person may lose some part of the body, organ, or tissue. One of the goals of modern science is to improve the quality of life of people in such situations. For this purpose, developments are underway to replace and restore damaged or lost tissues and organs using prostheses and implants. To achieve this result, neutron methods help to study the structural and mechanical properties of materials developed for the creation of implants [Cobo et al., 2015; Ahmed et al., 2011; Törnquist et al., 2021].

The main materials used are metal alloys, ceramic compounds, carbon materials (nanotubes, fullerenes, graphene) and polymers, as well as composite materials. Implants must be biocompatible, bioinert, resistant to corrosion and, in certain cases, biodegradable. Biodegradable materials are needed where implants perform a temporary function: bone fasteners, drug delivery devices, polymer matrix scaffolds for the restoration of living tissue, suture materials, monitors of vital signs of the body (temperature, pressure, oxygen and glucose concentration, etc.). Neutron investigations help to understand the behavior of such materials under various external conditions (e.g., under the influence of the environment of a living organism). Owing to neutron diffraction studies [Ahmed et al., 2011], it was found that, although heat treatment of the coating leads to a decrease in residual compressive stresses in the implant near the interface and increases the degree of crystallinity of the coating, further exposure to model body fluids again increases the level of residual stresses.

Neutrons also help to observe the aging processes of implants and their fusion with living tissues [Burns et al., 2014]. This process is well visualized by neutron tomography [Isaksson et al., 2017] (Figure 1.5). In certain situations, depending on the sample under study, neutrons have better contrast compared to X-rays, better detail and the absence of artifacts in the image (for example, for metal parts) [Isaksson et al. 2017; Metzke et al. 2011]. In addition, neutrons have a high penetrating power and make it possible to study samples with a large thickness.

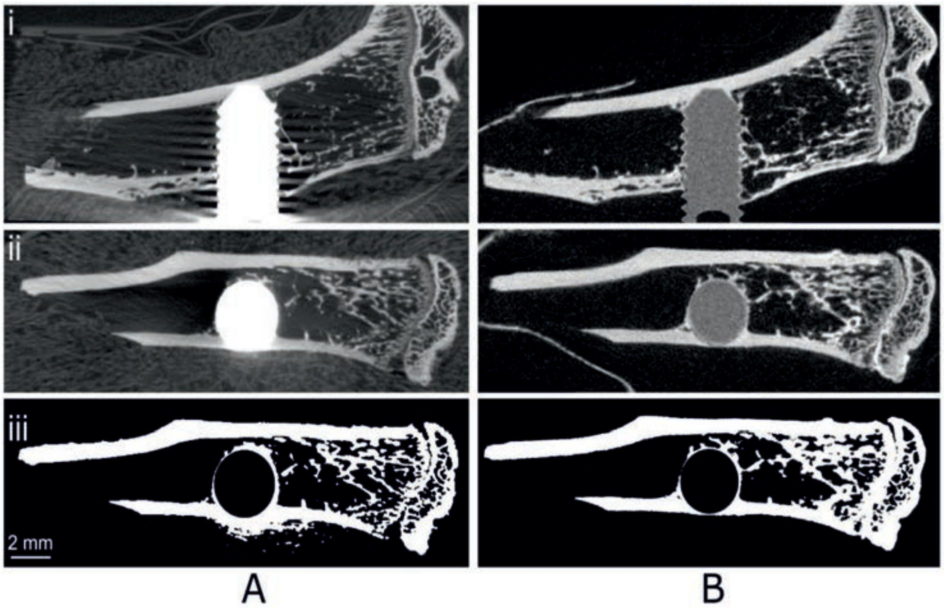


Fig. 1.5. Growth of bone tissue on a metal implant. Comparison of X-ray (left) and neutron (right) tomography results [Isaksson et al., 2017].

1.3. ENVIRONMENT, FOOD AND ECOLOGICAL PROBLEMS

As a result of human economic activity, the environment changes, often for the worse: pollution of the atmosphere, water, soil; climate change; extinction of some species of animals and plants; depletion of natural resources. Humanity is faced with the task of stopping pollution and getting rid of existing environmental contamination. The use of neutron methods in environmental studies plays an important role. In particular, neutron activation analysis is used to monitor the pollution of soil, air and seafood with heavy metals [Frontasyeva et al., 2020; Nekhoroshkov, et al. 2021] (Figure 1.6). Also, neutron methods help in the development of technologies for treating wastewater and water bodies [Zinicovscaia et al., 2020; Hellsing et al., 2014].

Neutron activation analysis has long been successfully employed at the IBR-2 reactor. Using this technique of elemental and isotopic analysis, it is possible to determine more than 70 elements with a ppm-level accuracy (10^{-6} g/g) [Nazarov, 1985]. The advantages of the method are high sensitivity and comparative ease of implementation at a research reactor.

At a fundamental level, neutrons can be used to study the impact of atmospheric pollution on climate and the production of environmentally friendly food [Jones, 2017; Thompson, 2013]. To avoid increasing pollution, it is necessary to develop new, efficient and safer technologies for the use of fertilizers and agricultural pesticides, as well as new active materials for the elimination of the consequences of man-made accidents. Neutron methods (small-angle scattering, diffraction, inelastic and quasi-elastic scattering, reflectometry, etc.) can help to solve these problems, making it possible to study the structural characteristics of such materials and their behavior under certain external conditions. For example, to observe the process of pesticide release from the micellar shell upon contact exclusively with the waxy coating of a plant leaf [Pambou, 2018] or the process of absorption of crude oil from the water surface by surfactant gels [Owoseni, 2018].

Fig. 1.6. Sampling map of moss biomonitors for monitoring heavy metal pollution. Studies using neutron activation analysis [Frontasyeva et al., 2020].

In the 21st century, neutron scattering methods have become widely used in research at the intersection of materials science, dietetics and food industry technology to improve production methods, improve the quality and value of food products [Lopez-Rubio & Gilbert, 2009]. In situ small-angle neutron scattering is used to study the dynamics of enzymatic degradation of starch, dissociation, aggregation, unfolding of various proteins contained in milk, including, for example, the main allergen of cow's milk — beta-lactoglobulin [Texeira, 2019; Wu et al., 2023].

The concept of glass transition is of great importance not only for polymer physics but also in food research [Odarchenko & Sergienko, 2015; Witek et al., 2021]. The combined use of neutron diffraction and deep inelastic scattering, as well as neutron transmission measurements, made it possible to determine the glass transition temperature of rice noodles, as well as the changes in the secondary structure of starch in dry noodles accompanying the glass transition [Witek et al., 2021]. Such studies are extremely useful for studying the quality and stability of frozen or freeze-dried food, as well as new food products and related processes, which we will undoubtedly encounter more and more often in the future.

Thus, to conduct effective research at the future advanced neutron source at JINR, which would contribute to environmental protection, solving problems in ecology and food industry, it is necessary to provide for the development and construction of a number of instruments: NAA facility, diffractometers, a quasi-elastic/inelastic scattering spectrometer, a reflectometer, and a small-angle scattering instrument. The enhancement of the fluence and neutron flux in extracted beams is critically important for such studies in order to increase the number of samples studied, improve statistics, and develop the methodology of neutron elemental analysis.

1.4. ADAPTABILITY AND RESISTANCE OF LIVING SYSTEMS TO STRESS

Living organisms encounter various stress factors during their life: radiation, active forms of oxygen, pressure changes, critical temperatures. At the same time, there are organisms in nature (archaea, bacteria, yeast, algae, fish) that live in conditions of high salt concentrations, extreme pH values, high or low temperatures, etc. In addition, it is known that cancer cells are also capable of adapting to stress conditions during antitumor therapy. Extremophiles are an incredibly interesting object for research and open up prospects in science, medicine, biotechnology, industry and space exploration. Studying biomolecules isolated from such organisms will help to understand the mechanisms that allow them to maintain their activity in the most extreme conditions. For example, it is possible to develop unique nanomaterials based on the adaptive principles of organisms adapted to harsh conditions. By studying antifreeze proteins, it is possible to develop cryoprotection technologies for industry and medicine. Understanding the mechanisms of resistance of some bacteria to high acidity will help in the fight against pathological organisms that survive even in the stomach environment, etc. The evolution of the dynamics and structural features of such living systems and their individual components (membranes, proteins, macromolecular complexes, etc.) can be traced using neutron methods. For example, neutron methods are already being used to study the features of the dynamics of intracellular water and proteins in extremophile cells [Tehei and Zaccai, 2007; Zaccai, et al., 2022], the role of osmolytes in cryo- and bioprotection [Al-Ayoubi, et al., 2017; Zaccai, et al., 2016; Magazù et al., 2012], oligomerization of sensory complexes depending on external conditions [Ryzhykau, et al., 2018]. 2021] (Figure 1.7), organization of cellular proteins under dehydration and high pressure [Erikamp et al., 2015; Minezaki Y. et al., 1996].

The tardigrade, a microscopic invertebrate, can survive extreme temperature changes, prolonged dehydration, ionizing radiation, and space vacuum. It has specific defense and repair systems. For example, its cells produce a large amount of a specific disordered protein, Dsup (damage suppressor), which binds to DNA and protects it from harmful effects of radiation and reactive oxygen species. Studying the complex formation of such proteins with DNA is an excellent task for neutron scattering, since such a system is heterogeneous for neutrons, and it is possible to use the contrast variation technique for structural and dynamic studies of both the entire complex and the individual behavior of the components in the complex. At present, there is a growing interest in disordered proteins. It has become clear that not all proteins need to have an ordered three-dimensional structure to perform their functions. It has turned out that about 30% of all eukaryotic proteins are disordered. They perform vital functions in cellular regulation and signaling. **An advanced high-flux neutron source will allow expanding the application of neutron methods for studying this and other groups of important proteins, since these systems have small scattering cross-sections, and the contrast variation technique reduces the scattering intensity. At the same time, time-resolved experiments with changing external conditions require high fluxes of the incident beam.**

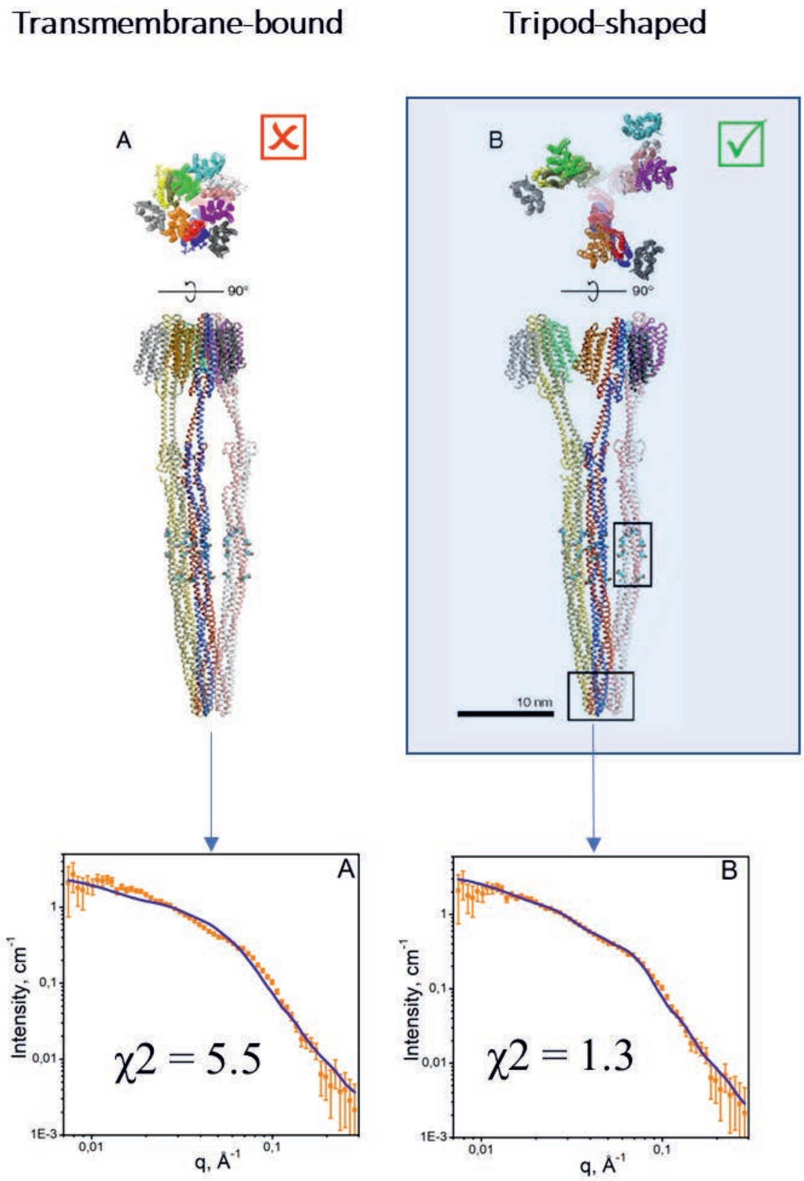


Fig. 1.7. Study of the oligomeric state of a photoreceptor using small-angle neutron scattering combined with the molecular dynamics method. The use of neutrons made it possible to study the protein complex under conditions of high salt concentration [Ryzhykau, et al. 2021].

1.5. BIOTECHNOLOGIES AND BIOROBOTS

Mechanisms and technologies invented by man already have their analogues in living systems. The cell has its own power plants, electrical networks, transport, chemical and processing plants, machine tools and machines, information storage and transmission systems, electrically conducting systems, etc. However, unlike human-made machines, biological mechanisms have nano- and micro-sizes. Therefore, biological prototypes can be used both to develop new nature-like technologies and to use cellular elements to produce nanorobots. This will help to solve problems in many areas — from medicine and ecology to information technologies: controlled drug delivery, biosensorics, microsurgery, monitoring of toxic compounds and cleaning the environment from them, development of new types of information storage and signal processing, conversion of different types of energy, creation of biofuel, optoelectronic and photonic devices, etc. (Figure 1.8). To implement such technologies, it is necessary to understand the structure of biological systems at the molecular level and their interaction, as well as the response of these systems to exposure to light, electromagnetic fields, changes in temperature and concentration of chemicals.

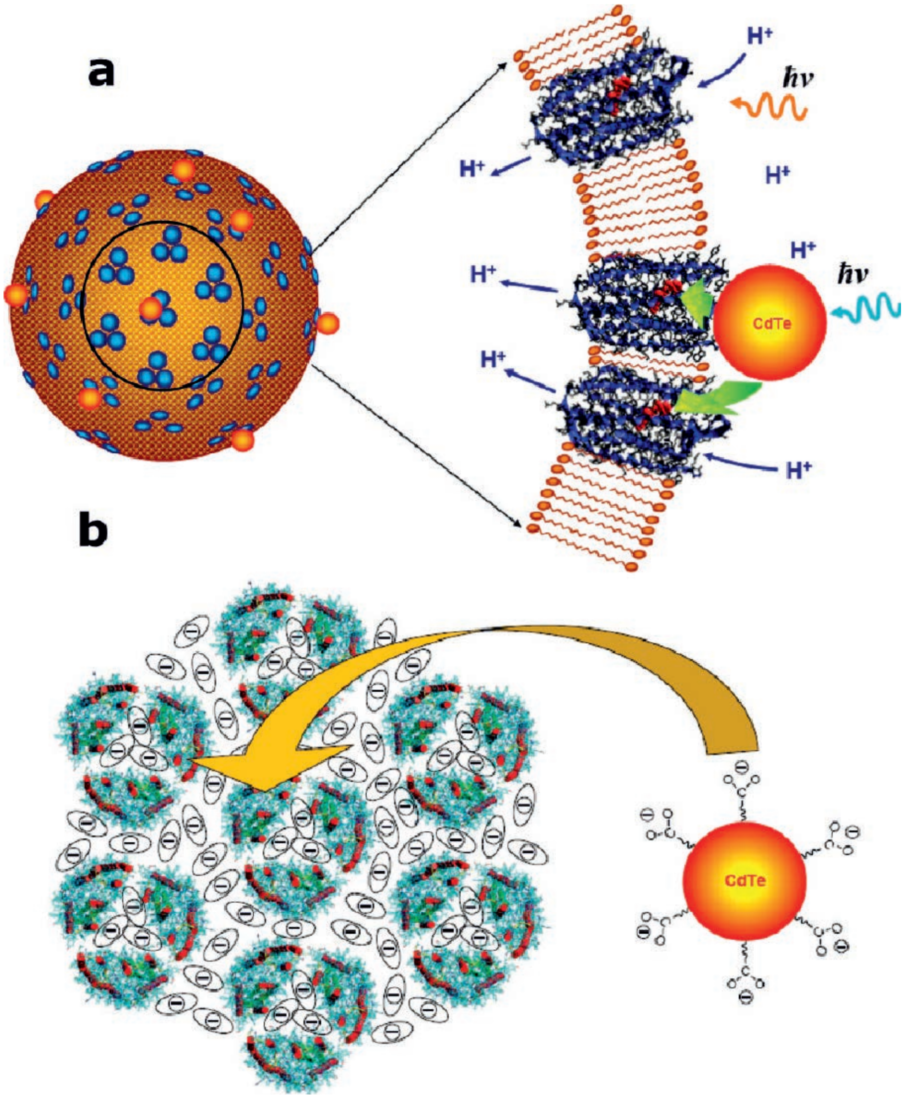


Fig. 1.8. Nanoscale solar energy converter developed on the basis of bacterial purple membrane and quantum dots [Rakovich, et al., 2010].

Nanorobots are biohybrid objects. To study such systems, it is desirable to use the neutron contrast variation technique. In addition, the interaction between components in these systems, their mutual motion, orientation and oscillatory movements can be studied in a wide range of amplitudes and times using neutron spectroscopy. In relation to structural characteristics, neutron methods can be used in studying the processes of nanorobot assembling, the synthesis of its individual components, in investigations of systems of toxic elements coated with an active biocompatible material, in monitoring structural/dynamic transformations in the system after its targeted modification or changes in external conditions [Toolan, 2022; Rakovich, 2010; Peters, 2016].

At present, technologies for growing organs on a chip are already being implemented, which are used for testing pharmaceutical and chemical compounds and biomaterials [Leung, 2022], as well as epidermal electronics, which make it possible to monitor vital signs and, depending on their values, administer the necessary drugs (for example, insulin patches) [Kim, 2011]. The components of these systems are materials that are actively studied by neutron methods, for example, widely known hydrogels and other polymers.

1.6. RADIOBIOLOGICAL RESEARCH USING NEUTRON SOURCES

1.6.1. Investigations of relative biological effectiveness of mixed radiation fields of neutron sources

In most fundamental radiobiological studies on the problem of relative biological effectiveness (RBE) of ionizing radiation, monoenergetic particle beams have been well studied. In practically important cases of man-made and natural neutron sources, as a rule, there is a continuous energy spectrum, which also includes gamma-rays. The solution to the problem of RBE of mixed radiation fields, firstly, should be based on the development of computational and experimental dosimetry methods that make it possible to determine the kerma and absorbed dose directly in biological objects with maximum accuracy, and secondly, on the assessment of biological effects using modern methods of molecular radiobiology, radiation genetics and radiation physiology. The organization of this kind of research should provide for the possibility of manipulating the radiation spectrum (isotope sources, neutron generators, extracted neutron beams), as well as placing biological objects (cell cultures and small laboratory animals) in special containers and holders. At the same time, it is necessary to observe radiation safety measures (in particular, prevent the activation of containers) and necessary sanitary standards in the room (cleanliness, temperature, humidity, etc.).

1.6.2. Studies of the mechanisms of action of radioprotectors on laboratory animals

The availability of a large number of man-made neutron sources raises the question of protective measures, in particular, the search for promising radioprotectors. Testing of the mechanisms and effectiveness of radioprotective drugs developed in specialized institutes of the JINR Member States can be organized using extracted beams of the reactor. In this case, it is necessary to conduct total irradiation of the body of small laboratory animals (mice, rats), which requires sufficient width and uniformity of the beam. The irradiated animals are then sent to the vivarium of the LRB, where studies are performed on their behavioral reactions using specialized test systems and pathomorphological changes in various critical organs and systems of rodents using modern histological and immunohistochemical methods.

1.6.3. Radiobiological aspects of neutron capture therapy of cancer

One of the promising methods of treating malignant tumors is neutron capture therapy. This type of therapy is based on the use of pharmaceuticals to deliver compounds of certain stable isotopes to tumor cells and subsequent irradiation with epithermal neutrons. High biological efficiency in the selective accumulation of an isotope in a cell is determined by short-range products of the neutron capture reaction, which, depending on the isotope, can be conversion and Auger electrons (gadolinium-157) or alpha particles (boron-10 and lithium-6). Radiobiological research in this area is aimed at finding biological mechanisms for the selective accumulation of these isotopes in tumor cells and other ways to ensure maximum biological efficiency of neutron-capture reaction products. The organization of radiobiological research on cell cultures and small laboratory animals requires the extraction of an intense beam of epithermal neutrons from a reactor with a minimal admixture of gamma-radiation or a neutron-producing target of an accelerator. Also, an important task is the development of methods for dosimetry and visualization of the accumulation of isotope-containing preparations.

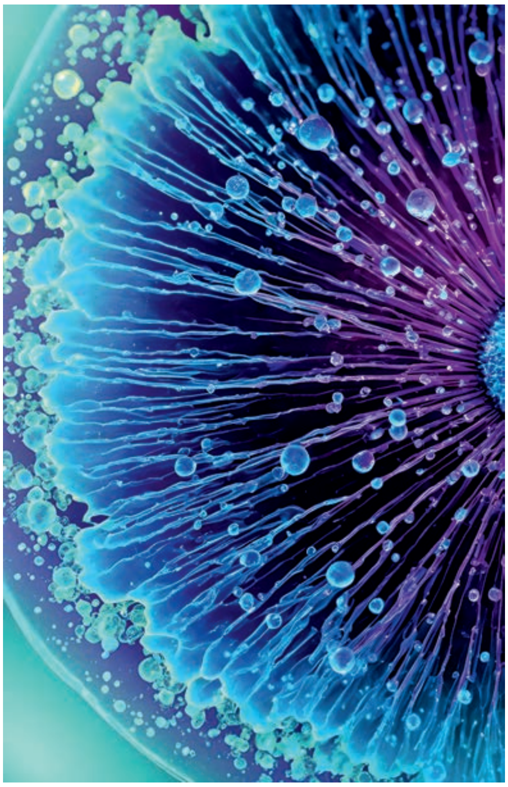
1.6.4. Structural studies of biological samples

Methods for structural studies of biological samples available at FLNP, in particular small-angle X-ray and neutron scattering, can be effectively applied to the analysis of radiation-induced effects in living systems. For example, studies of conformational changes in transmembrane proteins and damage to cellular organelles in the structures of the central nervous system can shed light on the mechanisms of radiation-induced neurodegenerative processes, which is very important in studying the side effects of radiation therapy, assessing the radiation risks of cosmic types of radiation, and studying the mechanisms of development of brain diseases. Studies of the mechanisms of transport into tumor cells of certain classes of molecular complexes for targeted delivery of radiosensitizers, contrast agents for tomography and drugs used in theranostics are of great importance for the development of medical radiobiology and nuclear medicine.

1.6.5. Astrobiological investigations

Investigations in the field of astrobiology are primarily aimed at studying the mechanisms of synthesis of prebiotic compounds of simple organic molecules (e.g., formamide) in the presence of meteorite matter or rocks of planetary systems under irradiation with hadron beams. Pioneering studies in this area using proton beams have revealed the formation of various prebiotic compounds in reaction mixtures including amino acids, carboxylic acids, sugars, nucleic bases, and even nucleosides. The mechanisms of such radiation catalysis are the subject of further detailed research. This raises a natural question whether such kind of synthesis is possible when samples are irradiated with neutron beams. Complementary astrobiological studies of the elemental and structural composition of cosmic matter to search for traces of organic compounds and remains of living organisms can be carried out using the FLNP infrastructure by neutron activation analysis and energy-dispersive X-ray spectroscopy techniques.

1.7. NEUTRON RESEARCH IN LIFE SCIENCES AND DEVELOPMENT OF SCIENTIFIC INFRASTRUCTURE



Currently, there is growing interest in understanding the architecture of living systems and the processes occurring in them. Such understanding will help to create new biomaterials and develop biotechnologies, control biosystems and organisms, develop systems with specified characteristics, and implement nature-like technologies. Main objects of research **at the advanced neutron source at JINR** are:

- macromolecules (proteins, DNA, RNA, lipids);
- biological membranes and membrane proteins;
- disordered proteins;
- multicomponent biocomplexes (enzymatic systems, protein-lipid, protein-nucleic acid complexes, etc.);
- signaling systems (receptors, photosystems);
- biohybrid materials;
- polymers;
- tissues;
- organelles and living cells.

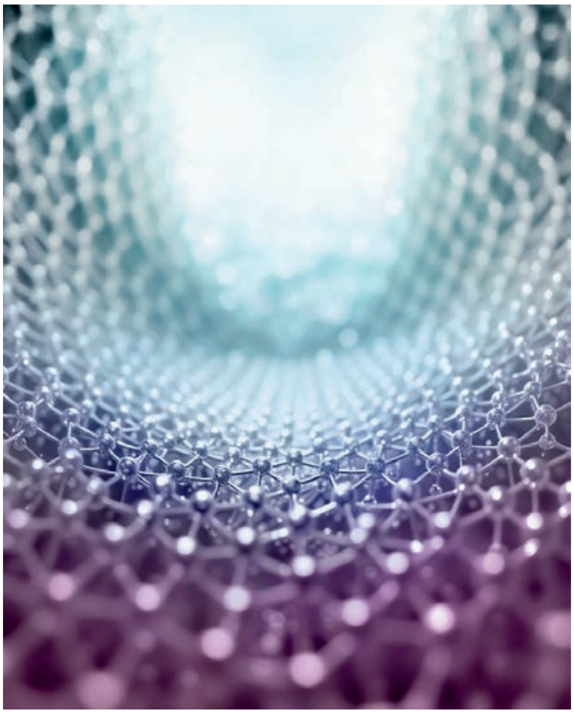
Such methods as small-angle neutron scattering, diffraction from macromolecular crystals, reflectometry, neutron spectroscopy (inelastic scattering, inelastic spin echo, quasi-elastic scattering, incoherent scattering), neutron tomography and neutron activation analysis have great potential for use in studying these objects.

It is also necessary to outline a number of technical and organizational tasks, the solution of which is required for more complete implementation of scientific research using neutron scattering methods:

- Creating a laboratory for the production of deuterated compounds and the deuteration of biological objects, crystallization of proteins.
- Creating a base for the joint use of several methods complementary to neutrons (X-ray scattering, nuclear magnetic resonance, electron and cryo-electron microscopy, molecular modeling, dynamic light scattering, etc.).
- Increasing computing power that will allow modeling complex multicomponent systems and comprehensively analyzing results obtained by several complementary methods.
- Development of infrastructure at scattering instruments for studying the structure and mechanisms of functioning of multicomponent complexes directly in the cell.

Extending possibilities for time-resolved experiments to study processes induced by light or signaling chemical molecules, as well as changes in ionic strength, pressure, temperature, etc.

Nanosystems and soft condensed matter



Nanosystems are the systems that have at least one dimension on the nanometer scale (1–100 nm). They include nanoparticles (NPs), nanocomposites and other nanoscale materials. Another group of nanosystems referred to as "soft matter" covers a wide range of materials and systems that have unique physical properties due to a high degree of internal disorder. These systems exist in the states that are not related to the "simple" liquid or crystalline states studied in classical solid-state physics. Soft matter includes polymers, colloids, liquid crystals, gels, surfactants, and others. All these systems can be classified in different ways basing on a variety of characteristics or properties, such as size, dimensionality, composition, functionality, etc. For example, depending on the materials incorporated into a system, they can be divided into carbon nanomaterials, inorganic and organic nanomaterials, composite nanomaterials. In terms of dimensionality, three-dimensional (3D), planar (2D), linear (1D) and nanodispersed (0D) materials, nanocomposites and supramolecular materials can be distinguished.

Among the current tasks of modern research of these systems, the following areas can be highlighted: synthesis of advanced nanomaterials/soft matter, application of nanomaterials (*in situ*, *in operando* research), basic knowledge (physical and chemical properties of nanosystems, interactions in ensembles of nanoobjects, irreversible processes in nanosystems), modeling of nanosystems and processes. In addition, environmentally friendly, biodegradable materials are of great relevance for almost all of the above mentioned systems.

The scientific program of the advanced neutron source at JINR in the area of soft matter and nanosystems is aimed at applying the possibilities and main advantages of neutron scattering to study the properties, structure and dynamics of a wide range of materials. The new pulsed neutron source is expected to start operation in the 2040s and will be equipped with a suite of modern instruments, including small-angle instruments, reflectometers and neutron spectrometers, which are essential for this area.

In the area of soft matter and nanosystems, materials such as polymers, surfactants, thin films, nanocomposites and complex multicomponent systems are of great interest to researchers. These materials play an important role in many areas of modern science and technology, including chemistry, physics, biotechnology, materials science and biomedicine. Using neutron scattering methods, users will be able to study basic properties of these materials and systems at the atomic and molecular levels, which will provide new insights into their behavior and potential applications. In this area, it is extremely important to understand both the slow dynamics and large-scale processes in multicomponent systems. The new neutron source instrumentation will make it possible to conduct experiments with a previously unattainable time resolution, which will allow a new level of study of the assembly of hierarchical structures, the dynamics of phase transformations and the kinetics of highly non-equilibrium processes in relevant nanosystems. The key factor will be the high neutron flux density on the samples under study. While continuing to exploit the advantages of neutrons (sensitivity to light elements and isotopes, non-destructive interaction, high penetrating power and magnetic scattering), **experiments at the new neutron source will enable efficient study of samples in an environment approximated to real industrial and natural processes and conditions.**

2.1. POLYMERS

Polymers represent a broad class of systems and a huge area of scientific research, related to a variety of practical applications in almost all types of human activity. Over the past decades, polymer synthesis technologies have come a long way, and it has become possible to synthesize complex copolymers, as well as polymers with low polydispersity [Lutz, 2016]. At the same time, the search for new polymerization methods remains a serious challenge for the chemistry of synthesis of new materials [Abd-El-Aziz, 2020]. Neutron scattering plays an important role in determining the structure and dynamics of complex polymers and polymer-based complex systems, as well as in studies of relaxation and behavior of polymer systems under various extreme conditions. For example, small-angle neutron scattering (SANS) was used to study three-armed polymers [Mortensen, 2018; Mortensen & Annaka; 2018]. A three-armed polymer with deuterated outer parts of the chains was synthesized from polystyrene, which makes it possible to effectively use the advantages of neutron contrast. Using SANS data from such a system, it is possible to effectively determine the orientation of individual copolymer chains in the melt. Among other things, there is also a fundamental interest in these studies: the results obtained make it possible to test the applicability of statistical physics models [de Gennes, 1971] to polymer systems under extreme conditions. Here, a heated copolymer sample was stretched, then cooled rather quickly, and the relaxation process was successively monitored. The SANS results are shown in Figure 2.1, where three stages of relaxation are observed. During the first stage, the horizontal SANS peaks are blurred and disappear (i.e. the characteristic distance between the 'legs' disappears). At the second stage, the vertical peaks smooth out and change shape, which indicates that the elongated arrangement of the polymer in the reptation tube is disrupted, the macromolecular chains become entangled, and the pronounced length and orientation disappear. Finally, at the third stage of relaxation, which lasts an order of magnitude longer than the previous ones, the microstructure of the melt passes into an isotropic state.

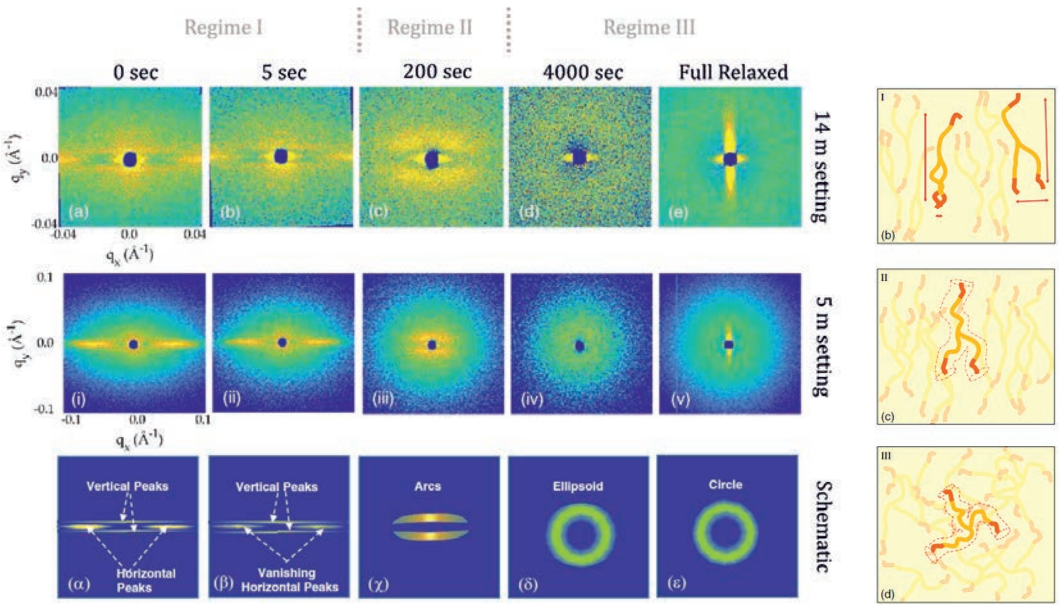


Fig. 2.1. Left: SANS data for the relaxation kinetics of a three-armed copolymer (polystyrene). Right: schematic representation of the characteristic structure of the system at different stages of relaxation [Mortensen et al., 2018; Mortensen & Annaka; 2018].

The combination of computer modeling and scattering experiments for high-precision studies of the structure and dynamics of polymers and polymer-containing systems will play an increasingly important role in the future research. First of all, this refers to the measurement of static and dynamic structure-factors. In this regard, the synergy of two methods — neutron scattering and molecular dynamics (MD) modeling — can be noted [Arbe et al., 2020], which has a wider range of scattering vectors and larger time ranges at the microscale. Thus, the research approach proposed in [Arbe et al., 2020; Colmenero et al., 2013; Genix et al., 2015] involves iterations of system modeling, adjusted through detailed comparison with neutron experiment data. After a sufficient number of iterations, a description of the system with acceptable quality is achieved. The MD model is then used as a basis for the next research stages of the study and description of the system. In this case, the contrast variation in the neutron experiment (due to deuteration of different parts of the polymers) allows for a more detailed comparison with MD (and, therefore, better fine-tuning of the simulation parameters). For example, in [Genix et al., 2006] polymethyl methacrylate (PMMA) was studied in detail, including the effective application of the neutron spin-echo (NSE) method at various temperatures (Figure 2.2). **It is important to note the great significance of the expansion of the experimentally achievable time range τ for NSE, which will be available at the new source. This will allow obtaining new dynamic information at different time scales for the systems (Figure 2.2).**

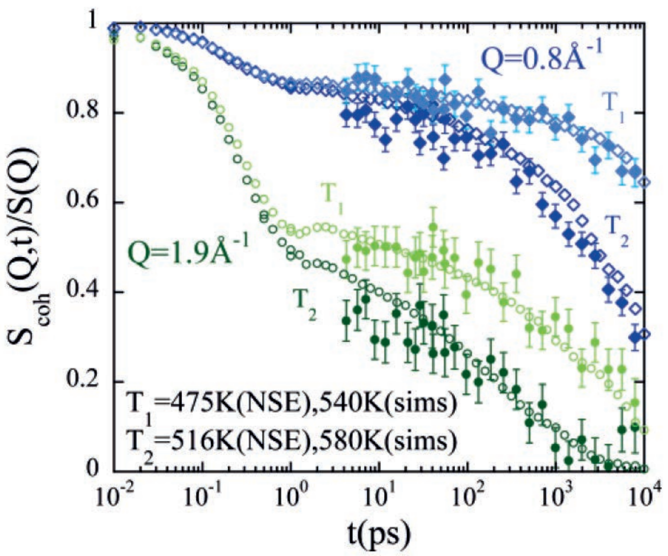


Fig. 2.2. Dynamic structure-factor of PMMA at different temperatures; comparison of experiment with MD simulation data [Genix et al., 2006].

Neutron scattering as a complementary method also plays an important role in studies of polymer glass transitions. For example, in [Chua et al., 2017], a number of measurements were performed using differential scanning calorimetry (DSC), while the neutron spin echo method was used to track the polymer dynamics in direct space. These measurements show that even at high temperatures, the structure-factor mainly exhibits a "plateau". Here, the extension of the time range provides additional and new information, so this is an important component of complex experiments. Regarding the studies of polymer glass transitions, this information is critical to achieve a full understanding and description of these physical phenomena. **Thus, to conduct detailed studies of the entire spectrum of excitations and relaxations in polymers at the new source, it is necessary to develop and construct several spectrometers that complement each other in terms of time range, energies and momentum transfer.**

2.2. SURFACTANTS

Modern research on surfactants focuses on the study of various micelles formed from these molecules. For instance, a typical example of nowadays systems are the so-called worm-like micelles. Such systems can form interesting structures with promising properties for various applications. Of particular interest are worm-like micelles formed by Gemini surfactants [Chen et al., 2017], [Fan et al., 2019]. In this case, various diamines are added to sodium dodecyl sulfate. This system was studied by SANS in combination with cryo-TEM. When the fraction of added diamines is small, the scattering is well described by the model of a solution of globular micelles. With an increase in the diamine concentration, the symmetric form-factor no longer fits the SANS data. It is observed that the micelles become elongated, and it is necessary to use an ellipsoidal model. Further, the ellipticity increases tenfold [Fan et al., 2019], which is indicative of the formation of worm-like micelles. In this case, SANS plays a key role in determining the morphology of the system.

In [Murphy et al., 2020], studies of worm-like micelles are complemented by the rheoSANS method [Eberle & Porcar, 2012]. The successful application of SANS for studying rheology and nanostructures in complex fluids is demonstrated in a wide (8 orders of magnitude) range of shear rates in capillaries hundreds of micrometers thick (Figure 2.3). In the absence of a flow, an isotropic scattering function $I(q_x,q_y)$ is observed. When liquid flows through a capillary, the SANS signal expands asymmetrically in the direction opposite to the flow. This suggests that there is a rearrangement of the internal structure induced by the hydrodynamic flow. After exceeding a certain flow rate threshold, the micelles align along the flow with the anisotropy factor reaching 65%. However, at even higher flow rates, this factor begins to decrease. This is explained by the fact that higher flow rates lead to the disruption and partial transformation of worm-like micelles into smaller cylindrical micelles that are less oriented and can rotate across the flow [Murphy et al., 2020].

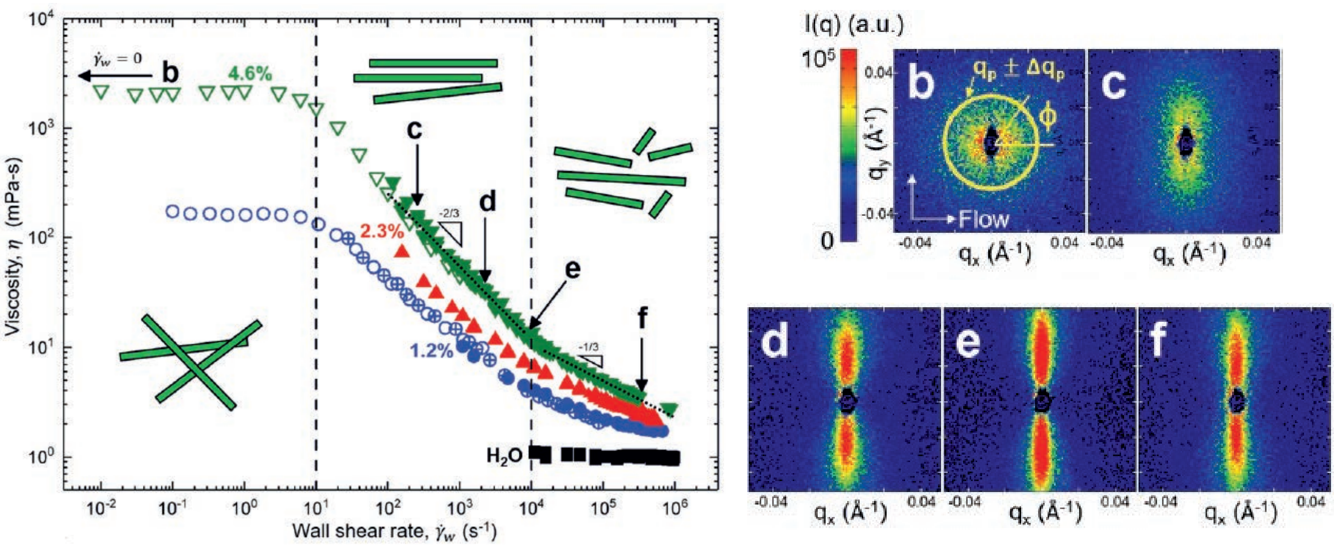


Fig. 2.3. Steady-state flow viscosity measurements of a solution of worm-like micelles at different concentrations. The corresponding 2D SANS data are shown on the right for different flow rates [Murphy et al., 2020].

It is worth mentioning that in such kind of in situ studies, flow rates are comparable to those in a number of industrial systems, which is of great practical importance. Accordingly, in addition to great fundamental interest, such studies also have significant practical value.

2.3. MAGNETIC FLUIDS

Magnetic fluids (or ferrofluids)—highly dispersed solutions of ferro- or ferrimagnetic nanoparticles (~3–30 nm in size)—have been studied for over 50 years [Vékás et al., 2007], [Avdeev et al., 2011]. A distinctive feature compared to magnetorheological fluids is that they do not undergo phase separation. Magnetic fluids are widely used in technical devices. The current tasks in this area, as in general for colloidal systems, are the development of methods for the synthesis of stable magnetic fluids with specified properties. In these studies, neutron scattering, including magnetic scattering, plays a major role [Avdeev et al., 2011]. Thus, in studies of magnetic nanoparticles, SANS and neutron reflectometry methods are actively used. For example, the structure of adsorption layers on silicon from magnetic fluids stabilized by oleic acid and polyethyleneglycol (PEG) was compared [Gapon et al., 2017], [Kubovcikova et al., 2017]. It was shown that nanoparticles are adsorbed from the magnetic fluid stabilized by oleic acid onto the silicon surface, which is manifested in a qualitative difference in the reflection curve from the Fresnel curve. If the magnetic fluids are stabilized by a polymer, such behavior is not observed, mainly due to the formation of aggregates in the bulk of the solution.

More recent studies have used chemical modification of the SiOx surface to initiate the adsorption of nanoparticles onto the substrate [Theis-Bröhl et al., 2020]. Using neutron reflectometry, a dense layer of nanoparticles is observed, the structure of which can be controlled using a magnetic field (Figure 2.4). The presence of an adsorbed monolayer of nanoparticles at the surface leads to the formation of a secondary layer of nanoparticle dimers when the field is turned on. In this case, the orientation and, accordingly, the packing density of these aggregates strongly depend on the field strength.

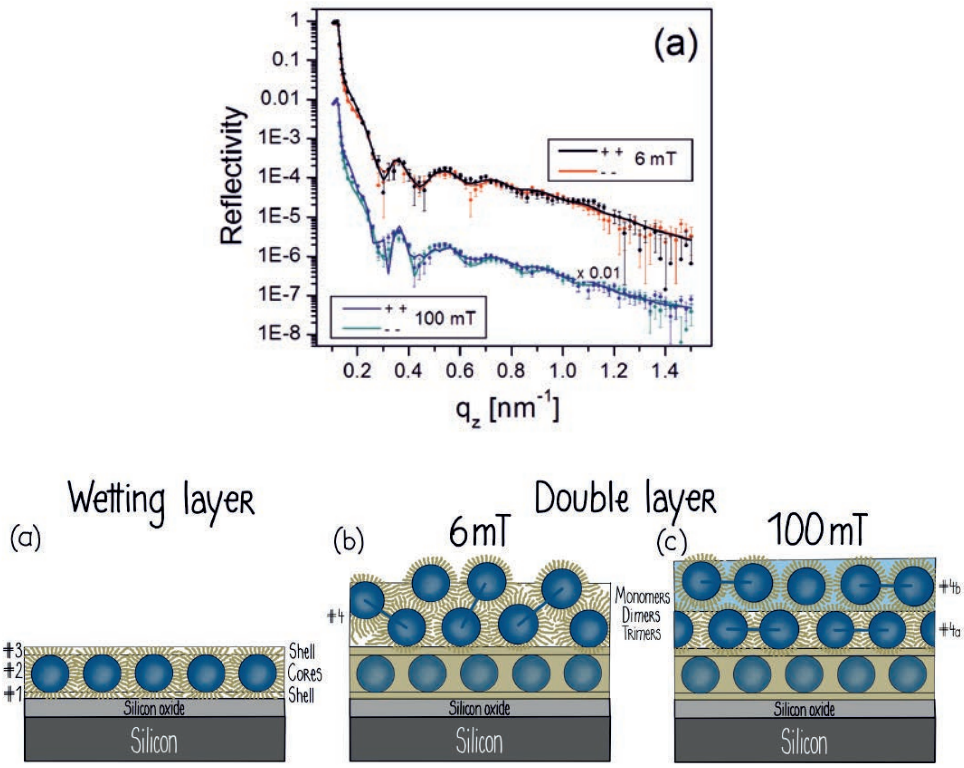


Fig. 2.4. Study of the structure of adsorption layers of magnetic nanoparticles on the treated silicon surface under external magnetic field [Theis-Bröhl et al., 2020].

2.4. KINETIC PROCESSES IN COLLOIDAL SYSTEMS

The development of new colloids and hybrid nanostructures opens up possibilities for new applications and allows the exploration of unusual phenomena arising due to the unique microscopic structure of new materials. A large developing area of research of colloidal systems is kinetic studies, the so-called *time resolved* SANS and SAXS. These methods have a number of advantages, for example, over fluorescence spectroscopy, which requires modifications of the studied molecules for labeling. One example of research is the study of the kinetics of nucleation and growth of gold and silver nanoparticles [Polte et al., 2012, Wuithschick et al., 2015]. A model description of the nature of the formation of nanoparticles was proposed by LaMer about 70 years ago (in turn, his studies are based on the classical theory of nucleation) [LaMer & Dinegar, 1950]. Using TR-SAXS, interesting results have recently been obtained which made it possible to identify four stages of nanoparticle growth [Polte et al., 2012], [Wuithschick et al., 2015]. The first stage is nucleation, while the second and third stages include coalescence, i.e., the fusion of aggregates. However, in the Lamer model, coalescence is not explicitly recognized. The difference between the growth of gold and silver nanoparticles, found in these studies, is that a metastable transition to a separate stage of fusion of nuclei was detected for Ag nanoparticles.

Another example in this area, in which neutron scattering was used, is the study of the kinetics of formation of mesoporous silica nanoparticles. Mesoporous silica is a topical object of research, which has applications, for example, in drug delivery. In [Hollamby et al., 2012], the growth mechanism of mesoporous silica nanoparticles was monitored and studied by time-resolved small-angle neutron scattering. While quite a lot is already known about the formation of pores in bulk macrosystems, the transition to the nanoscale may lead to new phenomena. Prior to neutron studies, two hypotheses were under consideration: the first one was that the formation mechanism is preserved during this transition; the second -'currant bun' model - was that silica nanoaggregates are formed, which are embedded between growing micelles and partially screen the interaction of surfactants. Within the framework of this model, the characteristic times of all occurring processes are comparable in order of magnitude, which affects the structure of the new nanoparticle. It was the SANS experiments that made it possible to determine in detail which of the proposed mechanisms takes place. Note that this was achieved by measuring the system at three different contrasts (Figure 2.5).

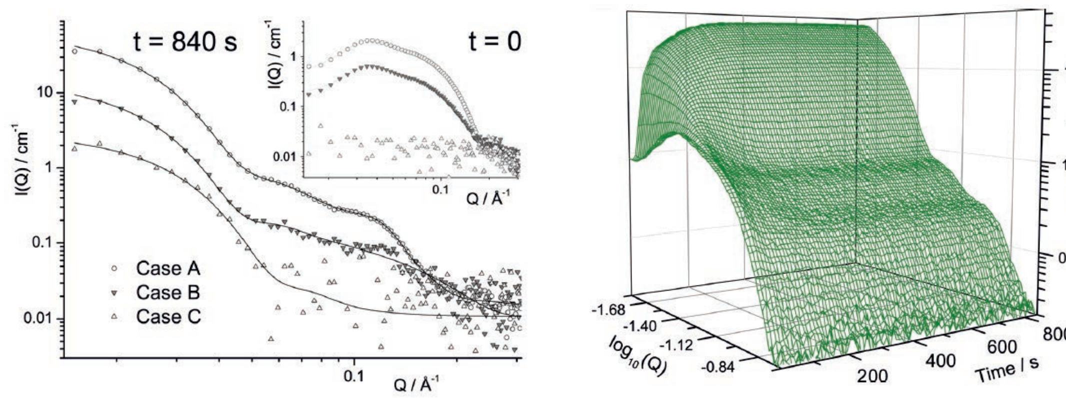


Fig. 2.5. SANS data for porous silica nanoparticles being formed. Left: three measurements with different contrasts 840 s after the start of nanoparticle growth (the inset shows measurements at the initial time point). Right: a set of curves measured during 15 min of nanoparticle growth [Hollamby et al., 2012].

Measurements of kinetic processes in colloidal solutions are more effective at higher neutron fluxes at the sample position on corresponding instruments on extracted beams of the neutron source.

2.5. ADSORPTION LAYERS AT THE LIQUID-AIR INTERFACE

The study of adsorption layers of biomolecules, surfactants and polymers at the liquid-air interface is a highly relevant task that allows us to obtain new fundamental knowledge and develop practical applications. In fact, the surface properties of complex mixtures often determine the characteristics of cosmetic and medical products, as well as the stability of conventional foods. A useful method for studying such systems is neutron reflectometry with a vertical scattering plane (horizontal sample plane). For example, in [Gochev et al., 2019], the adsorption layers of β-lactoglobulin were investigated as a convenient model system for studying the adsorption properties of proteins in liquid. One of the questions that neutron reflectometry made it possible to solve was "what happens near the isoelectric point?". Measurements in the "zero" contrast mode turned out to be indispensable for the answer. Figure 2.6 shows the resulting representation of the structure of the surface layer at the water-air interface: a formed monolayer of "flattened" protein at the surface, under which is a loose layer of β-lactoglobulin dimers formed upon reaching the isoelectric point.

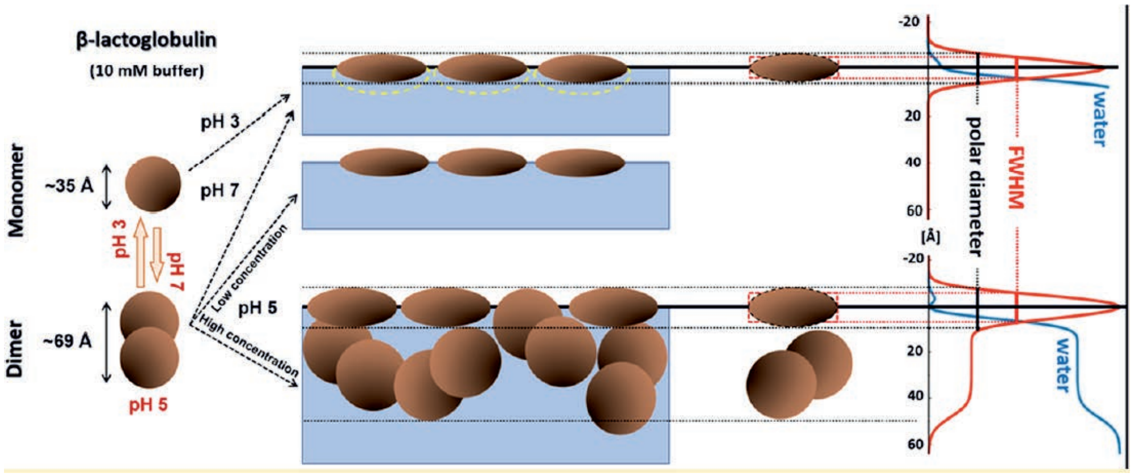


Fig. 2.6. Structure of the adsorption layer of β-lactoglobulin on the water surface and the corresponding scattering length density profiles of the system [Gochev et al., 2019].

Another example is the study of the interaction of a polymer and a surfactant at the liquid-air interface [Slastanova et al., 2022]. A PEG-g-PVAc copolymer was synthesized, which forms tardigrade-type structures in solutions. The synergistic effect of this copolymer on the structure of the surfactant layer on the water surface was studied: the surfactant concentration was varied at a fixed polymer concentration. Neutron reflectometry measurements for three different contrasts showed that the synergistic effect manifests itself only up to a certain critical concentration. Above this limit, a dense surfactant monolayer is formed on the surface, from which the polymer is completely displaced; this leads to the loss of its effect on the surface tension of the system.

The neutron flux density at the sample position plays a decisive role in such kind of experiments: high fluxes at extracted beams of the advanced neutron source will enable the use of specular reflection with a resolution close to the atomic level. In addition, studies with good time resolution are crucial for determining how surfactant molecules self-assemble into micelles and how such structures transform into various objects relevant for applications. It should also be expected that in 20 years, a common feature of high-performance neutron reflectometry experiments will be a combination with detailed non-specular scattering and grazing-incidence small-angle neutron scattering (GISANS), providing quantitative information about particles from micron to nanoscale, their form-factors and distribution. So, at the advanced neutron source, for studying both adsorption layers and thin films, it is important to build high- and medium-resolution reflectometers for precise sample characterization and for studying kinetics, respectively, as well as reflectometers specializing in non-specular scattering modes.

2.6. NANOCOMPOSITES AND THIN FILMS

Nanocomposites are a hot area of research, and over the next 20 years we can expect to see the development of new systems, improvements in synthesis methods, and progress in controlling their properties. At present, nanoparticles are often incorporated into polymers or fibrous materials to provide increased strength or elasticity (e.g. in plastics). In this case, the dispersion state and aggregation of nanofillers have a significant impact on the resulting final properties.

An example is the research on nanocomposites with metal nanoparticles [Faupel et al., 2010], which show no dependence on preparation procedures. With an increase in the fraction of nanoparticles in a polymer, an increase in the size of nanoparticles from units to tens of nanometers is observed. These nanocomposites have a number of applications based, in particular, on optical (plasmon resonance; absorption peak position is regulated by varying the Ag/Au ratio) and antibacterial (when interacting with water, silver ions actively affect bacteria) properties. At low concentrations of nanoparticles, these materials are non-toxic.

Another example of a complex system is thin films of polystyrene/fullerene polymer nanocomposites [Yaklin et al., 2008; Tropin et al., 2021]. As shown by neutron scattering data [Tropin et al., 2021], fullerenes are concentrated in a rather dense layer at the silicon-polymer interface. In [Yaklin, et al., 2008], inverted films removed from mica were studied using neutrons, and the diffusion movement of C60 fullerenes into the bulk of polystyrene from the interface with air was observed (Figure 2.7).

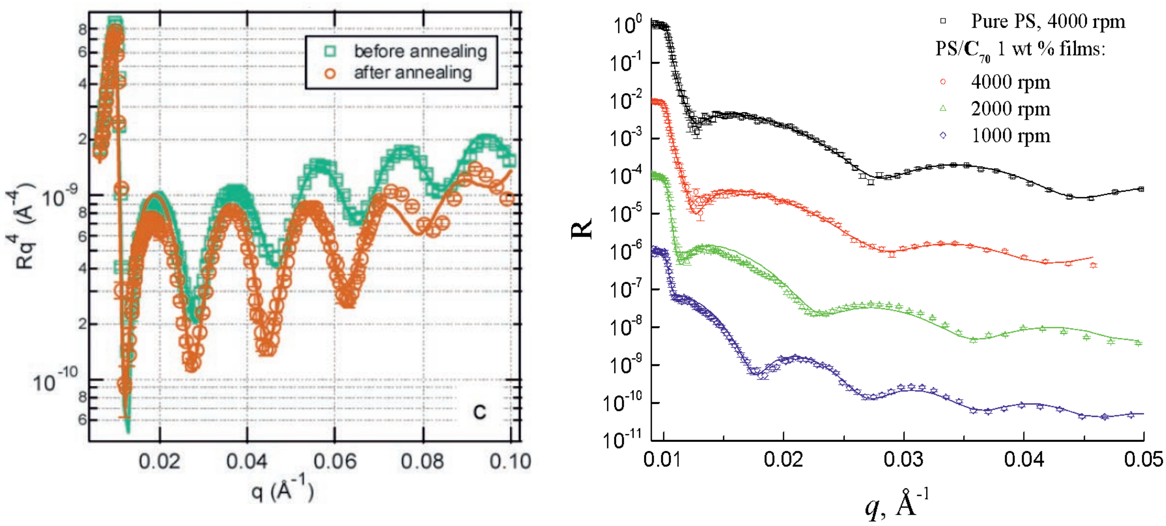


Fig. 2.7. Left: neutron reflectometry of polystyrene/C60 nanocomposites inverted on a silicon substrate before and after annealing [Yaklin et al., 2008]. Right: neutron reflectometry data (IBR-2, GRAINS) of polystyrene/C70 thin films of different thicknesses [Tropin et al., 2021].

Composite materials often have structures at different levels from nanometer to micrometer scales. High flux and wide q-range in SANS for small volume samples will be an increasingly important requirement in the study of nanocomposite materials both in their final state and during preparation/processing.

2.7. THE ROLE OF NEUTRON METHODS IN STUDIES OF SOFT MATTER

The implementation of the scientific program at the new neutron source in the area of soft matter and nanosystems will make a major contribution to these research topics and will have a significant impact on our understanding of these materials and their potential applications. The program will unite researchers from various fields, including materials science, chemistry, physics and biotechnology. With the support of an international scientific user community and the latest advances in neutron scattering methods, the program will open new horizons in research of materials science, will facilitate the achievement of new breakthrough results and the development of new systems relevant for practical applications. One of the key factors here will be the high flux density at the instruments on beamlines of the new source.

Let us note the modern trends in the field of nanosystems and soft matter, the development of which can be expected over the next 20 years. The first growing tendency is the continuous complication of the systems under study including multicomposition, heterogeneity and multilevel hierarchy. The second trend is the increasing complexity of the dynamics of the systems being studied. In order to obtain functional materials, new systems must respond to changing external parameters and, therefore, be in a non-equilibrium state. Therefore, scientists need to study non-equilibrium processes, rearrangements, dynamics in flows and phenomena that are hierarchical in time. Fundamental research will also remain relevant (until a deep understanding of the interactions and processes in nano- and mesosystems is achieved).

One of the main complex tasks for neutron scattering will be a detailed characterization of the structure and dynamics of materials on scales from ~1 nm to ~10 µm. Key neutron methods for these tasks are small-angle scattering, reflectometry and neutron spectroscopy (inelastic scattering). High neutron flux density at beamlines will allow obtaining new information about the systems under study, thereby opening up opportunities for developing new relevant systems and gaining a fundamental understanding of interactions and non-equilibrium processes in complex structures.

To effectively solve these problems, high-flux small-angle and ultra-small-angle instruments with fast 2D position-sensitive detectors will be required. For the first type of instruments, a wide available q-range is also important. Also, the possibility for building a spin-echo small-angle setup should be considered. For reflectometry, high-resolution and low-background instruments (minimum reflectivity detected down to 10^{-8}) in both kinds of geometries (vertical and horizontal scattering planes), as well as a medium- or low-resolution reflectometers with a horizontal plane for kinetic studies, will be useful. It is also important to construct additional instruments for efficient measurements of non-specular scattering (characteristic structure sizes of ~10-10^{5} nm) and grazing-incidence small-angle scattering (GISANS) on scales from subnanometers to hundreds of nanometers. To study relaxation and energy spectra of nanosystems and soft matter, it will be necessary to create a complex of neutron spectrometers, including spin-echo spectrometers.

It is also worth mentioning the continuous growth in the quality of computer modeling methods. It can be expected that in 20 years, the use of modeling in neutron research will become “not an advantage, but an obligation” at all stages of the experiment (preparation, measurement and processing of results). At present, research into nanosystems and soft matter is developing rapidly and extensively, aiming to cover a large number of hybrid materials, as well as complex systems based on existing materials. This trend will continue, and in the future, the creation of “libraries” (possibly controlled by AI systems) to automate the development of new materials is inevitable. One of the main general tasks here is the regular development of self-assembling structures for solving complex problems in medicine, technology, food industry and other industries. This task requires the development of a comprehensive understanding of the structure and dynamics of the constituent components at all scales of size and time with good resolution. To solve these problems, neutron scattering methods are indispensable.

Magnetism and superconductivity

3.1. MAGNETISM AND SUPERCONDUCTIVITY IN MAGNETIC LAYERS AND THIN FILMS

Due to the rapid development of nanotechnology and a number of major discoveries in the field of physics of low-dimensional systems (the giant magnetoresistance effect, properties of graphene, etc.), in recent years increased attention has been paid to the study of magnetism in magnetic layers and thin films. The most striking examples demonstrating the importance of studying these phenomena include the indirect exchange interaction between ferromagnetic layers through intermediate (paramagnetic, semiconductor) layers, the effect of exchange-bias magnetization upon contact of ferromagnetic and antiferromagnetic layers, the effect of exchange-spring coupling between magnetically hard and soft layers, spin-orientation phase transitions, and proximity effects of ferromagnetic and superconducting layers. The most important of these phenomena were studied using polarized neutron reflectometry, since this method is sensitive to the morphological and magnetic features of layered nanostructures. Some of these effects, such as exchange bias and exchange interaction through intermediate layers, have already been studied quite well for existing technological systems. However, with their continuing miniaturization, these effects will manifest themselves on smaller scales with an increasing role of interfaces and their influence on the electron system. Understanding the role of new interaction mechanisms will not only lead to an understanding of the fundamental laws of low-dimensional magnetism, but will also allow one to use them for designing systems with desired magnetic and transport properties, for example, for magnetic memory devices, polarized electron injectors, etc.

The applied aspect in studies of thin-film structures using polarized neutron reflectometry is also connected with the fact that special attention in recent years has been paid to the problems of spintronics and the creation of quantum computers, with which the next industrial revolution is associated. The presence of spin in electrons is already used to read information from hard drives in commercial devices based on the giant magnetoresistance effect. In the future, with the development of spintronics, the fundamental limitation of electronics associated with the loss of energy when a charge moves may be removed, since spin current is possible at zero charge current. The effective magnetic field induced by the spin-orbit interaction acts only on spins. This fact can contribute to solving problems in spintronics, in particular, the creation of spin transistors in which the spin current is controlled, and their usage in processors, read-only memory devices, and even in qubits — elements of quantum computing.

In connection with the development of superconducting spintronics, superconducting quantum computing and superconducting neuromorphic computing, the study of the interaction of superconductivity and ferromagnetism is of particular interest. The interaction of the two phenomena was first addressed theoretically by Ginzburg in 1957, who pointed to great difficulties in realizing a superconducting ferromagnet. Later, it was noted that the coexistence of phenomena with ferromagnetic and superconducting order parameters is possible in inhomogeneous systems. It was pointed out that the phenomena of ferromagnetism and superconductivity in inhomogeneous ferromagnetic-superconducting systems are modified. For instance, the review [Nikitenko & Zhaketov, 2022] provides an overall picture of magnetic phenomena caused by the interaction of ferromagnetic and superconducting order parameters in layered nanostructures.

An important result on the interaction of superconductivity and ferromagnetism in a layered periodic structure, obtained using polarized neutron reflectometry, is described in [Khaydukov et al., 2019]. It was shown that structures based on Nb/Gd bilayers are stable due to the absence of mutual dissolution of the elements. Gadolinium, having a low Curie temperature, is a relatively weak ferromagnet, and niobium has a relatively high superconducting transition temperature and is a strong superconductor. So, one can expect a significant effect of superconductivity on ferromagnetism in Nb/Gd. Along with this, gadolinium has a large cross-section of interaction with neutrons, as a result of which, when neutrons are captured by gadolinium nuclei, secondary radiation is produced — gamma-rays with energies of hundreds of keV. Detection of this kind of radiation allows one to additionally obtain a spatial profile of gadolinium, and then niobium, which is important for determining which element is associated with changes in the magnetization distribution at the ferromagnet-superconductor interface. To date, studies have been done for periodic structures [Nb(25nm)/Gd(x = 1.2, 3, 5 nm)]$_{12}$, in which the thickness of gadolinium layers was less than or of the order of the correlation length of superconductivity in gadolinium (Figure 3.1). A coherent action of the superconducting layers was observed, manifesting suppression of the magnetization of the gadolinium layers (superconducting diamagnetism of the periodic F/C structure). Thus, the periodic structure is superconducting. The penetration depth of the magnetic field into the structure was 180 nm, which is greater than the value of 120 nm for superconducting solid niobium. The suppression of the magnetization magnitude, as expected, increased with a decrease in the thickness of the ferromagnetic gadolinium layers.

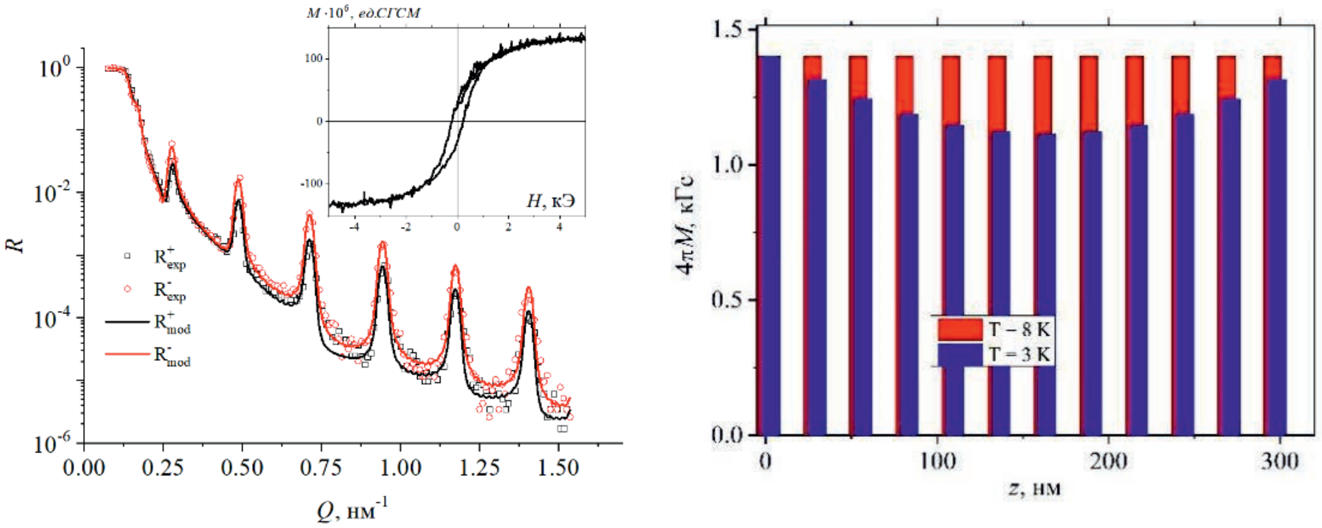


Fig. 3.1. (a) Experimental dependence (dots) of neutron reflection coefficients for the [Gd(2 nm)/Nb(25 nm)]$_{12}$ sample at T=7 K and H=4.5 kOe. Solid lines show model curves. The inset shows the magnetic hysteresis measured at T=7 K with a SQUID magnetometer. (b) Magnetization of the periodic structure of [Gd(2 nm)/Nb(25 nm)]$_{12}$ at H=661 Oe.

For neutrons, the main interactions are absorption and scattering by atomic nuclei and atoms. The decay of nuclei after neutron capture is accompanied by the emission of radiation in the form of gamma-rays, charged particles and nuclear fragments (Figure 3.2). The type, intensity and energy of radiation are different for isotopes of elements and, thus, can be used in the isotope characterization. In real layered structures, the interface is relatively stretched (1–10 nm). In this regard, in the vicinity of the interface, the interaction potential is determined by the sum of the interaction potentials of neutrons with the elements in contact. To determine the spatial distribution of a particular element, it is necessary to detect both primary (neutrons) and secondary (from nuclei) radiation. Primary radiation is reflected neutrons that have passed through the structure. The intensity of secondary radiation is determined by the absorption of neutrons. The partial neutron absorption coefficient can be determined directly if the spatial distribution of a particular isotope is known. [Аксенов, В.Л. и др., 2023]

The change in the magnetization distribution at the superconductor/ferromagnet interface during the superconducting transition was studied in [Khaydukov et al., 2013]. For the Cu(32 nm)/V(40 nm)/Fe(1 nm)/MgO(001) structure, measurements of the spatial profile of the interaction potential of neutrons with matter revealed the emergence of positive magnetization during the superconducting transition. The proximity effect in ferromagnet-superconductor heterostructures is responsible for the interference phenomena that determine their thermodynamic and transport properties. For reflectometric measurements of the Cu(32 nm)/V(40 nm)/Fe(1 nm)/MgO(001) structure, the developed mode of enhanced standing neutron waves was used. The experimental data are consistent with the assumption of the inverse effect, when a positive magnetic moment arises in the superconducting layer. It should be noted that this work also presents data showing that iron atoms are completely located in the vanadium layer. The relative concentration of iron atoms is in the range of 0-20% in about 10-nm layer from the side of vanadium. It is known that in the FeV alloy, vanadium atoms are magnetized and their moments are oriented anticollinearly to the magnetic moments of iron atoms. In this regard, due to the complex magnetic structure, other scenarios for changing the magnetic moment during the superconducting transition are not excluded. In particular, this may be diamagnetic compensation during the superconducting transition of the magnetic moment of vanadium atoms. Detection of secondary radiation from elements in contact at the interface, in addition to neutron reflection, can help in identifying the mechanism of magnetization of the structure. **The advanced neutron source with a high neutron flux on extracted beams will make it possible to determine with high accuracy the correlation between the distribution of element concentrations and magnetization for a wide range of elements, and to study subtle magnetic effects associated with a change in magnetization of less than 1%.**

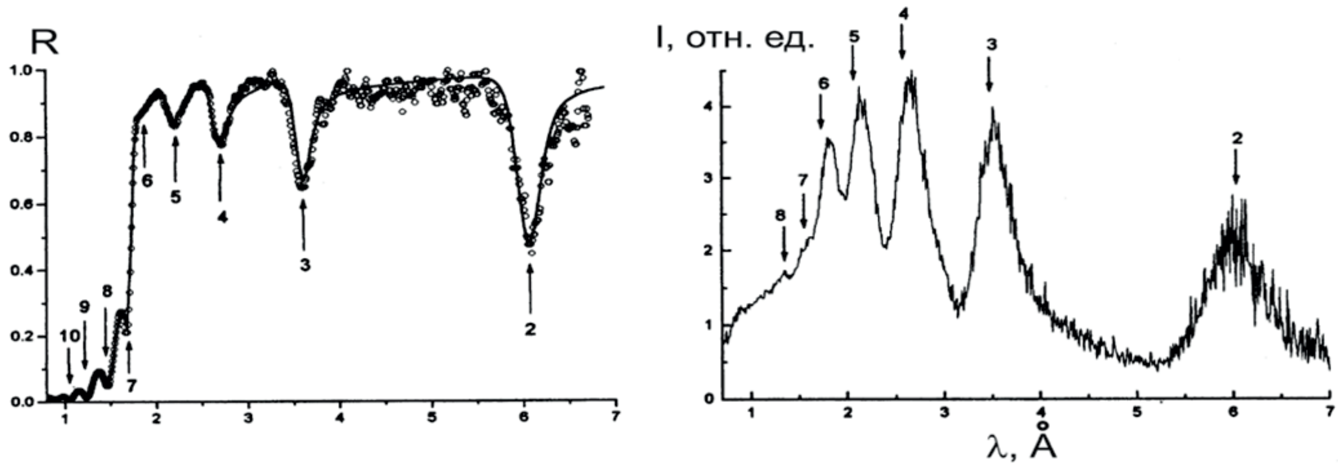


Fig. 3.2. Long-wave dependences of the neutron reflectivity (left) from the ^{6}LiF(20nm)/Ti(200nm)/Cu(100nm)/glass structure and the yield of charged particles (right) caused by the capture of neutrons by nuclei of the ^{6}Li isotope.

Another important and promising area of research is the study of systems with non-trivial magnetic ordering. Thus, in a series of studies on the REMUR reflectometer at the IBR-2 reactor, heterostructures with layers of helically ordered rare-earth magnets Dy and Ho were studied. The paper [Devyaterikov et al., 2022] presents the results of studies of the periodic structure of [Dy(6 nm)/Ho(6 nm)]$_{34}$. The helical magnetic structure is formed in bulk Dy in the range between the Curie temperature (T_c = 85 K) and the Neel temperature (T_N = 178 K), in bulk Ho — in the range between T_c = 18 K and T_N = 132 K. Due to the size effects and epitaxial stresses in low-dimensional heterostructures based on Dy and Ho, the magnetic structure exhibits features such as a change in the Curie and Neel temperatures and different values of the helicoid periods compared to bulk materials. It is important that in superlattices with alternating Dy and Ho layers, two different magnetic helicoids are formed, coherently propagating in the Dy and Ho layers. Figure 3.3a shows a neutron reflection pattern for the [Dy (6 nm)/Ho (6 nm)]$_{34}$ structure obtained at T=100 K. Accordingly, the periods of the magnetic helicoids, the Neel and Curie temperatures for Dy and Ho in the superlattice differ from the characteristic periods and characteristic temperatures of single crystals and thin single-component films of Dy and Ho (Figure 3.3b). It is concluded that for Ho in the [Dy (6 nm)/Ho (6 nm)]$_{34}$ superlattice, the magnetic phase transition from the helical phase to the conical phase is suppressed below the Curie temperature, T_c. For the Dy layers, compared to T_c in single-crystal Dy, an increase in the Neel temperature T_N in the Ho layers is observed.

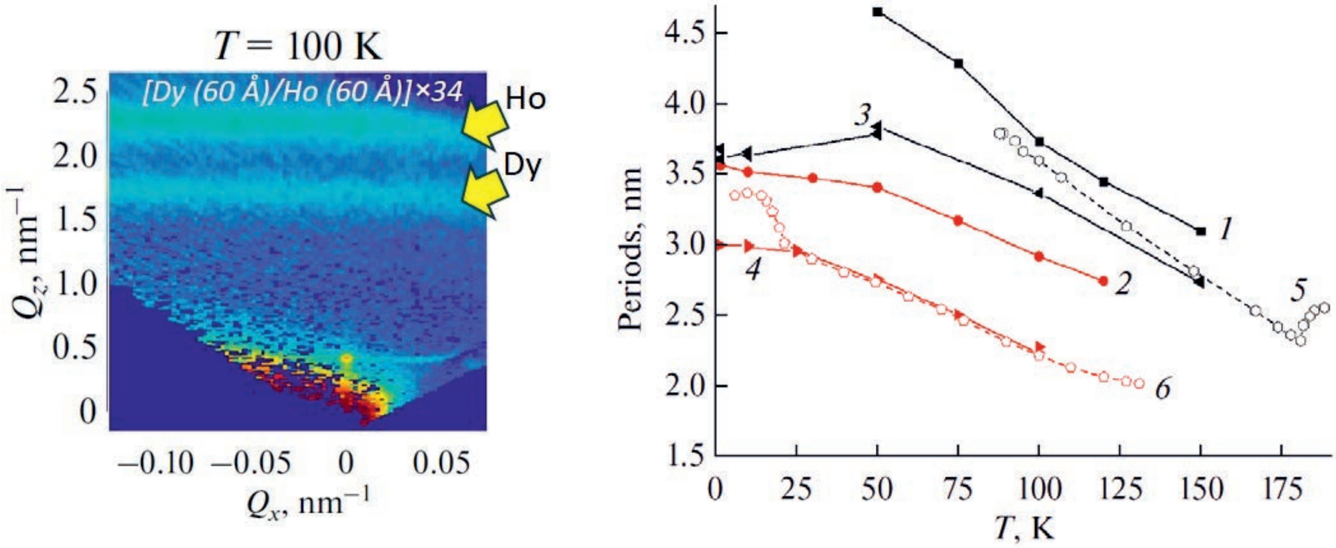


Fig. 3.3. (a) Reflectometric spectra for the [Dy (6 nm)/Ho (6 nm)] × 34 superlattice in the coordinates of the transferred wave vector Q_z-Q_x. (b) Temperature dependence of the helicoid period in bulk Dy (1) and Ho (2) single crystals, in thin (200 nm) Dy (3) and Ho (4) films, and in Dy (5), Ho (6) as part of the superlattice.

Use of neutrons also allowed a detailed analysis of low-temperature measurements for the Al_2O_3(11 ¯02)/Nb(40 nm)/[Dy(6 nm)/Ho(6 nm)]$_{34}$/Nb(10 nm) structure obtained at a temperature below T_c(Nb) [Zhaketov et al., 2023]. Neutron measurements were carried out on the REMUR time-of-flight reflectometer for polarized neutrons. Figure 3.4a shows the difference in the neutron specular reflectivity $S=R_+-R_-$, which is proportional to the magnetic moment. The data are given for the first-order Bragg peak obtained on the superlattice period. The sample was cooled in a magnetic field of H=1 kOe, and the measurement was carried out in the same field. It is evident that with decreasing temperature the parameter S increases, which is indicative of the fact that the helical magnetic ordering is transformed into a fan-shaped structure, since the collinear component of magnetization increases (Figure 3.4b). But at T= 1.5K<T_c (Nb) the opposite behavior is observed, i.e. a decrease in S, which means the system restores the helical magnetic phase. This behavior is due to the fact that the helical magnetic phase is energetically more preferable for the existence of superconducting correlations. The total macroscopic value of the magnetic induction in a helical magnet is zero, while for a magnet with fan-shaped magnetic ordering this value is non-zero. Obviously, the first case is more preferable for superconducting correlations, which are thus responsible for the magnetic ordering.

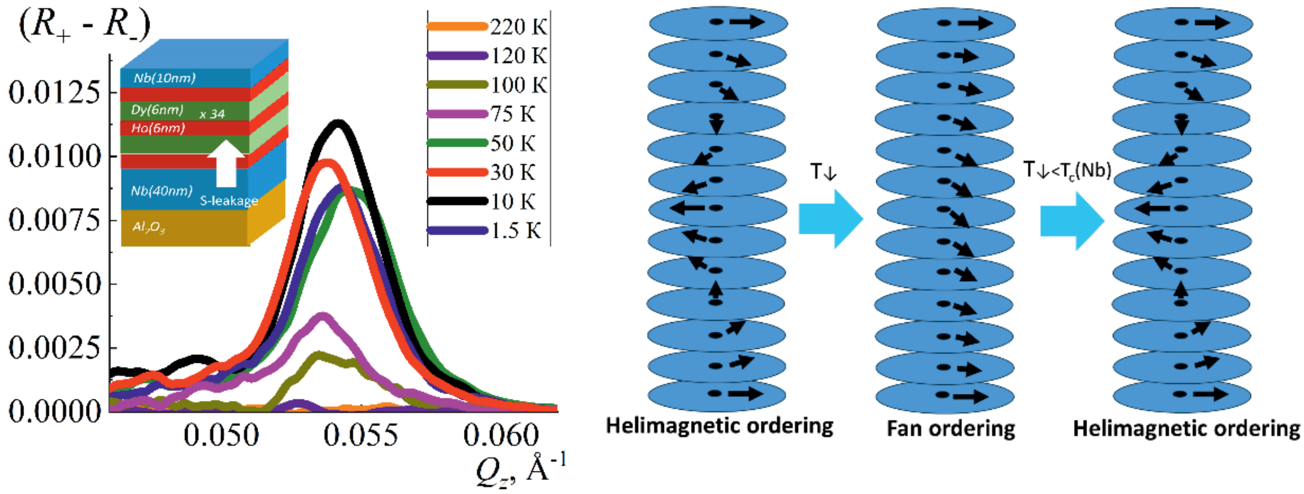


Fig. 3.4. (a) Difference in neutron specular reflection coefficients obtained at different temperature values in a magnetic field of *H*=1 kOe. (b) Change in the magnetic ordering upon cooling of the structure: magnetic helicoid is transformed into magnetic fan, under the influence of superconductivity magnetic fan is transformed into magnetic helicoid.

It is worth noting the studies of a complexly ordered non-coplanar magnetic system [Tatarskiy, 2020], which show that the antisymmetric Dzyaloshinsky-Moriya interaction affects the reflection of polarized neutrons from a multilayer structure with random magnetic anisotropy. It was observed that the antisymmetric exchange leads to the emergence of a polarization-dependent asymmetric term in the reflection. **In this kind of studies, small-angle neutron scattering in grazing geometry should be detected at a level of less than 1% of the reflected beam intensity. So, experiments require a high neutron flux on the sample, which can be provided by the advanced neutron source with state-of-the-art reflectometers on extracted beams.**

3.2. SPIN DYNAMICS OF STRONGLY CORRELATED ELECTRON SYSTEMS

A promising area of application of inelastic neutron scattering (INS) is spin dynamics of strongly correlated electron systems (SCES). An example is the study of magnetic dynamics of the intermediate valence compound $CePd_3$ [Goremychkin et al., 2018]. The experimental determination of the 4D scattering law function S(Q, ω) and its comparison with theoretical calculations in the DFT+DMFT theory made it possible to conclude about the origin of the features in the band structure and, in turn, about the anomalous magnetic and transport properties. The first experiments with single-crystal $CePd_3$ showed the presence of an unusual evolution of magnetic excitations in (Q,ω)-space. Figure 3.5 presents the experimentally determined 2D cross-sections of the imaginary part of the generalized susceptibility χ″(Q, ω) ~ S(Q,ω)(1-exp(-ω/kBT) at energies of 35 meV (panel A) and 65 meV (panel B).

The comparison of the data in panels (A) and (B) unexpectedly shows a strong dependence of the scattering intensity on *Q*. The first-principles calculations (panels C and D) show good quantitative agreement with the experiment. They also answer the question about the origin of the features in the scattering law S(Q, ω): electron-hole excitations (electron transitions between electron and hole pockets) and their location in the (Q,ω)-space are due to the features of the band structure. In fact, it can be stated that measurements of the 4D scattering law S(Q, ω) by the INS method make it possible to study the electronic structure of SCES. In particular, the degree of coherence of the electron bands can be seen in the temperature dependence of S(Q, ω). Figure 3.6 presents the INS data for two temperatures of 6 K and 300 K. At room temperature, all specific features in the scattering practically disappear, while at 6 K three well-defined peaks are observed.

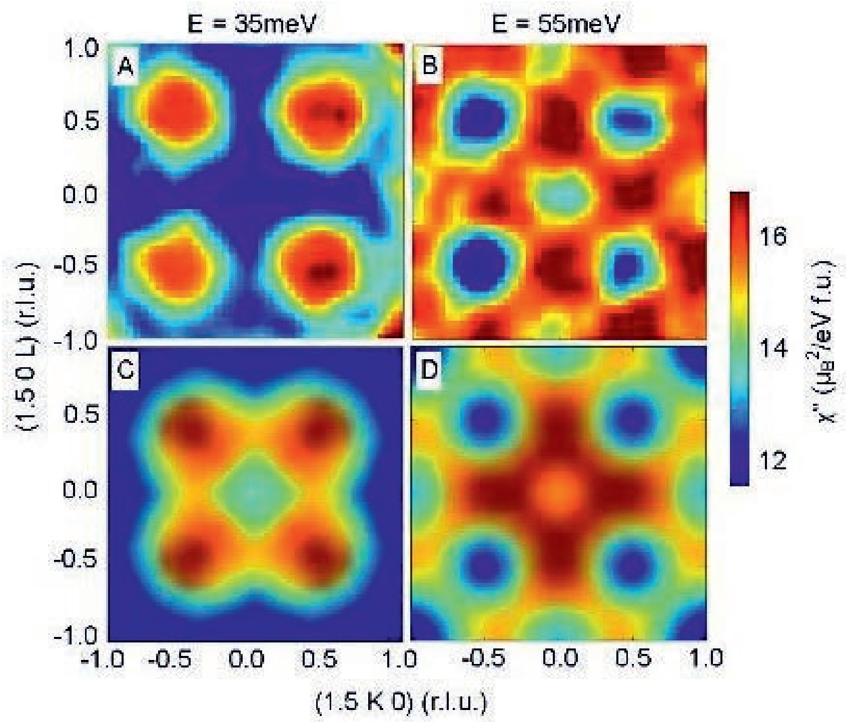


Fig. 3.5. Magnetic scattering intensity at energies of 35 meV and 65 meV in the plane (1.5 K L). Panels A and B are the data of the INS experiment at *T*=5 K. Panels C and D are the results of theoretical first-principles calculations using the DFT+DMFT method. [Goremychkin et al., 2018].

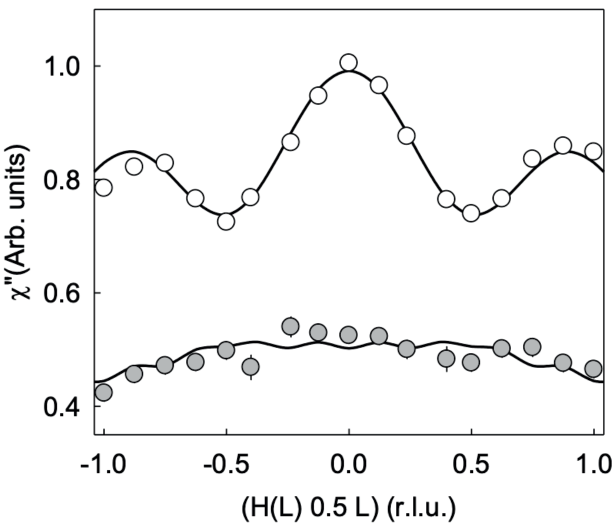


Fig. 3.6. Temperature dependence of the dynamic magnetic susceptibility of $CePd_3$. Filled (gray) circles are INS measurements at 6 K (300 K) and an energy transfer of 60 ± 10 meV, K = 0.50 ± 0.25. Lines are the results of DFT+DMFT calculations. [Goremychkin et al., 2018].

This evolution of the scattering intensity is very well described by DFT+DMFT calculations, which reflects a significant loss of coherence of the 4*f*-bands in the vicinity of the Fermi level at high temperatures. This result is very important, since it is a direct spectroscopic confirmation of the evolution of the 4*f* moments from the mode of free paramagnetic states at high temperatures to the mode of strongly bound 4*f* states with conduction electrons (*d*-electrons of palladium) at low temperatures. **Experiments of this kind require the availability of inelastic neutron scattering spectrometers with a large coverage area in the (Q,ω)-space and high neutron flux density on the sample at the advanced neutron source of JINR, which will allow measurements of the 4D scattering law $S(Q_x, Q_y, Q_z, \omega)$. In the future, the INS technology will undoubtedly be further improved and satisfy an ever-growing demand from the user community.**

Another interesting example of the successful application of 4D neutron spectroscopy is the investigation of the spin dynamics of molecular magnets [Chiesa, 2017]. If in the previous example, measurements were made in the energy range of thermal neutrons ~10-200 meV, then for molecular magnets, the spectrum of magnetic excitations is much smaller and covers the energy range of ~1-10 meV, so in this case, experiments are carried out on high-resolution spectrometers located at cold neutron sources. Here, the example concerns a molecular nanomagnet containing a cluster of 12 manganese atoms (Figure 3.7), which is abbreviated as Mn_{12} with the full chemical formula:

$$\{Mn_{12}O_{12}[O_2CCD_2C(CD_3)_3]_{16}(CD_3OD)_4\} \cdot (C_2H_5)_2O$$

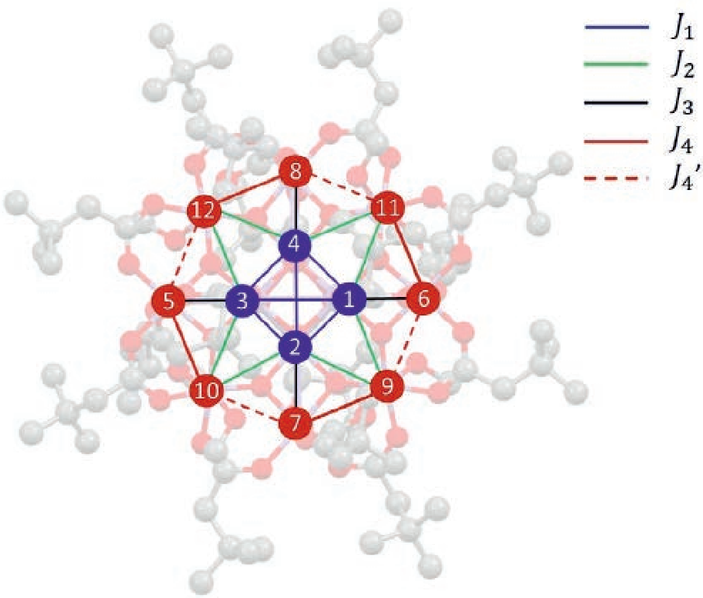


Fig. 3.7. Scheme of the Mn_{12} molecule. Blue circles are Mn^{+4} ions (1 — 4, s=3/2), red circles are Mn^{+3} ions (5 — 12, s=2). The lines connecting the manganese atoms represent different exchange interactions. The total number of exchange constants is five. Their list is given in the upper right corner. [Chiesa, 2017].

This is a very unique nanomagnet, since it contains an isolated cluster of 12 magnetoactive ions of different valence and, accordingly, having different values of spin (magnetic moment). The phenomenological Hamiltonian describing the magnetic dynamics of Mn_{12} will contain five exchange constants and the most reliable way to determine them is to measure the 4D scattering function by the INS method and quantitatively compare the experimental data with the magnetic dynamics calculations using the model Hamiltonian. As can be seen in Figure 3.8, there is very good agreement between the measured and calculated cross-sections $S(Q_x, Q_y)$ in almost the entire energy range, which clearly indicates the high quality of the obtained values of the spin Hamiltonian parameters. This is absolutely necessary for understanding the physical properties of nanomagnetic materials and their possible practical applications.

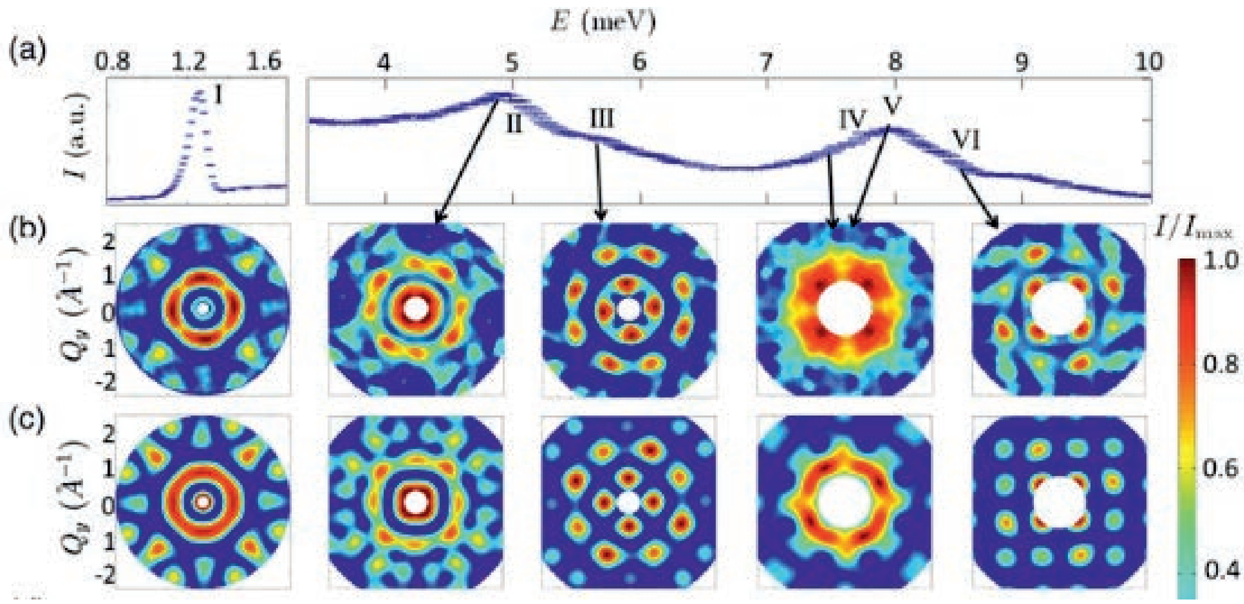


Fig. 3.8. (a) INS spectrum measured at the LET spectrometer, ISIS, at incident neutron energies of 4.2 meV and 15.4 meV and a temperature of 1.5 K. (b) 2D cross-section $S(Q_x, Q_y)$ obtained by integrating over the entire Q_z-range. (c) Calculated 2D intensity distribution with a set of exchange parameters of the model Hamiltonian determined in the INS experiment [Chiesa, 2017].

3.3. HIGH-TEMPERATURE SUPERCONDUCTIVITY

High-temperature superconductors (HTSCs) are of great current interest all over the world. The potential discovery of materials showing HTSC properties at room temperature and normal pressure could lead to a real industrial revolution. This ambitious task will certainly be a subject for study at the advanced neutron source. Several theories of superconductivity have been proposed to date (e.g., Bardeen et al., 1957; Aksenov et al., 1992; Bozin et al., 2015). In particular, important studies on the physics of high-temperature superconductors are based on the use of neutron scattering methods. Thus, in [Smolyaninova, 2015; Smolyaninova, 2019] it was demonstrated that a metamaterial with an effective permittivity tending to zero, consisting of Al nanoparticles coated with an Al_2O_3 shell (total diameter of 18 nm) has a critical superconductivity temperature 3.25 times higher than that of pure aluminum. Inelastic neutron scattering made it possible to establish that this increase is associated with an increase in the electron-electron interaction due to an additional hybrid plasmon-phonon excitations occurring in a metal-insulator metamaterial.

INS studies of spin dynamics in HTSCs have revealed a number of interesting features in spectra of elementary magnetic excitations and their relation to superconductivity. An example is the occurrence in the superconducting state of the so-called neutron resonance (a peak in the scattering law $S(Q_{res},\omega_{res})$) at a certain point of the Brillouin zone (Q_{res}), the energy (ω_{res}) of which correlates with the temperature of the transition to the superconducting state. A good illustration of the role of INS in the study of HTSCs is the research of magnetic dynamics in the so-called 'iron' superconductors discovered in 2008. Figure 3.9 shows the evolution of the scattering law depending on temperature [Christianson et al., 2008].

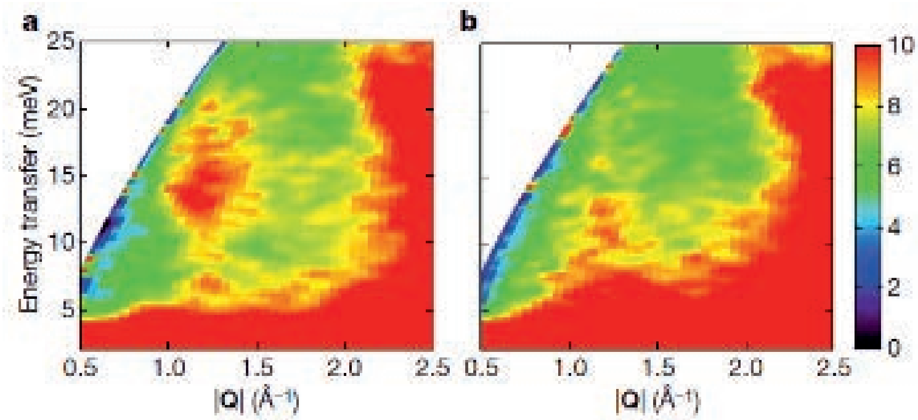


Fig. 3.9. Scattering law of the HTSC compound $Ba_{0.6}K_{0.4}Fe_2As_2$ in $\mathbf{Q} - \omega$ coordinates for two temperatures, in the superconducting state (a, 7K) and in the normal state (b, 50K). [Christianson et al., 2008]

As can be seen in this figure, at 7 K in the superconducting phase, there is a feature in the spectrum of magnetic excitations at an energy transfer of 14 meV and a momentum transfer of 1.15 $Å^{-1}$. The analysis showed that this feature is a neutron resonance, previously established in INS studies of copper HTSCs. Observation of neutron resonance in combination with photoemission spectroscopy analysis allowed us to conclude about the symmetry of the Cooper pair $s_{\pm}$ in this class of HTSC compounds.

Of great interest is the phenomenon of superconductivity in hydrides (e.g. H_3S, LaH_{10}, YH_9, etc.) at high (~10-100 GPa) pressures and at temperatures close to room temperature, discovered in the 2010s. Work is underway to search for new hydrides with an even higher critical temperature at relatively low pressures, for example, among ternary systems (La-Ce-H, [Chen et al., 2023]). The physical mechanism of superconductivity in hydrides is actively studied together with the development of an appropriate theory that should explain the observed effects, for example, a huge decrease in the critical temperature when replacing hydrogen with deuterium (~70 K), significant temperature hysteresis of electrical resistance (~15 K), extremely high critical magnetic fields (>100 T) [Eremets et al., 2022]. Due to the sensitivity of scattered thermal neutrons to hydrogen, experiments on elastic [Haberl et al., 2023] and inelastic [Antonov et al., 2022] neutron scattering at high pressures are expected to provide unique information on the structure and dynamics of superconducting hydrides. **It should be noted that high-pressure experiments require measurements of extremely small sample volumes (~ 0.01 mm^3 and below). Therefore, they require a high-flux neutron source.**

3.4. MAGNETIC PROPERTIES OF MATERIALS AT HIGH PRESSURES

Recently, there has been significant progress in the study of materials under extreme conditions. High pressure often gives rise to new physical phenomena in materials, including, in addition to pressure-induced superconductivity, various changes in magnetic states, insulator-metal transitions, spin crossover, structural and electronic phase transitions. In addition, high-pressure studies offer unique opportunities to study microscopic mechanisms of the formation of physical phenomena in functional materials by analyzing the response of various properties to changes in structural parameters during compression of the crystal lattice. Also, under high pressures and temperatures, it is possible to synthesize new metastable forms of materials with unusual properties. The nature of the interaction of neutrons with matter determines a number of advantages of neutron diffraction as compared to the corresponding X-ray methods in structural studies: high sensitivity to the positions of light atoms in the crystal structure, such as hydrogen and oxygen, especially under conditions of structural disorder; the possibility to study the magnetic structures of materials; high penetrating power. [Kozlenko et al., 2021]

Nowadays, the study of van der Waals magnets is one of the most developing areas in condensed matter physics and materials science, since such substances are actually magnetic analogues of graphene, a unique 2D material, the discovery of which was awarded the Nobel Prize in Physics in 2010. Studies of 2D forms of van der Waals magnets have shown that magnetic ordering in them can be maintained at fairly high temperatures up to the limit of an atomic monolayer. In addition, a wide variety of new physical phenomena have been discovered in these materials with changes in thermodynamic parameters (temperature and pressure), including superconductivity, topological spin excitations, skyrmion states, etc.

Studies of the structural and magnetic properties of the $CrBr_3$ compound, which were conducted at the IBR-2 reactor using the neutron diffraction method, revealed a number of unusual effects, including anomalous behavior of the structural characteristics in the region of the ferromagnetic ordering temperature T_C and negative thermal expansion of the volume of the crystal lattice of quasi-two-dimensional van der Waals layers in the temperature range $T < T_C$. It should be noted that negative thermal expansion is a relatively rare physical effect, found only in a few classes of materials. While most crystalline substances exhibit an increase in the volume of the crystal lattice and characteristic interatomic distances with increasing temperature□positive thermal expansion, in exceptional cases, as for $CrBr_3$, in a certain range of thermodynamic parameters, the opposite effect can be realized — negative thermal expansion, when with increasing temperature there is a decrease in the volume and interatomic distances (Figure 3.10) [Kozlenko et al., 2021]. It is interesting to note that graphene also exhibits negative thermal expansion, and the coefficient of linear thermal expansion of atomic layers in $CrBr_3$ in the region $T < T_C$, $\alpha l = 1.6 \cdot 10^{-5}$ K^{-1}, turned out to be close to the corresponding value for graphene in the low-temperature region. The obtained result indicates good compatibility of materials such as CrX_3 and graphene, in terms of the prospects for developing heterostructures based on them. The practical use of such kind of systems can become an important step towards the development of an advanced generation of spintronics, nanoelectronics, information recording and storage devices. [Kozlenko et al., 2021]

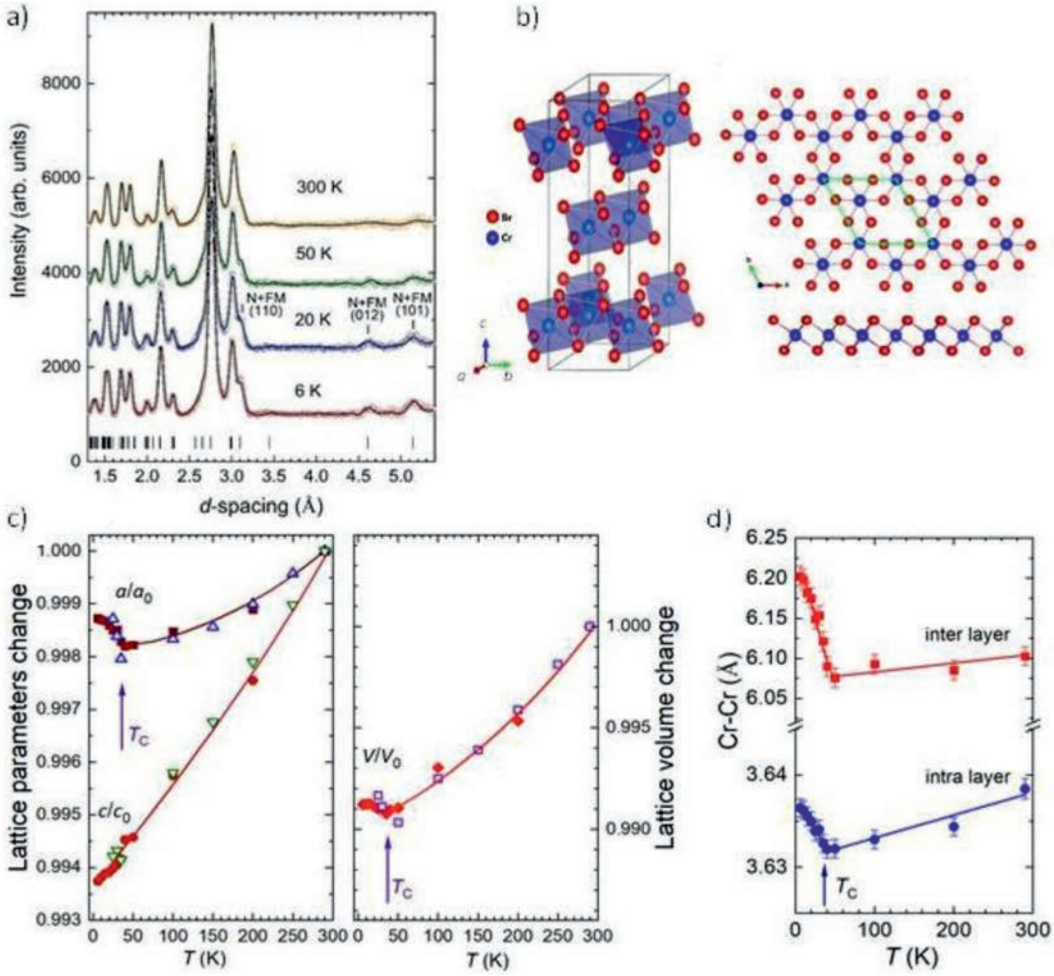


Fig. 3.10. a) Neutron diffraction patterns for $CrBr_3$ measured at different temperatures and profiles calculated by the Rietveld method. b) Rhombohedral crystal structure of $CrBr_3$ with R*3* symmetry. The top and side views of the van der Waals atomic layers are shown on the right. c) Temperature dependences of the lattice parameters and the unit cell volume of $CrBr_3$, normalized to the corresponding values at room temperature. d) Temperature dependences of distances between magnetic Cr ions inside van der Waals layers (intra-layer) and between layers (inter-layer) [Kozlenko et al., 2021].

The mineral magnetite Fe_3O_4 is one of the first magnetic materials used by mankind since ancient times, and now it also finds wide application in the development of advanced technologies. It exhibits a number of unusual physical phenomena that have been the focus of extensive research for more than a century. In particular, anomalous behavior of physical properties of magnetite at high pressures in the vicinity of the structural phase transition at 20–25 GPa has recently been revealed. To clarify the nature of this phenomenon, the magnetic and electronic properties of magnetite were studied using neutron diffraction and ^{57}Fe synchrotron Mössbauer spectroscopy in the pressure range of 0–40 GPa and temperature range of 10–300 K [3]. In the high-pressure phase, the formation of ferrimagnetic ordering at a temperature of T_{NP} ~ 420 K was observed and its symmetry was deduced. The structural, magnetic, and electronic phase diagram of magnetite was determined in the studied range of thermodynamic parameters (Fig. 3.11). [Kozlenko, et al., 2019]

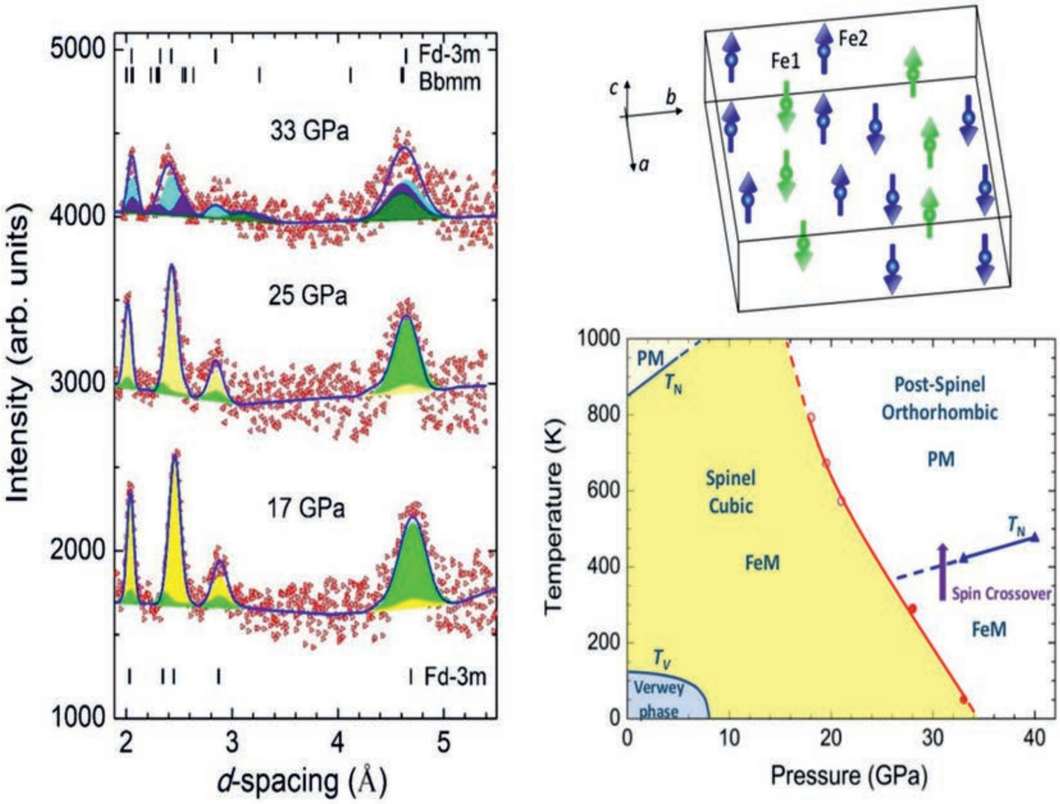


Fig. 3.11. *Left*: Neutron diffraction patterns of magnetite measured with a diamond anvil high-pressure cell at pressures of up to 33 GPa on the DN-6 diffractometer and treated using the Rietveld method. *Right*: Magnetic structure of high-pressure orthorhombic phase of magnetite (top) and structural, magnetic and electronic phase diagram of magnetite (bottom). [Kozlenko, et al., 2019]

The development and construction of the advanced neutron source will make it possible to enhance the intensity of the neutron flux on microsamples for experiments to study the atomic and magnetic structures and properties of functional materials under extreme external conditions (high pressure and low temperature), which will be an important factor for conducting such research at a new, higher quality level.

3.5. NEUTRON METHODS IN RESEARCH OF MAGNETIC AND SUPERCONDUCTING MATERIALS

The above examples of studies of magnetic dynamics demonstrate, first of all, the need for inelastic neutron scattering spectrometers that allow measurements of the scattering law in four dimensions and covering a large solid angle and the energy transfer range of ~1–200 meV. These examples do not encompass all areas of studies of strongly correlated electron systems, since these systems demonstrate a large variety of ground states, which is constantly expanding. Thus, in the last four decades, a lot of new SCES materials have been discovered, including HTSC (copper, iron), superconductors with heavy fermions, CMR, GMR, a large variety of quantum magnets, spin liquid, spin ice, quantum critical points, etc. The “industry” of creating new materials with exotic properties also continues to develop actively. An example is the intensive search for HTSC with room transition temperature at normal pressure. There is no reason to assume that interest in the research using the inelastic neutron scattering method will ever decline due to following three circumstances:

- The neutron has a magnetic moment, and magnetic inelastic neutron scattering is beyond competition in comparison with inelastic scattering approaches at synchrotron sources.
- Magnetic INS allows obtaining detailed, spectroscopic information about the dynamics of the studied material at the microscopic level, which cannot be achieved by any other method.
- Synthesis of new materials containing magnetoactive atoms gives rise to many new interesting systems that require a detailed study of magnetic dynamics both for the purpose of understanding their fundamental physical properties and for their use in applied problems.

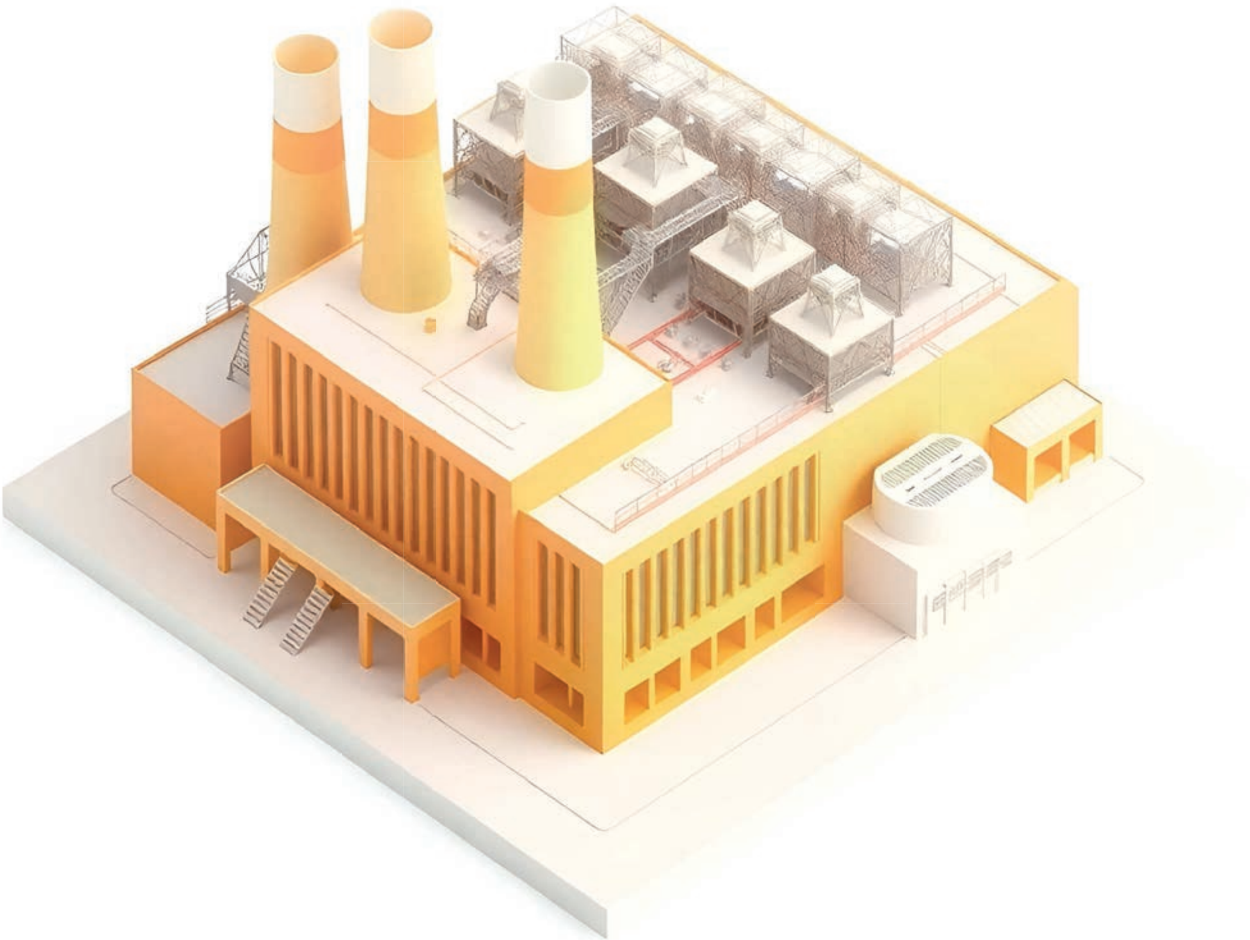
The examples given in this section also demonstrate a number of areas with a range of tasks, the solutions of which require the presence of several reflectometers at the promising neutron source at JINR for studying superconducting and magnetic layered heterostructures. The intense neutron flux at the extracted beams will allow determining with high accuracy the correlation of the distribution of the element concentration and magnetization for a wide range of elements, and studying subtle magnetic effects associated with variations in magnetization of <1%.

The development and construction of the advanced neutron source will also make it possible to increase the intensity of the neutron flux on microsamples for experiments to study the atomic and magnetic structures and properties of functional materials under extreme external conditions (external high pressure and low temperature), which will be an important factor for conducting investigations at a new, higher quality level. There is no doubt that the suite of instruments at the new neutron source should comprise diffractometers for studying micro samples under external extreme conditions (high pressure, low temperatures, etc.).

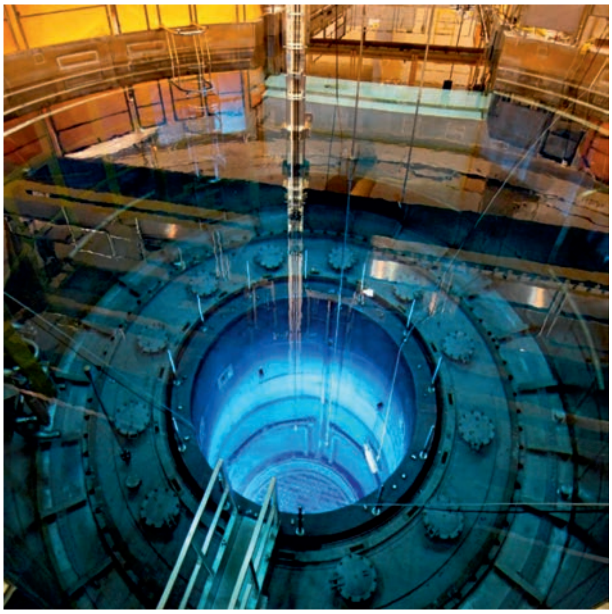
Compared to the IBR-2 reactor, an increase in the neutron flux density at the sample position at instruments of the advanced neutron source will make it possible to realize the following possibilities:

- reduction of statistical measurement error for a given measurement time, resolution and wave vector interval;
- reduction of measurement time for a given resolution in a certain range of the neutron wave vector;
- increase in resolution due to beam collimation and increase in flight path;
- increase in statistically supported range of neutron wavelengths;
- reduction of sample size to less than $5 \times 5\ mm^2$;
- real-time measurements.

Energy production and storage, chemical power sources



4.1. MATERIALS FOR NUCLEAR POWER ENGINEERING



The unique properties of thermal neutrons make them useful for studying materials important for energy production and storage. A number of studies have been carried out using neutron scattering methods for the development of nuclear power industry. In particular, internal stresses in reactor vessel samples were investigated. The neutron diffraction method was used to study internal stresses in samples cut from a real vessel of the VVER-1000 reactor. Thin and thick templates (flat samples cut from a bulk product) were studied, and the effect of the volume factor on the stress distribution was revealed. Tangential stresses in ferrite at the ferrite-austenite interface of the coating are compressive, which allows us to consider the product as having high resistance to stress corrosion cracking [Sumin et al., 2010].

Neutron diffraction finds its application in studying the distribution of residual stresses, dislocation densities and crystallite sizes in 18MND5-steel surveillance specimens that are used to assess the radiation embrittlement of nuclear reactor pressure vessel material [Bokuchava & Petrov, 2020]. In some cases, surveillance specimens that have been subjected to the mechanical Charpy impact test need to be reconstituted and placed back in the immediate vicinity of the reactor pressure vessel. Therefore, it is desirable that the process of specimen reconstitution (welding) introduces minimal changes to the stress-strain state and microstructure of the material. Neutron diffraction experiments were carried out by scanning samples along the depth and length with a small gauge volume with dimensions of 2×2×10 mm^3 (Figure 4.1). It was shown that electron beam welding generally induces the lowest residual stresses compared to other methods. However, it leads to the formation of areas with increased dislocation densities near the welds and reduces the size of steel grains more than other methods, which significantly increases the yield strength of the material near the welds.

Due to excellent mechanical properties, corrosion resistance and low neutron absorption, Zr-Nb alloys are widely used in nuclear reactor engineering. The crystallographic texture formed during thermomechanical processing of these alloys determines the anisotropy of the physical properties of products and influences the mechanisms of their degradation (for example, the preferential orientation of hydride precipitates, radiation creep or swelling). Neutron diffraction was used to study crystallographic textures in high-pressure tubes made of Zr+2.5%Nb alloy using a multi-step process, including extrusion at 800°C, air cooling at room temperature, cold pilger rolling and annealing at 400°C for 24 h [Malamud et al., 2018]. It was found that a specific microstructure and a sharp single-component texture are formed in the tubes with a preferred orientation of [0001] axes of the alloy in the tangential direction, and normals to the {10-10} planes in the axial direction of the tubes (Figure 4.2). The texture at the end of the tube was found to be somewhat sharper than at the front. Measurements on various neutron diffractometers have demonstrated that the errors in determining the position, volume and width of texture components using neutron diffraction are small and comparable to those expected in the tube manufacturing process. This study confirmed that neutron diffraction allows textures to be studied in the bulk of the sample, providing excellent grain statistics and superior accuracy.

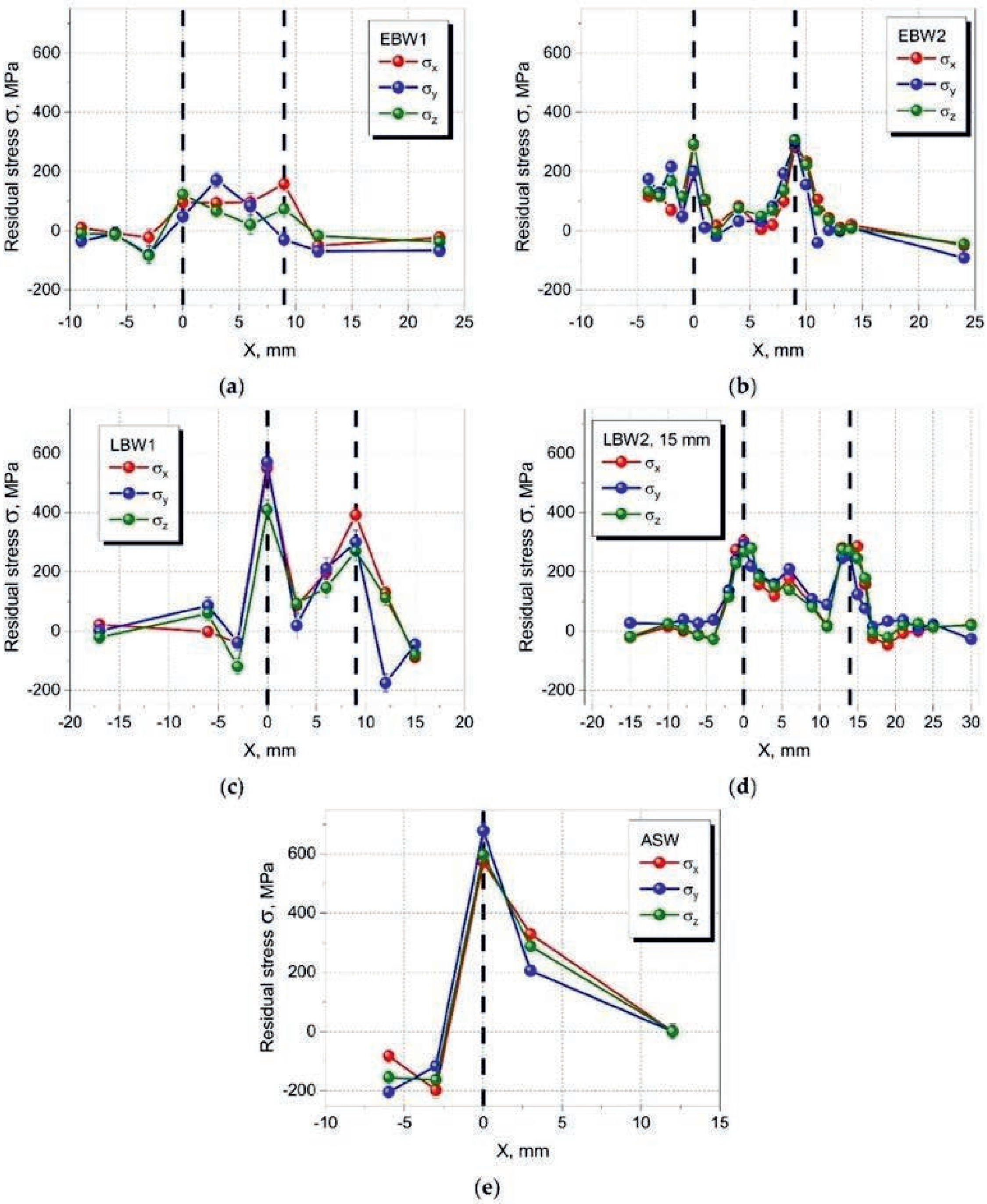


Fig. 4.1. Main components of the first-order residual stress tensor in 18MND5 steel specimens reconstituted by welding after the Charpy test. Different welding techniques are shown: arc stud welding (ASW), electron beam welding (EBW), laser beam welding (LBW). The X-axis of the coordinate system is directed along the specimens perpendicular to the welds, the Z-axis — perpendicular to the surface of the specimens. The dashed lines indicate positions of the welds [Bokuchava & Petrov, 2020].

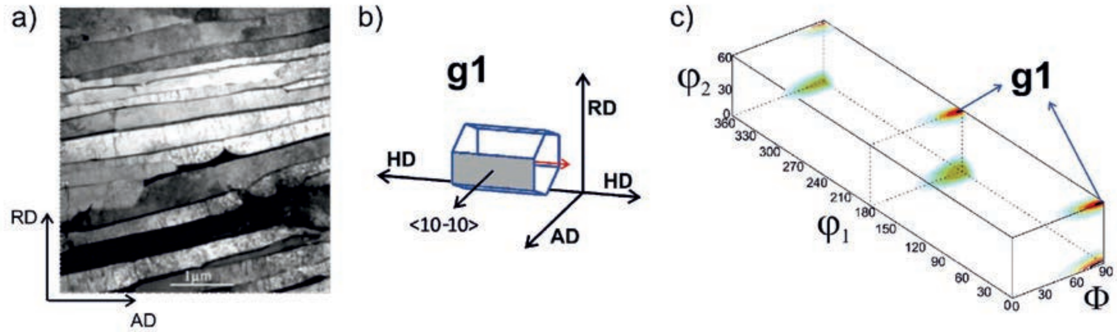


Fig. 4.2. Microstructure and texture of a high-pressure tube made of Zr+2.5%Nb alloy: SEM results (a), schematic representation of the main texture component g1 (b), distribution of orientation intensity in the orientation space in the Bunge notation (c). RD — radial, AD — axial and HD — tangential directions to the tube [Malamud et al., 2018].

The development of energy sources of the future is inextricably linked with controlled thermonuclear fusion in thermonuclear reactors (tokamaks), the operation of which, in particular, requires accurate measurement of magnetic fields. In tokamaks, fairly reliable inductive converters based on metal receiving coils with integrators are mainly used to measure the topology of the magnetic field distribution. Inductive converters are suitable for this function in tokamaks with a pulse duration of a magnetic field of no more than a few tens of seconds. Increasing the pulse duration to 3600 s for new-generation tokamaks, such as ITER, leads to an increase in the stationary part of the pulse, which results in a significant decrease in the accuracy of measuring the magnetic field. In addition, high neutron fluxes can generate radiation-induced signals in integrators, introducing an additional component of magnetic field measurement error. Investigations of radiation resistance of materials and devices that operate in high radiation fields require conducting the necessary studies on experimental facilities with conditions similar in characteristics. For example, a number of studies were conducted to study Hall sensors based on InAs/i-GaAs nanogeterostructures when irradiated with fast neutrons and gamma-rays at the IBR-2 reactor (FLNP JINR) [Bolshakova et al., 2015].

To carry out studies on the radiation resistance of materials and electronics under irradiation with fast neutrons and gamma-rays, as well as to conduct methodological work, at the future advanced neutron source it is necessary to make provision for an experimental beamline with access to irradiation positions in the immediate vicinity of the source with the possibility of *in situ* measurement of signals.

4.2. SOLAR ENERGY CONVERTERS

One of the possible directions of energy development is the use of organic solar panels. Lightweight, flexible, translucent and potentially cheap batteries could become a widely used renewable energy source. However, more research is needed to improve their efficiency and long-term stability.

In organic solar cells, conversion occurs through the absorption of photons in a donor polymer (e.g., poly(3-hexylthiophene), P3HT) to produce an exciton. It, in turn, dissociates into free charge carriers at the donor-acceptor interface. Small molecules, such as a fullerene derivative [6,6]-phenyl-C61-butyric acid methyl ester (PCBM), are commonly used as acceptors. To improve battery performance, it is necessary that the distance between the donor-acceptor interfaces in the active layer be comparable to the exciton diffusion length (~ 20 nm). Time-of-flight grazing-incidence small-angle neutron scattering has proven to be the best method for studying the morphology of the active layer. Using it, for example, it was shown that the addition of 1,8-octenedithiol to the P3HT:PCBM system (Figure 4.3) improves the solubility of PCBM in amorphous P3HT and reduces the average distances between PCBM regions and the size of P3HT regions, which simplifies the formation of excitons [Wienhold et al., 2020]. As a result, the conversion efficiency is improved and the short-circuit current of the battery increases.

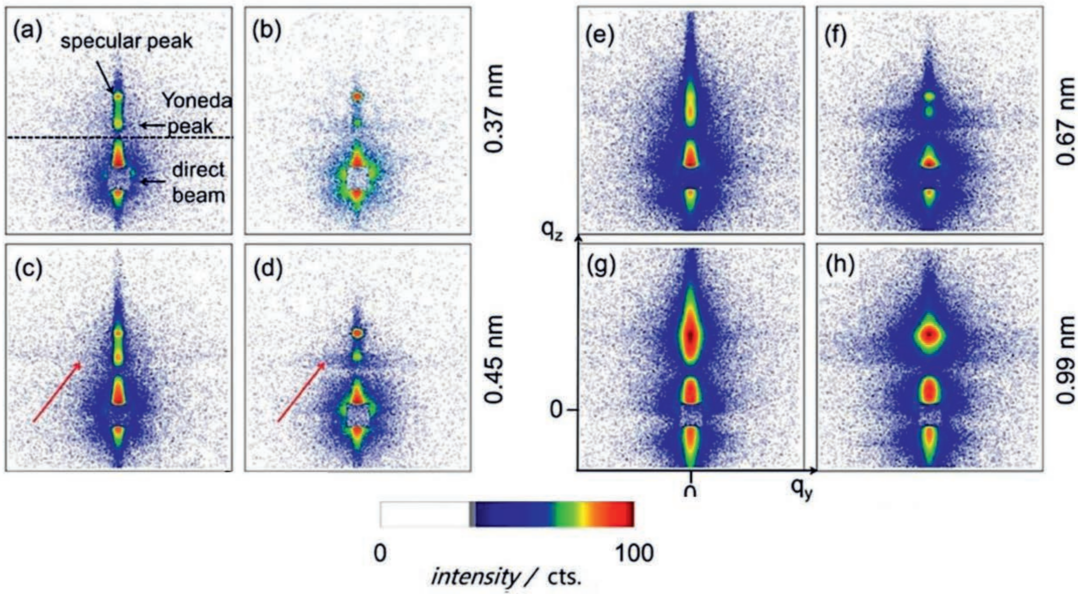


Fig. 4.3. Time-of-flight grazing-incidence small-angle neutron scattering from a thin film P3HT:PCBM without the addition of solvent (a, c, e, g) and with the addition of 5 vol% 1,8-octenedithiol (b, d, f, h). (a) shows the sample surface (dotted line), direct beam, specular peak and Yoneda peak; (g) shows the orientation of the scattering vector components [Wienhold et al., 2020].

The quasi-elastic neutron scattering method, which is extremely sensitive to hydrogen fluctuations in polymers due to the large incoherent scattering length of the hydrogen atom, has proven to be indispensable for studying the dynamics of the structure of the active layer of organic solar batteries. The presented examples are the initial stage of studying organic materials for use in solar batteries. The construction of new neutron sources with high-luminosity instruments on extracted beams will contribute to more active development of research in this direction.

4.3. CHEMICAL CURRENT SOURCES

It is no longer possible to imagine our daily life without mobile devices, electric cars, electric scooters and other devices that use solid-state batteries as energy sources. The main requirements for such energy sources are capacity or continuous operation time without recharging, durability, weight, dimensions, operating temperature range, etc. A huge number of studies of materials for lithium-ion batteries have been performed using neutron scattering methods, in particular [Avdeev et al., 2019; Kosova et al., (2015)].

Lithium-ion batteries are widely used in a variety of applications. However, the relatively low lithium content in the Earth's crust and the predicted depletion of economically viable lithium reserves by the middle of the 21st century make it necessary to develop new types of batteries. Currently, active research is underway into electrode materials for the creation of commercial sodium-ion batteries. Due to the high penetrating power of thermal neutrons, sensitivity to light atoms in the structure, and the fact that the energy of thermal neutrons is comparable to typical excitation energies of the crystalline structure, neutron scattering methods are widely applied in these studies [Shah et al., 2021].

For example, using the *operando* neutron diffraction technique for an electrochemical $Na_{0.5}Ni_{0.25}Mn_{0.75}O_2$ +hard carbon cell (Figure 4.4), a local ordering of Ni and Mn ions was revealed, which is associated with a large difference in their valence. The sequences of phase transformations in the cathode material were also determined and it was found that at a voltage of more than 4 V, the cathode is transformed into a new structural phase O3s, which is a completely Na-depleted O3 phase (space group R-3m) [Liu et al., 2020].

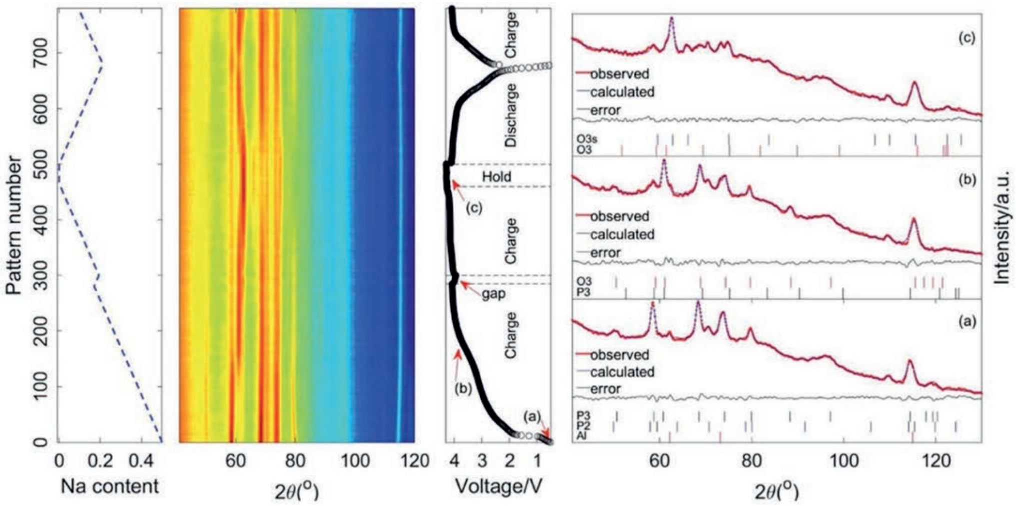


Fig. 4.4. Neutron diffraction patterns of $Na_{0.5}Ni_{0.25}Mn_{0.75}O_2$+hard carbon cell (intensity is shown in color: the highest is red, the lowest is blue), measured *in operando* during cycling at 10 mA/g. Shown are the calculated sodium content, cell voltage, and diffraction patterns for different cell states, which are marked with red arrows [Liu et al., 2020].

Inelastic neutron scattering experiments made it possible to measure the phonon density of states in a promising cathode material. A correlation was established between changes in the dynamics of sodium ions and the discovery of one- and two-dimensional sodium diffusion paths during structural phase transitions in the layered oxide $Na_{0.7}CoO_2$ [Juranyi et al., 2015]. Neutron diffraction studies are also carried out in the development of new solid electrolytes in order to reduce the cost of sodium-ion batteries, improve operational stability and enhance safety [Gao et al., 2023]. There is no doubt that the search for new materials for chemical power sources will continue in the future, and neutron scattering methods will play a significant role in the study of such materials. For example, for potassium-ion batteries or multivalent metal-ion batteries [O'Donnell & Greenbaum, 2020].

4.4. HYDROGEN ENERGY

The use of hydrogen for energy production, storage and consumption is of great interest in terms of radical reduction of greenhouse gas emissions. One of the most important tasks of materials science in this area is the development of new materials for hydrogen storage, including various hydrides and porous materials. To solve this problem, neutron scattering methods are needed, in particular diffraction, inelastic and quasi-elastic scattering [Zhang et al., 2022; Klein et al., 2023]. The advantage of neutrons in such studies is their sensitivity to the isotopic substitution of deuterium for hydrogen, which opens up additional possibilities for the technique. So, the *in situ* neutron diffraction technique allows us to study the structure and hydrogenation kinetics of MgD_2-TiD_2 nanocomposites [Ponthieu et al., 2013]. Cheap and environmentally friendly magnesium hydride has the capacity for (reversible) uptake of up to 7.6 wt.% hydrogen, but the kinetics of hydrogen adsorption and desorption are extremely slow. Reactive ball milling makes it possible to synthesize hydrogen-rich MgD_2-TiD_2 nanocomposites with excellent hydrogen adsorption and desorption kinetics, which is due to the limitation of grain growth of Mg and MgD_2 phases by TiD_2 nanoinclusions and the coherence of interfaces between MgD_2 and TiD_2 (Figure 4.5), which allows for short hydrogen diffusion paths in the Mg matrix during reversible hydrogen loading.

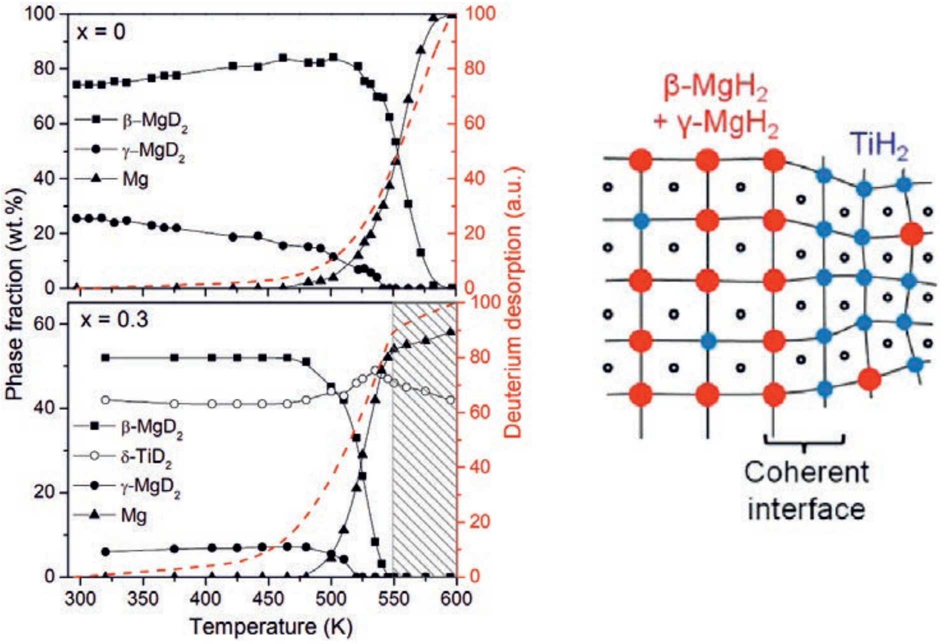


Fig. 4.5. *Left*: changes in the phase composition of MgD_2 and 0.7 MgD_2 + 0.3 TiD_2 nanocomposites during thermal desorption of deuterium upon heating at a rate of 0.5 K/min (dashed line shows the fraction of desorbed deuterium). *Right*: a schematic representation of the interface between phases [Ponthieu et al., 2013].

Neutron scattering plays an indispensable role in studying chitosan, which is considered as a promising material for electrodes or proton-exchange membranes for various fuel cells. It is a naturally occurring polysaccharide found in fungi, algae, sponges, worms, and mollusks, which shows good proton conductivity under humid conditions. Using quasi-elastic neutron scattering, the proton dynamics in hydrated chitosan was studied. It was demonstrated that hydrated chitosan exhibits proton conductivity at temperatures > 238 K. More specifically, proton transfer from the hydroxyl and amino groups of chitosan to the surrounding hydration water molecules plays a key role in the proton conductivity, as do the slow dynamics of the hydration water. It was shown that mobile hydration water assists protonation due to almost identical activation energies of the protonation process and the jump diffusion of hydration water [Hirota et al., 2022].

Due to the high penetrating power of neutrons and the high sensitivity of neutron scattering methods to hydrogen, neutron radiography makes it possible to visualize the change in water distribution during the operation of hydrogen fuel cells (Figure 4.6) [Nasu et al., 2022].

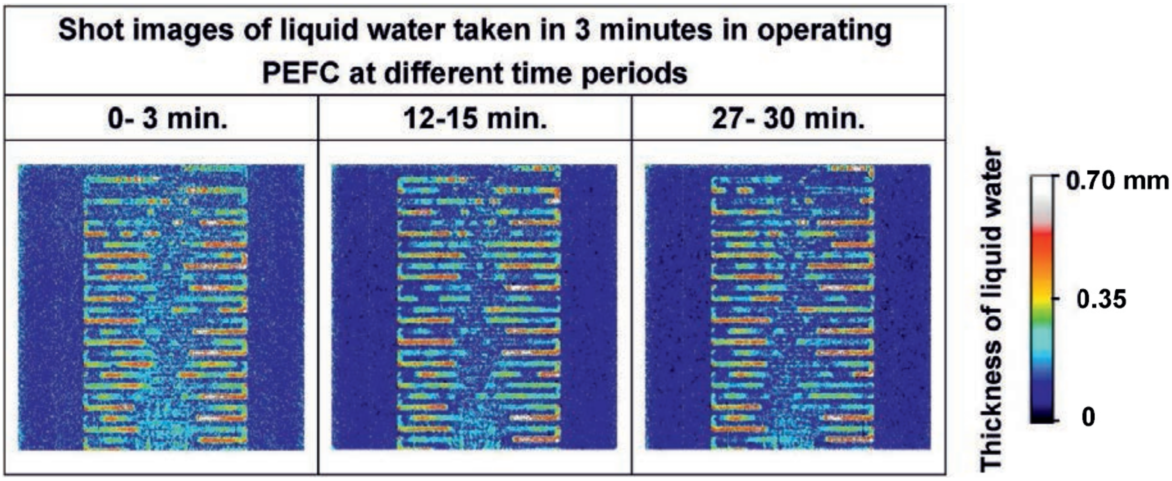


Fig. 4.6. Distribution of liquid water in an operating polymer electrolyte fuel cell with a water-repellent gas diffusion layer as a cathode at different time periods. The current density is 1 A/cm^2, the cell temperature is 75°C, and the relative gas humidity is 73% [Nasu et al., 2022].

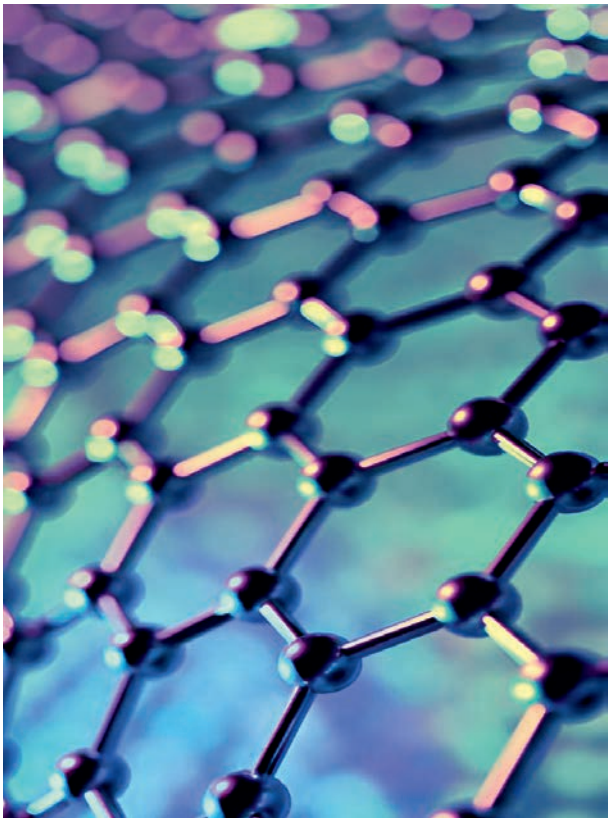
Such experiments are indispensable for solving the problems of developing powerful, stable and safe hydrogen fuel cells.

4.5. APPLICATION OF NEUTRON METHODS IN RESEARCH OF MATERIALS FOR ENERGY PRODUCTION AND STORAGE

Neutron scattering allows solving a huge number of problems in various areas of materials science that are relevant for the development of energy generation and storage, including those that will be of interest in the coming decades, such as the development of nuclear and thermonuclear energy, investigations of new materials for hydrogen energy and promising current sources (for example, K-ion, multivalent metal-ion batteries). The development of alternative energy sources and improvement of their efficiency, durability and environmental friendliness, such as solar energy converters, require the search and study of new materials, as well as their structure and dynamics.

In view of such a wide variety of tasks, the solution of which may take more than one decade, the instrument suite on extracted beams of the new advanced neutron source should include small-angle scattering instruments, diffractometers, inelastic and quasi-elastic scattering spectrometers, setups for studying radiation resistance and conducting methodological work. Studies of *in situ* processes require the development of appropriate sample environment instrumentation comprising fuel hydrogen cells and chemical current sources, loading machines, etc. In many cases, studies need to be carried out in real time, which requires high neutron fluxes.

Materials science



Materials science is an interdisciplinary science that studies the relationship between the composition, structure, processing and properties of materials in order to optimize the production and use of finished products in medicine, energy, construction, mechanical engineering and other industries. Materials science is concerned with a wide range of compositions and structures, both of well-known and widely used metals, steels, alloys, glasses, cements, ceramics, semiconductors, etc., and those that have emerged and attracted attention in recent decades: high-entropy alloys and alloys with giant magnetostriction, superduplex steels, bulk metallic glasses, metal-organic frameworks, nano- and biomaterials, metamaterials, etc. For the production of finished products, both classical methods of mechanical and thermal processing, welding, etc., as well as new ones, such as intensive plastic deformation processes or additive technologies, are used. Despite the fact that even in the first studies using thermal neutron scattering, one of its disadvantages was noted — the small number of available neutron sources compared to X-ray and electron sources [Shull & Wollan, 1948], diffraction, small-angle and inelastic neutron scattering, neutron radiography and tomography, as well as reflectometry, are widely used in the study of the structure and microstructure, phase state and composition, preferred grain orientations, residual mechanical stresses, dynamics of atoms and molecules of all kinds of materials. The sensitivity of neutron scattering to light elements, especially hydrogen, different isotopes of the same chemical element, and magnetic neutron scattering prove extremely useful. Due to the high penetrating power of thermal neutrons, it is possible to study bulk (> 100 cm^3) samples, which is important when gradients of phase composition, crystallographic texture, etc., or surface effects may exist in the material. In this case, the use of surface-sensitive methods, such as X-ray diffraction analysis of crystal structures, may lead to incorrect conclusions about the relationship between the structure of the material and its properties (Figure 5.1) [Sumnikov et al., 2022]. It should be noted that the application of the reverse time-of-flight technique makes it possible to achieve excellent resolution and symmetrical shape of diffraction peaks, which opens up the possibility of precise determination of structural parameters (determination of the density of dislocations of different types, distribution of crystallites of the material by shape and size, various stacking faults) from neutron diffraction data [Bokuchava, 2020].

The range of problems that can be solved using neutron scattering methods in investigations of various materials is very wide. We will consider only a few examples, distributed by research topics. This division is rather arbitrary. For example, shape memory alloys are widely used in medicine, aerospace industry, robotics, and neutron scattering methods are employed not only to study changes in their crystal structure, crystallographic texture, microstructure, internal mechanical stresses, etc. during thermoelastic martensitic transformation, which is responsible for the shape memory effect, but also to investigate their formation in the process of manufacturing finished products from these materials (including using additive technologies) or in the manufacture of products using welding.

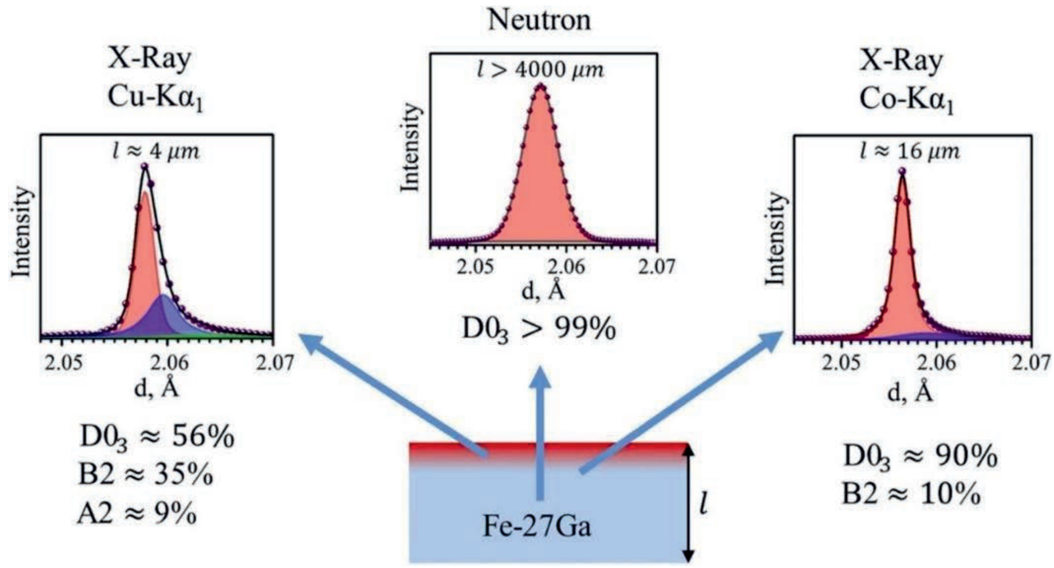


Fig. 5.1. Dependence of the phase composition of the magnetostrictive Fe-Ga alloy measured using diffraction methods on the penetration depth of the radiation used [Sumnikov et al., 2022].

5.1. STRUCTURAL MATERIALS

5.1.1. Steels

Neutron scattering methods have found wide application in the study of structural materials in all branches of industry: aerospace, chemical, oil and gas, mechanical engineering, machine tool building, metallurgy, construction, etc. In particular, much attention is now being paid to the study of various types of steel: structural, tool, and especially special-purpose steels.

For example, in the study of two duplex stainless steels, ^{22}Cr-^{5}Ni (2205) and ^{25}Cr-^{7}Ni (2507), which have excellent strength and resistance to aggressive environments and are therefore used in the chemical and oil and gas industries, the small-angle neutron scattering method was used to investigate the formation of phase separation induced by long-term aging (up to 6000 hours). The consequence of this process is the strengthening of the ferrite component of steel, an increase in its hardness and a change in the mode of its deformation under load [Xu et al., 2019]. Further studies are needed to determine whether the mechanism of steel embrittlement is temperature dependent and to define the mechanism of phase transformation in ferrite at high temperatures, which may be either spinodal decomposition or nucleation and growth.

In [Liang et al., 2020], the effect of hydrogen embrittlement of UNS S32760 super duplex stainless steel was investigated using neutron diffraction. It was shown that in austenite, hydrogen saturation increases the dislocation density, resulting in plastic deformation of the austenite component of the steel. In ferrite, on the contrary, after hydrogen saturation, the dislocation density decreases slightly (Figure 5.2).

Along with fractography analysis of the samples, neutron diffraction studies allowed us to propose a model describing the process of hydrogen embrittlement in super duplex stainless steels. Research into hydrogen embrittlement of various structural materials appears to be very promising in connection with the potential use of hydrogen fuel and the need to design appropriate pipelines, storage facilities, etc. [Wang et al., 2022a]. Neutron scattering techniques will help to create models that can predict the service life of structures, estimate critical loads, and optimize the microstructural design of duplex stainless steels.

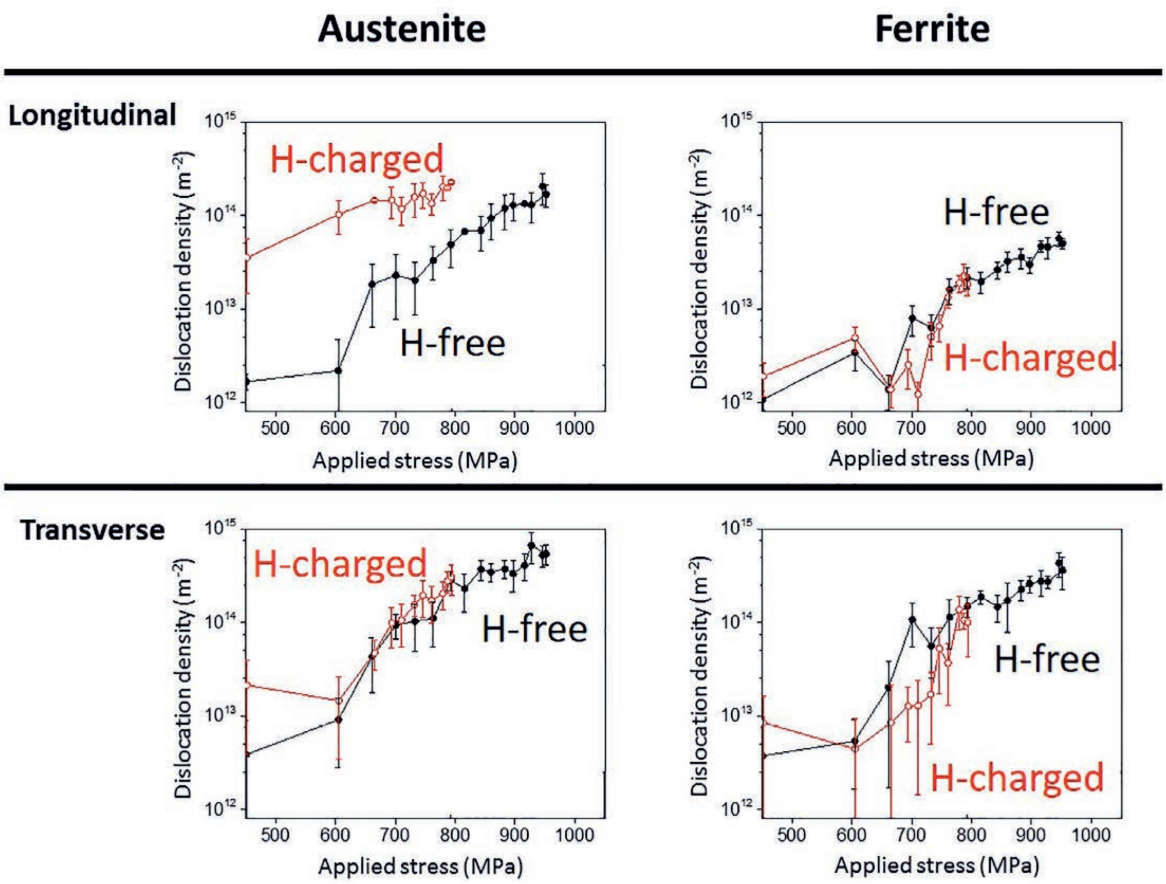


Fig. 5.2. Evolution of dislocation density in austenite and ferrite of super duplex stainless steel UNS S32760 before and after hydrogen saturation at a strain rate of 10^{-4} s^{-1} [Liang et al., 2020].

5.1.2. Alloys

Neutron scattering methods are actively used to study various alloys. Of interest are both their atomic and magnetic structures, their ordering and characteristic defects, as well as the characteristics of finished products: phase composition, crystallographic structure, microstructure. Due to the high penetrating power of thermal neutrons, studies are carried out on bulk samples.

One of the widely used structural materials is lightweight aluminum alloys. Their strength can be increased, for example, by thermomechanical treatment, which significantly increases the density of vacancies and dislocations in the structure. As a rule, this leads to a decrease in the plasticity of the material. However, the formation of wide low-angle boundaries in aluminum allows obtaining a lightweight, ductile alloy with a high tensile strength. Using the neutron total scattering technique, it was shown that in the alloy Al + ≈1 wt.% ZnO nanoparticles (20 nm), aluminum-oxygen bonds are formed (Figure 5.3), with oxygen atoms occupying interstitial positions in the aluminum lattice [Joo et al., 2023]. Oxygen-saturated regions form wide low-angle boundaries, which in turn form clusters of dislocations that facilitate dislocation glide at the initial stage of plastic deformation. With an increase in the degree of deformation, the exit of dislocations onto the surface of the low-angle boundary contributes to dislocation strengthening.

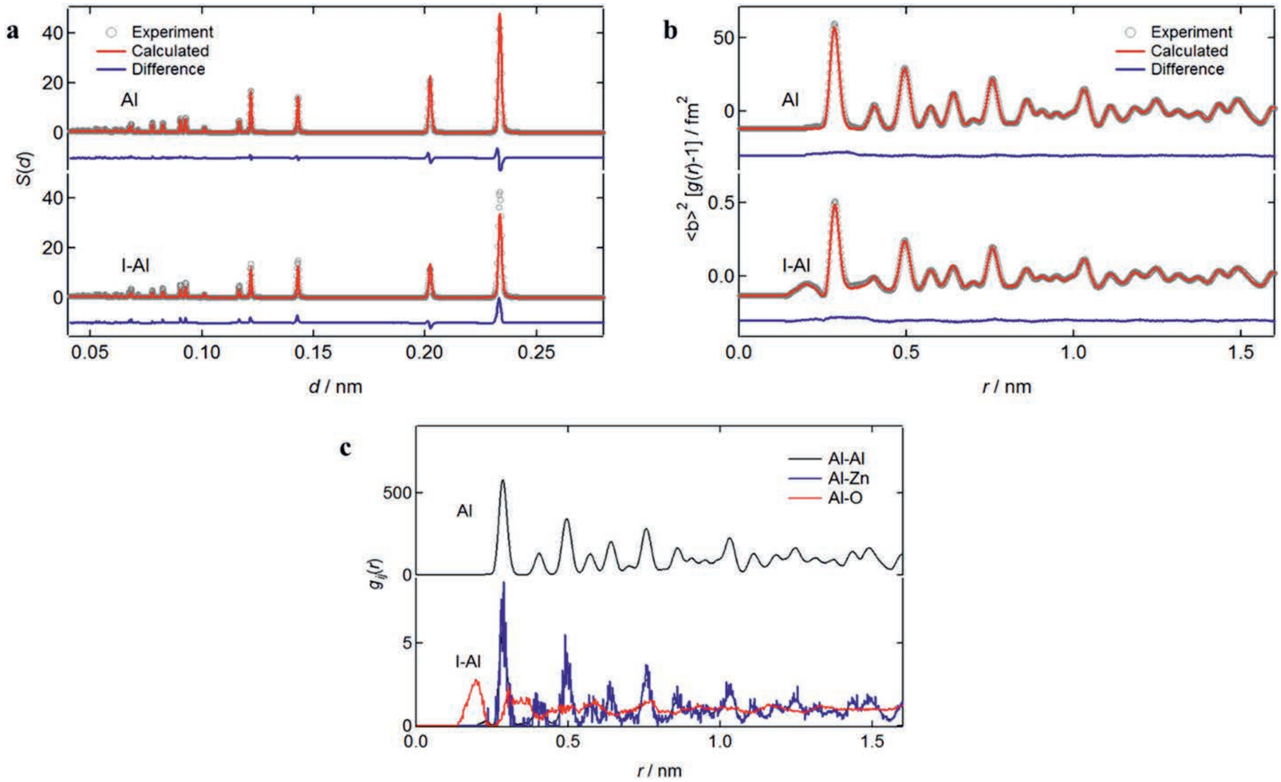


Fig. 5.3. Neutron diffraction patterns of pure aluminum and aluminum with interstitial oxygen atoms (a); corresponding pair correlation functions (b); partial pair distribution functions for different pairs of atoms (c) [Joo et al., 2023].

In the 2010s, interest in high-entropy alloys, i.e. alloys containing at least five elements, with the amount of each element being in the range of 5-35 at.%, increased significantly. Such materials are characterized by high entropy of mixing, so their properties and the processes occurring in them differ significantly from known metals and alloys. Potentially, it is possible to obtain high-entropy alloys with extremely high hardness, heat resistance, corrosion resistance, ductility, etc., over a wide range of temperatures and other conditions. Neutron scattering techniques are extensively used in research to develop high-entropy alloys with improved characteristics. For example, using *in situ* neutron diffraction, the process of inelastic deformation was studied for fine-grained (≈ 6 μm) high-entropy alloys with nominal compositions of $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$, $Co_{35}Cr_{20}Mn_{15}Ni_{15}Fe_{15}$ and $Co_{35}Cr_{25}Mn_{15}Ni_{15}Fe_{10}$ with a strain rate of 1×10^{-3} s^{-1} [Wei et al., 2022]. Analysis of the positions and profiles of diffraction peaks made it possible to calculate the elastic deformations of the crystal structure, dislocation density, probabilities of the existence of stacking faults and twins in the structure (Figure 5.4) at various stages of deformation. The latter two alloys have better plastic and strength properties (the tensile strength of $Co_{35}Cr_{25}Mn_{15}Ni_{15}Fe_{10}$ is 40% higher than that of $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$), which, however, is due to different physical mechanisms, as established using neutron diffraction on bulk samples of high-entropy alloys.

It should be noted that the possibility of producing high-entropy alloys using different isotopes of the same chemical element, which are clearly distinguishable using neutron scattering, can significantly facilitate the task of studying the atomic ordering and dynamics of these alloys.

There are also many tasks to be solved in the field of thermomechanical processing of high-entropy alloys, as well as, for example, the development of technologies for their welding [Li et al., 2021], in which the use of neutron scattering methods will play a significant role.

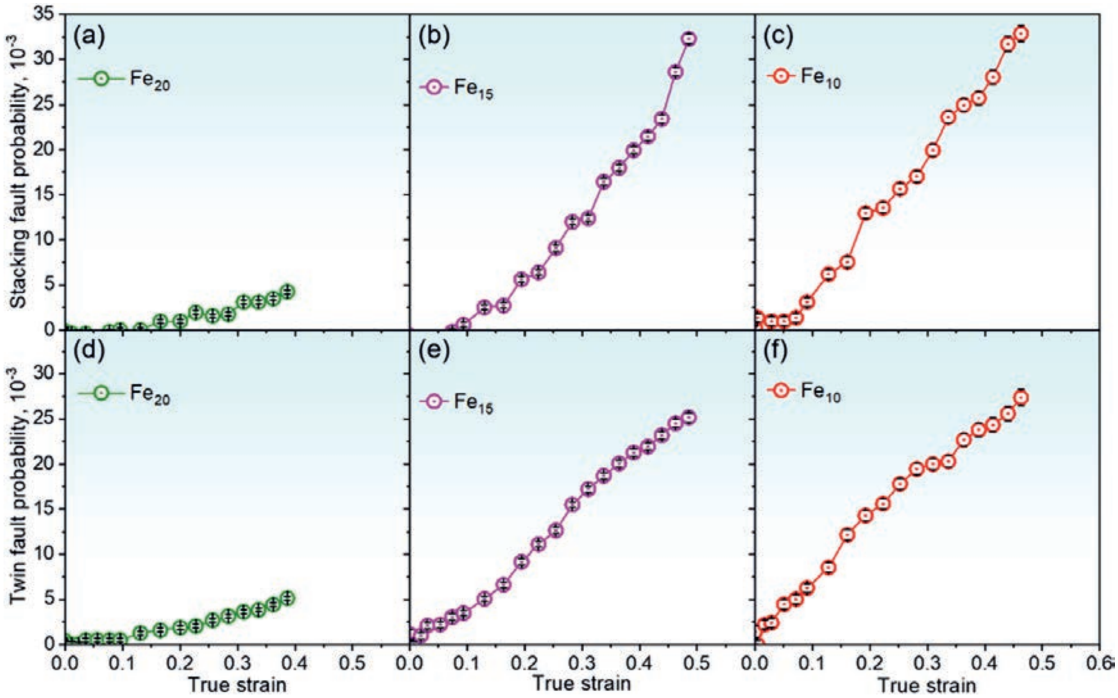


Fig. 5.4. Stacking fault probability (a, b, c) and twin fault probability (d, e, f) calculated from neutron diffraction data for $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$ (designated as Fe_{20}), $Co_{35}Cr_{20}Mn_{15}Ni_{15}Fe_{15}$ (Fe_{15}) and $Co_{35}Cr_{25}Mn_{15}Ni_{15}Fe_{10}$ (Fe_{10}). [Wei et al., 2022]

Obviously, to optimize the production processes of finished products, it is necessary to study the crystallographic textures of a large number of samples processed under various conditions. At present, the characteristic times for texture measurements on the specialized neutron diffractometer at FLNP JINR are about a day, whereas on neutron sources with higher fluxes, texture measurements can be performed within a few minutes (e.g., [Onuki et al., 2016]).

A significant increase in the neutron flux at the sample position at neutron scattering instruments of the new neutron source of FLNP JINR will make it possible to measure crystallographic textures for large series of samples and study changes in the textures of materials *in situ*, during plastic deformation, recrystallization or phase transformations.

5.1.3. Concretes and glasses

Using *in situ* neutron tomography, moisture migration processes in concrete subjected to gradient heating up to 300°C can be explored to study the physical causes of spalling in concrete exposed to high temperatures and to develop a technology for enhancing the structural stability of concrete structures during fires [Dauti et al., 2018]. Due to the high sensitivity of thermal neutrons to hydrogen, it was possible to directly track the movement of the drying front and the accompanying accumulation of moisture behind this front due to dehydration, evaporation, condensation and mass transfer caused by temperature and pressure gradients along microcracks in concrete. This moisture accumulation causes pore pressure build-up and may result in concrete spalling. It was found that the drying rate of concrete and the size of the area with increased moisture content depend on the maximum size of concrete aggregate particles (particles of sedimentary and metamorphic rocks). Concrete with a maximum aggregate particle size of 8 mm dries faster due to a more branched system of microcracks, however, the size of the area with increased moisture content in it is almost twice as large as in concrete with a maximum aggregate particle size of 4 mm (Figure 5.5).

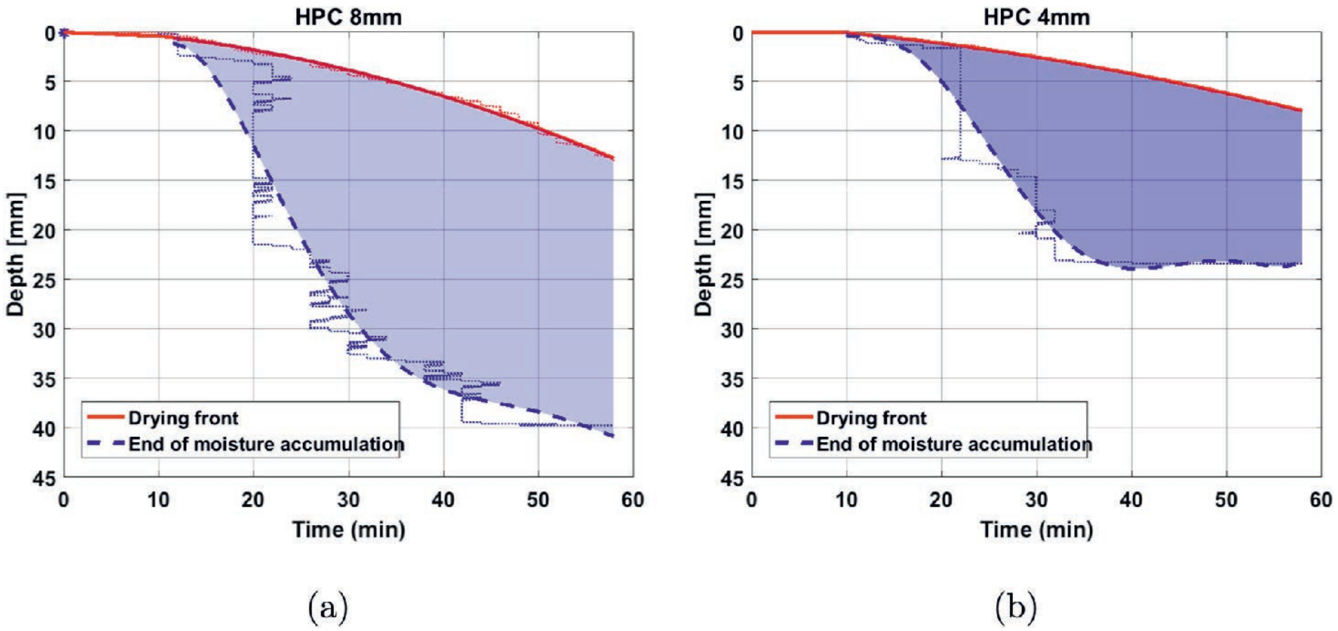


Fig. 5.5. Areas with increased moisture content during drying of concrete with a maximum aggregate particle size of 8 mm (a) and 4 mm (b) from neutron tomography data [Dauti et al., 2018].

The acquisition time for one 3D neutron image is only one minute, but this can be achieved by binning the acquired data and the concomitant deterioration of spatial resolution to 200 μm. To study fast processes with better spatial resolution (20–50 μm), a significant increase in the neutron flux on the instrument is necessary. **Given that hundreds of radiographic images are required to reconstruct 3D tomographic data, at higher fluxes on the instruments of the advanced pulsed neutron source it will be possible to achieve subsecond time resolution while maintaining good spatial resolution for *in situ* tomography experiments.**

The use of industrial waste and a number of natural materials as additional binding components in the production of concrete can be beneficial not only from an economic and environmental point of view, but also lead to the development of more durable concrete that is stable in various aggressive environments. For example, the addition of certain types of volcanic ash to cement leads to the formation of calcium aluminosilicate hydrate (C-A-S-H) as a binding component of durable concrete that is resistant to seawater. Using quasielastic neutron scattering [Kupwade-Patil et al., 2016], bound water indices, self-diffusion coefficients and mean jump distances of atoms in the early stages of hydration of Portland cement and volcanic ash with different average particle sizes were obtained. It was found that the addition of a small amount of finer volcanic ash particles (10 wt.%, grain size 14 μm) increases the bound water index (Figure 5.6) and the self-diffusion coefficient, indicating a higher concentration of bound immobile water in the material. An increase in the size of ash particles or an increase in their concentration leads to an acceleration of hardening, but at the same time the amount of free and mobile water in the material increases and it can be assumed that volcanic ash is not fully involved in the hydration process. The optimal hardening regime and the required final strength of concrete can be achieved by selecting the concentration and particle size of volcanic ash.

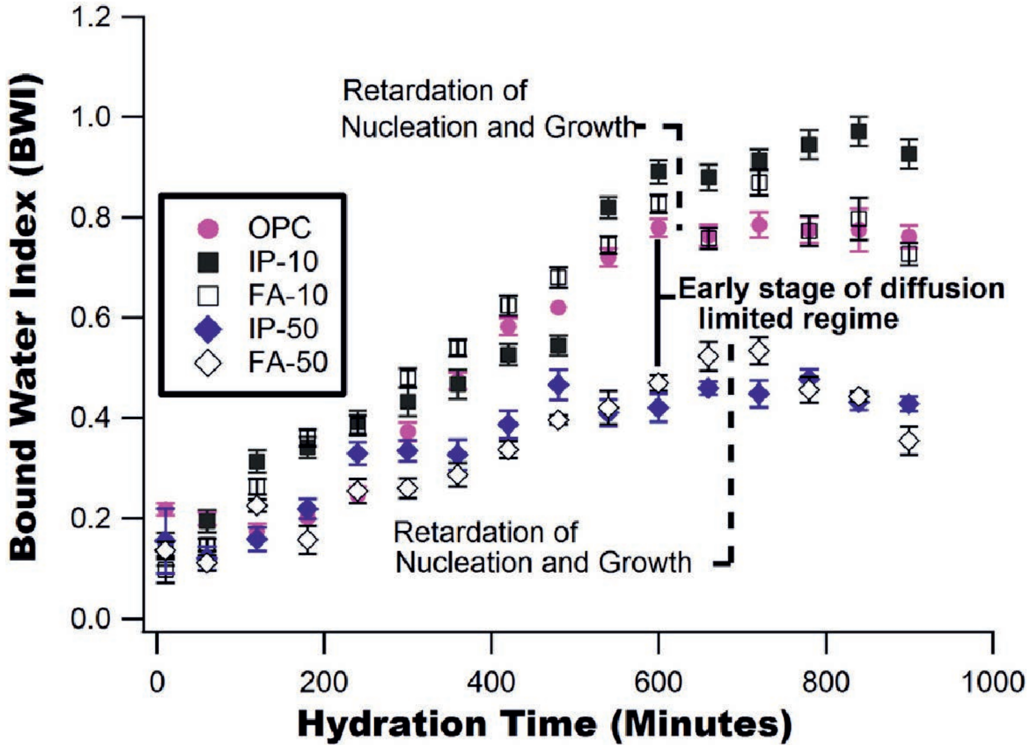


Fig. 5.6. Change in the bound water index during hardening of Portland cement (OPC) and mixtures of Portland cement and volcanic ash with grain sizes of 17 μm (IP) and 14 μm (FA). Index 10 indicates that the mixture contains 10 wt.% volcanic ash, and index 50 — 50 wt.% [Kupwade-Patil et al., 2016].

Glasses based on the CaO-MgO-Al_2O_3-SiO_2 (CMAS) system have high mechanical properties, excellent optical characteristics and chemical resistance. Therefore, they are promising candidates for a wide range of applications such as industrial and nuclear waste encapsulation, high performance glasses, ceramics, and cements. There is also evidence that CMAS glasses are important constituents of the Earth's lower crust and mantle, and their studies will contribute to a better understanding of the conditions and processes occurring in the lithosphere. The physical properties of glasses are determined by their chemical composition and structure. In [Gong et al., 2021], neutron total scattering and synchrotron radiation were used in combination with molecular dynamics simulations and density functional theory calculations to study the structure and generate detailed structural representations for a CMAS glass with a chemical composition of 42.3 wt% CaO, 32.3 wt% SiO_2, 13.3 wt% Al_2O_3, and 5.2 wt% MgO (Figure 5.7). It was found that for the nearest-neighbor bonding environment with oxygen atoms, Al is mainly in IV-coordination with a small proportion of V-fold, whereas Ca and Mg atoms exhibit a much wider distribution of coordination states, with an average of ~6.73 and ~5.15, respectively. Analysis of the next nearest neighbors revealed that there is slight preference for Ca atoms to associate with Si and Al atoms, which form the aluminosilicate network of the structure. Analysis of the oxygen environment revealed the violation of the Löwenstein's rule of Al-O-Al avoidance, preferential association of non-bridging oxygen atoms with Si atoms and other interesting structural features. It should be noted that for a full understanding of the relationship between the composition, structure and properties of such glasses in different conditions, further research is needed, including *in situ* total scattering experiments, which require high neutron fluxes over a wide range of momentum transfer and low background. **Both the neutron flux and the background conditions on the instruments of the new source should be significantly improved, which will open up the possibility of conducting such experiments.**

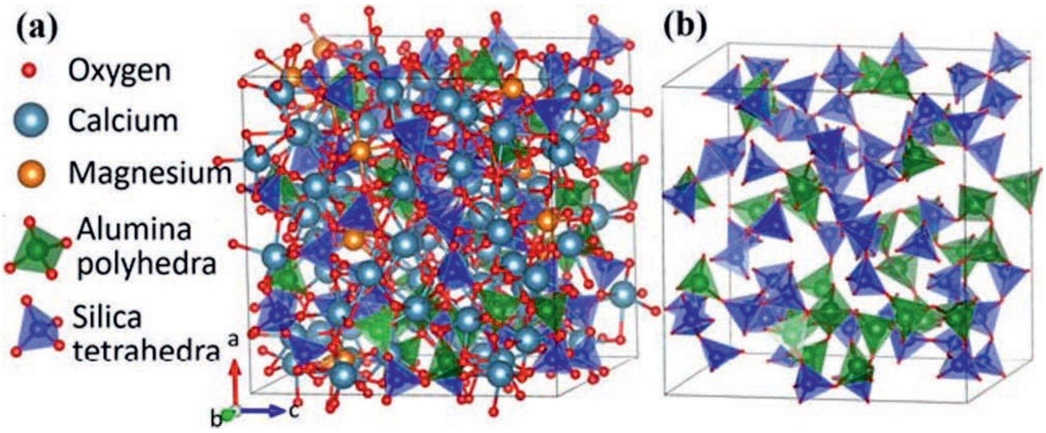


Fig. 5.7. (a) A representative final structure of the CaO-MgO-Al_2O_3-SiO_2 glass obtained after DFT geometry optimization. (b) The aluminosilicate network of the CMAS glass structure in (a) [Gong et al., 2021].

5.2. FUNCTIONAL MATERIALS

The term "functional materials" covers a huge number of very diverse materials that have their own specific properties and functions. Functional materials include metals and alloys, polymers and ceramics, nanocomposites and metal-organic frameworks, magnetic fluids and other materials that are piezo-, pyro- or ferroelectric, have magnetostriction or shape memory effect, are capable of adsorbing various gases, and so on. Even review articles devoted to the study of functional materials by neutron scattering methods usually cover only a small part of all the materials, properties and methods being studied (e.g. [Peterson & Papadakis, 2015]). Therefore, here and below, only some examples of studies of interesting materials and systems will be considered.

5.2.1. Shape memory alloys

The most commonly used shape memory alloy is nitinol (Ni-Ti with a nickel content slightly higher than 50 at.%), which has high strength, corrosion resistance, shape recovery coefficient, and good biocompatibility. Using *in situ* neutron diffraction, for $Ni_{55}Ti_{45}$ samples, it was shown that despite the different microstructure and texture of as-cast and hot-swaged samples, the development of preferred grain orientations during inelastic deformation occurs in them in the same way: [010] directions are oriented along the applied mechanical load (Figure 5.8) [Wang et al., 2021]. Neutron diffraction data made it possible to construct a model of deformation of the shape memory alloy, taking into account elastic deformations, reversible and irreversible plastic deformations during the reverse martensitic transformation, and also including the orientation of various martensite variants relative to the external load.

It should be noted that the temperature range of thermoelastic martensitic transformation in Ni-Ti alloys is below 100°C. For some applications, such as in the aerospace industry, it is necessary to develop cheap, strong, corrosion-resistant shape memory alloys that can function at temperatures up to 400°C [Ma et al., 2010]. For these purposes, NiTi(Hf,Zr) alloys are among the most promising candidates. *In situ* neutron diffraction studies of the $Ti_{29.7}Ni_{50.3}Hf_{10}Zr_{10}$ alloy during its cycling in the martensitic transformation temperature range made it possible to reveal 10% of retained austenite in the material, which does not participate in martensitic transformation [Shuitcev et al., 2022]. In addition, it was found that the retained austenite is partially disordered and simultaneously with the reverse martensitic transformation in this alloy, the austenite becomes ordered (Figure 5.9). Since the Ti atom has a negative thermal-neutron coherent scattering length, the fundamental diffraction peaks of austenite in $Ti_{29.7}Ni_{50.3}Hf_{10}Zr_{10}$ are only an order of magnitude more intense than the superstructure ones. In the case of X-ray scattering or synchrotron radiation, the difference in the intensities of such parasitic peaks is more than three orders of magnitude, so thermal neutron diffraction seems to be the preferred method for studying ordering in such systems. However, the presence of Ti atoms, as well as the large cross-section of thermal neutron absorption by Hf atoms, lead to low neutron scattering intensity and the need for long-term measurements. For example, the time for measuring the crystallographic texture of $Ti_{29.7}Ni_{50.3}Hf_{10}Zr_{10}$ samples at the SKAT diffractometer of the IBR-2 reactor at FLNP JINR can be estimated at ~10 days, and taking into account the texture is necessary for correct structural studies. **A significant increase in the neutron flux at the scientific instruments at the new source of FLNP JINR will make it possible to measure the crystallographic textures of high-temperature shape memory alloys based on NiTi(Hf,Zr) and other alloys in a significantly shorter time and with greater accuracy.**

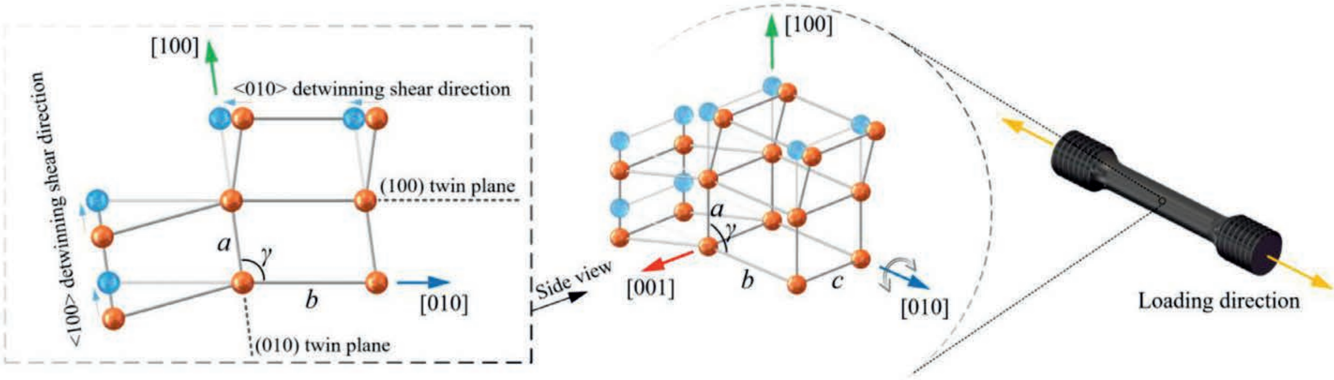


Fig. 5.8. Schematic illustration of detwinning of the (010) + (100) compound twin structures of martensite B19' $Ni_{55}Ti_{45}$: grains reorient with the [010] direction parallel to the loading direction and distribute homogeneously around the [010] pole, thus accommodating the detwinning shear strain along the loading direction [Wang et al., 2021].

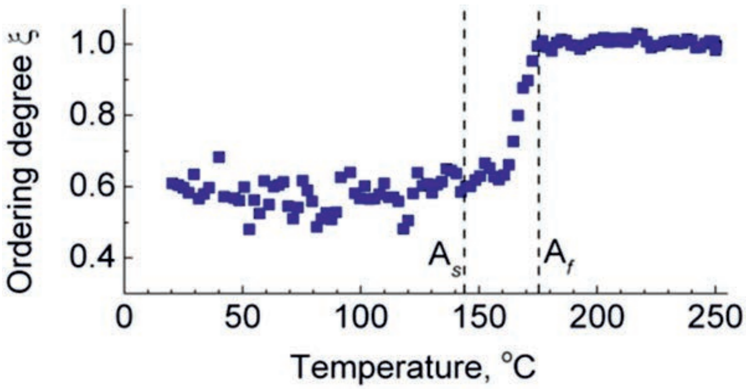


Fig. 5.9. The ordering degree of austenite during reverse martensitic transformation in the $Ti_{29.7}Ni_{50.3}Hf_{10}Zr_{10}$ alloy (without taking into account the weak crystallographic texture) [Shuitcev et al., 2022].

Functional alloys based on Mn-Cu are characterized by the shape memory effect with a small hysteresis of reversible thermal deformation, so they can be used for many temperature cycles without significant loss of functional properties. Small-angle neutron scattering measurements of the Mn-13Cu alloy made it possible to reveal that ageing for 1-120 h in the temperature range of 400—560 °C is accompanied by the decomposition into a Mn-rich matrix containing only 3.5-6.5 at.% Cu and Cu-rich clusters with a Cu content of 40-46 at.% [Sun et al., 2021a]. The volume fraction of clusters with increasing time or temperature of ageing remains practically unchanged, but the average volume of clusters increases significantly, i.e., merging of smaller clusters occurs. Also, it was found that higher ageing temperature or longer ageing time leads to the formation of α-Mn inclusions, which can affect the functional properties of the alloy. A linear relationship between phase transition temperatures and the Mn content in the matrix was established. The use of *in situ* neutron diffraction (Figure 5.10) made it possible to reveal that in the binary Mn-13Cu alloy the temperatures of the magnetic and structural transitions coincide, and the tetragonal distortion of the structure changes smoothly in proportion to the square of the long-range magnetic order parameter, which corresponds to the semi-phenomenological theory for such alloys.

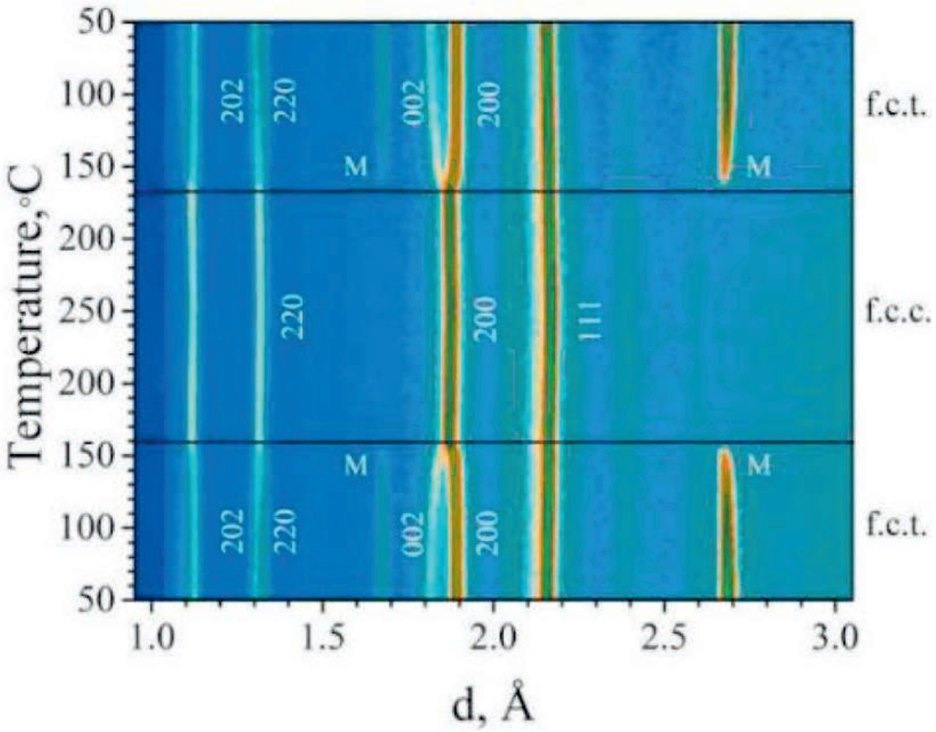


Fig. 5.10. Evolution of neutron diffraction patterns during a heating-cooling cycle of the Mn-13Cu alloy aged for 8 h at 440°C, in the region of martensitic transformation from the face-centered tetragonal phase to the face-centered cubic phase and back. Antiferromagnetic peaks are indicated by M [Sun et al., 2021a].

The addition of 3 at.% chromium to the Mn-12Cu alloy leads to a noticeable decrease in the martensitic transformation temperatures in the alloy and an increase in the transformation temperature hysteresis, and also destroys the direct proportionality of the tetragonal distortion and the square of the long-range magnetic order parameter [Sun et al., 2021b].

These studies conducted at the IBR-2 reactor show that in order to establish the relationship between the composition of functional alloys, the processes of their thermomechanical treatment and the desired physical properties, measurements of a large number of samples by neutron scattering methods are required. It should be noted that due to the negative length of coherent scattering of thermal neutrons by the Mn atom, the collection of neutron diffraction data for Mn-Cu-based alloy samples takes a significant amount of time. Diffraction patterns measured with relatively low statistics (Figure 5.11) make it possible to determine the phase composition of the alloy and the main structural parameters, but do not allow a quantitative analysis of the microstructural features of the material even using simple integral width methods. It can only be noted that the magnetic peaks are significantly wider than the nuclear ones, so the size of the coherent magnetic scattering regions is apparently significantly smaller than the coherent nuclear scattering regions. It can also be seen from Figures 5.9 and 5.10 that the antiferromagnetic peaks in Mn-Cu alloys are comparable in integral intensity to the nuclear peaks, which makes it possible to analyze both crystallographic and magnetic textures with equal accuracy. Studies of magnetic textures, as well as their changes during plastic deformation in the presence of a magnetic field or near the temperatures of magnetic and structural phase transitions, can help in understanding the physics and improving the characteristics of Mn-Cu alloys and products made from them.

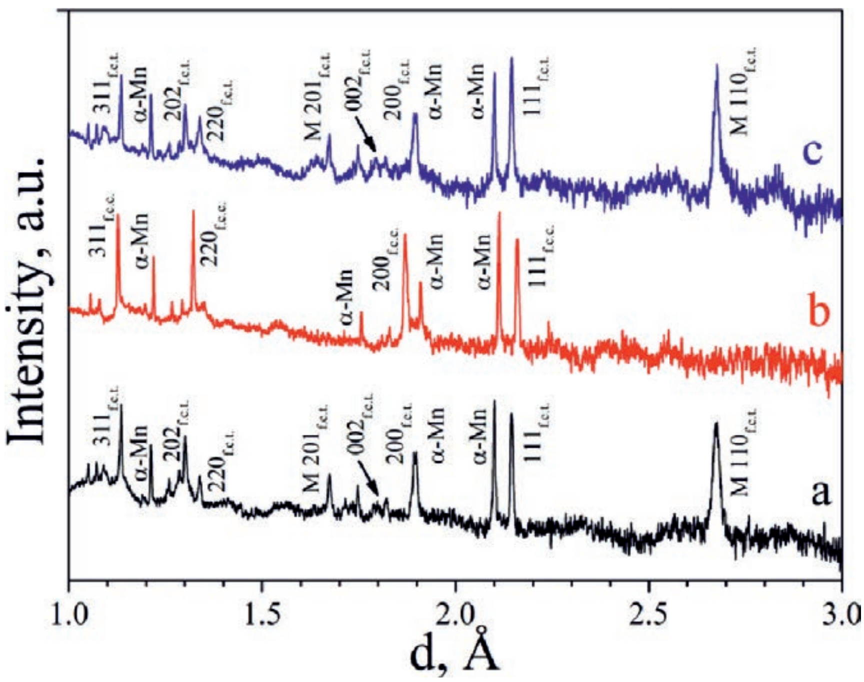


Fig. 5.11. High-resolution diffraction patterns of Mn-10Cu-4Cr alloy aged for 8 h at 440°C, measured at room temperature before heating (a), at 250°C (b), and at room temperature after cooling (c) [Sun et al., 2021b].

A relevant class of functional alloys with a shape memory effect, in the study of which neutron scattering methods (small-angle scattering, diffraction, reflectometry, tomography) play a significant role, are alloys with a magnetic shape memory effect [Río-López et al., 2021]. As a rule, these are Heusler alloys, among which the most interesting for industrial and medical applications is the Ni-Mn-Ga system, in which it is possible to achieve record-breaking characteristics, for example, significant (> 10%) magnetically induced deformations or high (> 300 °C) martensite transformation temperatures. Here, the most interesting and unique possibilities can be provided by energy-dispersive neutron imaging (Figure 5.12), which allows studying the morphology of twins in Ni-Mn-Ga-based Heusler alloys, which are formed as a result of the application of an external magnetic field, as well as the mosaic microstructure of the crystals of these alloys [Kabra et al., 2016].

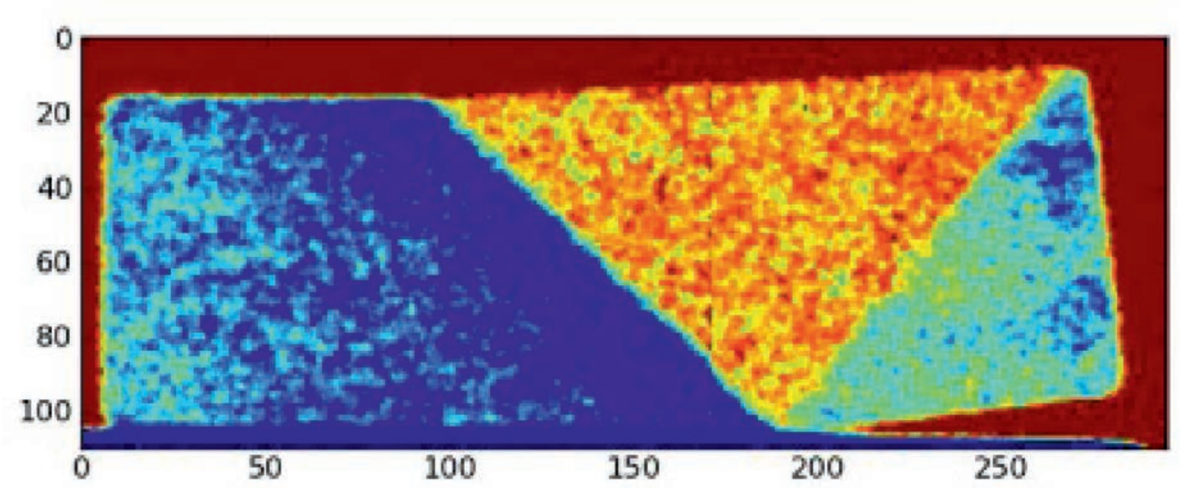


Fig. 5.12. Neutron image of a Ni_2MnGa single crystal demonstrating spontaneous twinning in a magnetic field [Kabra et al., 2016].

5.2.2. Self-healing materials

An interesting research area that has developed in the 21st century is the development and study of materials that can locally "heal" damage to their structure. These materials can be used to produce more reliable and durable structures. We already know self-healing polymers, concrete, ceramics and even electrode materials. Work on developing self-healing alloys is also of considerable interest and importance [Zhang et al., 2020a]. Examples of such alloys include the Fe-Au and Fe-Au-B-N systems. These alloys with 8% and 24% pre-strain were studied by *in situ* small-angle neutron scattering during isothermal aging at 550 °C [Zhang et al., 2013]. These experiments showed that Au atoms continuously precipitate from the alloy matrix during aging in the deformed samples (Figure 5.13). The addition of boron and nitrogen is found to retard the kinetics of Au precipitation. Au precipitates are formed exclusively at dislocations and along grain boundaries due to the high nucleation energy of Au in the Fe matrix. Due to the effective "healing" of defects by Au atoms, the creep time in the Fe-Au alloy is significantly higher than in the Fe-Cu alloy, which does not have this property (Figure 5.13).

Self-healing materials are of increasing interest in terms of developing new radiovoltaic devices. The output power of betavoltaic batteries using beta-emitting isotopes is low. Power cells using alpha-emitting isotopes can have an energy density six orders of magnitude higher than that achievable in electrochemical cells and function for hundreds of years, which ensures their use in the space industry, for powering equipment in remote and hard-to-reach regions. However, heavy alpha-particles seriously damage solid-state semiconductors, which leads to their rapid degradation. This limits the development of alphavoltaic devices. A solution could be to use a liquid self-healing semiconductor to convert the energy of emitted particles into electricity. In [Nullmeyer et al., 2018], using the total neutron scattering method, it was shown (Figure 5.14) that the atomic coordination in the liquid Se-S semiconductor remains practically unchanged up to the maximum radiation dose of 4×10^{11} Gy used in the experiment. It was concluded that liquid Se-S has the ability to self-heal radiation damage, and, as a result, its properties are virtually not subject to degradation even at high radiation doses.

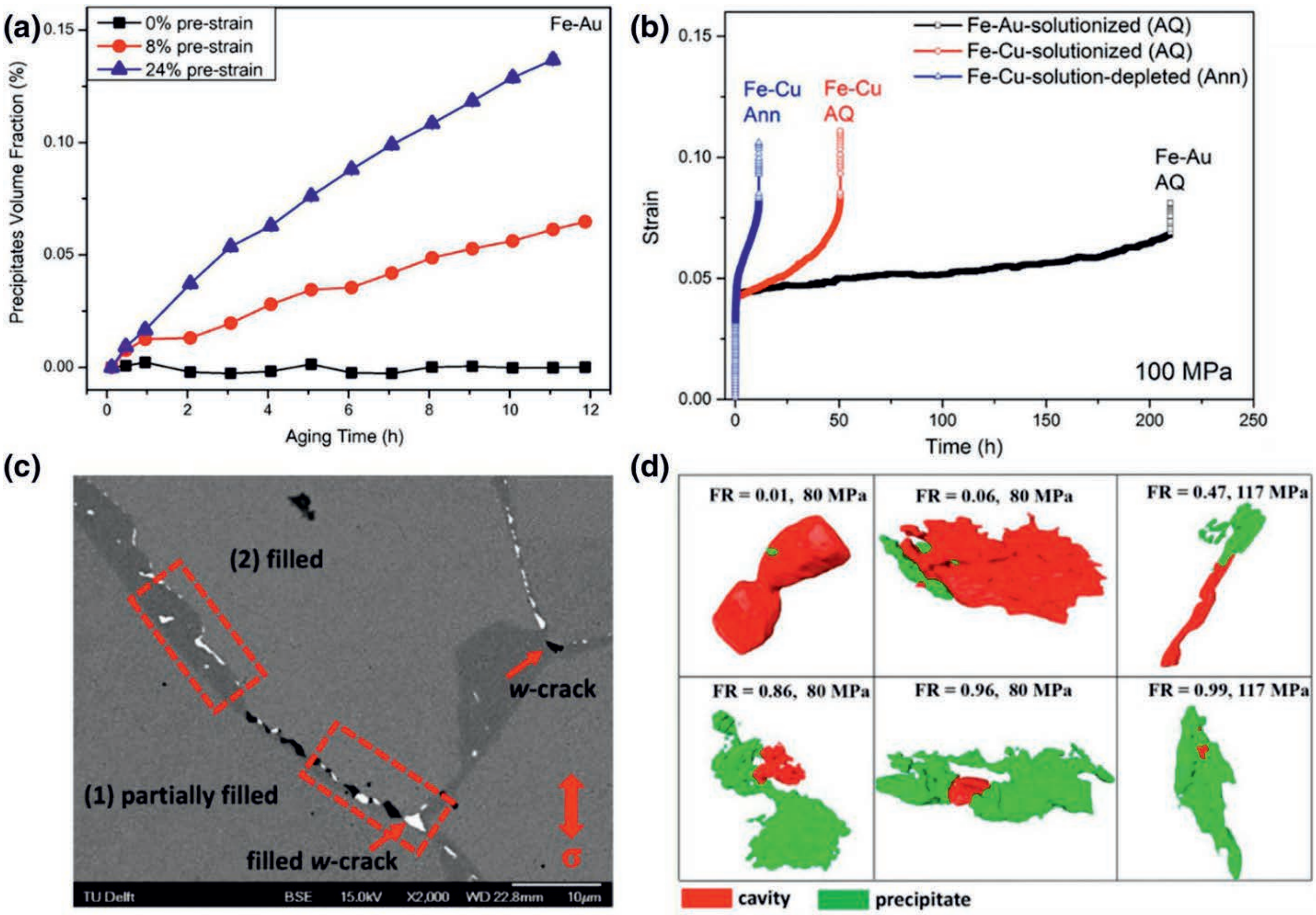


Fig. 5.13. Volume fraction of Au-rich precipitates in the Fe-Au alloy depending on the magnitude of preliminary deformation (a); comparison of the creep curves for the Fe-Cu and Fe-Al alloys (100 MPa) (b); micrograph of cavities and microcracks filled and partially filled with gold after creep (c); synchrotron microtomography of cavities with different filling ratios (FR) (d) [Zhang et al., 2020a].

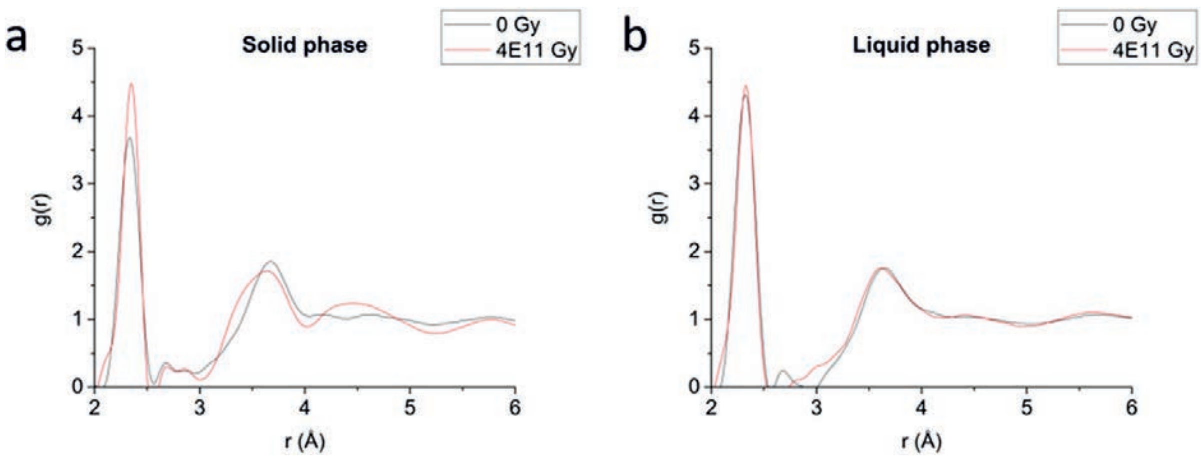


Fig. 5.14. Pair correlation functions of Se-S in the solid (a) and liquid (b) phases. In the solid phase, differences in the atomic coordination before and after irradiation are visible, while in the liquid phase they are minimal [Nullmeyer et al., 2018].

5.2.3. Metamaterials

Metamaterials are rationally designed composites composed of one or more constituent bulk materials and engineered to have properties, including those rarely observed in naturally occurring materials, which are derived not from the properties of the base materials but from their newly designed structures. Schematically, the principle of construction of metamaterials is shown in Fig. 5.15.

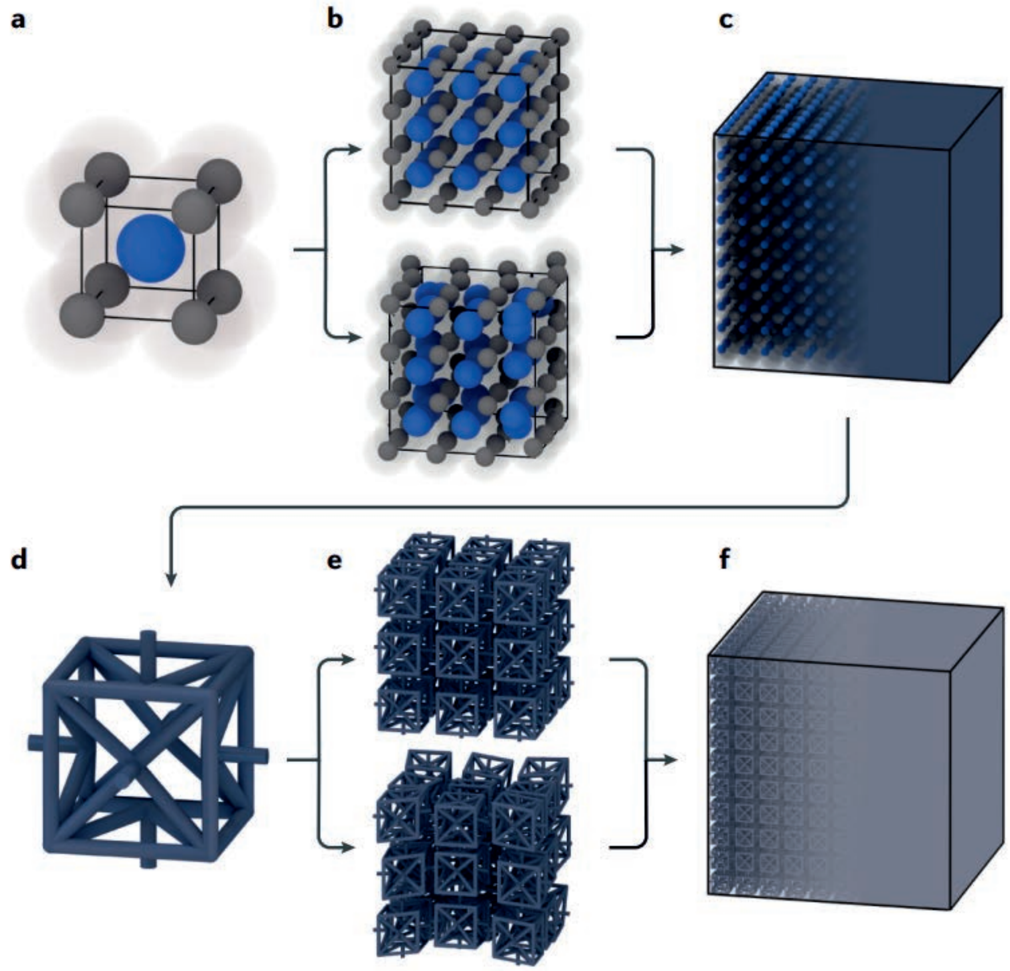


Fig. 5.15. From atoms via 3D materials to designed unit cells and 3D metamaterials. (a) and (b) Ordinary crystalline or amorphous materials are built up from atoms. (c) To compress the underlying complexity, materials are often treated as fictitious continuous media with associated effective parameters such as the electric conductivity, the optical refractive index, or the mechanical Young's modulus. (d) These effective media are used as the elements for rationally designed artificial unit cells. (e) Out of these, periodic or non-periodic 3D metamaterials are assembled. (f) Again, to compress complexity, metamaterials are mapped onto fictitious continuous media. Notably, the resulting effective metamaterial properties can go beyond those of the element materials, qualitatively and/or quantitatively. The example unit cell shown in (d) leads to auxetic behavior [Kadic et al., 2019].

Modern technologies already make it possible to produce three-dimensional metamaterials with various properties, including auxetic behavior (negative bulk moduli), negative mass density, near-zero shear modulus, mechanical chirality, exotic electromagnetic and optical properties, etc. [Kadic et al., 2019]. The potential applications of metamaterials are also wide and include “self-aware” filters, sensors and actuators that operate in the absence of conventional power sources and electronic components [Barry et al., 2021], lenses, radio-transparent surfaces, invisibility cloaks, earthquake-resistant structures, etc.

At present, there are only a few examples of studies of metamaterials using neutron scattering methods. However, diffraction, small-angle neutron scattering, reflectometry, tomography, and other methods can successfully be used to characterize the structure and microstructure of metamaterials at various “levels” of their structure, which are illustrated in Figure 5.15 (a–d).

5.3. ADDITIVE TECHNOLOGIES

Additive manufacturing technologies have gained immense popularity in the last decade. The advantages of this approach are the possibility of manufacturing parts and components of complex geometry, as well as the minimization of production waste. There are already examples of complex products manufactured entirely using additive manufacturing technologies, such as a fully functioning rocket engine with cooling channels 3D printed inside the rocket body [Nickels, 2018]. Modern additive technologies, such as selective laser melting, selective laser sintering, etc., make it possible to produce parts and components from several metals, such as stainless steel, titanium and aluminum alloys, etc. [Hasanov et al., 2021]. There are a number of difficulties and problems associated with the further development of additive technologies, such as the specific microstructure and shape of the grains of the material being manufactured, the possible presence of significant residual stresses, defects and pores in the material, and often low fatigue strength. Neutron scattering methods are also used to solve these problems.

In [Sofras et al., 2022], the deformation behavior of bulk samples produced by laser-powder bed fusion (L-PBF) from 304L stainless steel powder under an argon atmosphere were studied using *in situ* neutron diffraction and *ex situ* electron backscatter diffraction (EBSD). It was shown that the L-PBF process parameters make it possible to control the crystallographic texture of the samples, which largely determines the behavior of the material under plastic deformation. At a strain rate of 0.01 s^{-1} in the plastic regime, the sample with a predominant <111> crystallographic texture along the loading direction displays the highest fraction of α'-martensite, which also increased with increasing deformation faster than in other samples. Based on theoretical calculations, the best deformation properties in terms of phase transformation-induced plasticity were expected for specimens with the <110> crystallographic orientation parallel to the loading direction, but experimental data have shown that the <111> crystallographic texture along the loading direction is the most favorable for facilitating the effects of phase transformation-induced plasticity under tension. It is noteworthy that the preferred grain orientations determined using neutron diffraction and electron backscatter diffraction in some samples are completely different (Fig. 5.16), which indicates the need to use methods sensitive to the volume of the material (in this case, neutron diffraction) to study the characteristics of products manufactured by additive methods.

At present, additive technologies are one of the most dynamically developing areas of digital manufacturing. The principle is that the product is made layer by layer, by adding material in various ways, for example, by fusing or depositing metal powder, composite or other material. The development of additive technologies requires the use of modern control methods, such as neutron tomography (Podurets, K.M. et al., (2021)). The transition from the use of additive technologies for prototyping and manufacturing individual parts or units of devices to their industrial application in mass production will require a huge amount of research, including for further optimization of serial production. The unique possibilities offered by neutron scattering methods are already highly popular in this area of materials science and there is no doubt that the demand for the use of neutron scattering will only increase in the coming decades. **One of the new potential opportunities at the advanced neutron source at FLNP JINR will be to conduct *in situ* neutron diffraction studies directly during the manufacturing of parts and components at relatively low manufacturing speeds.**

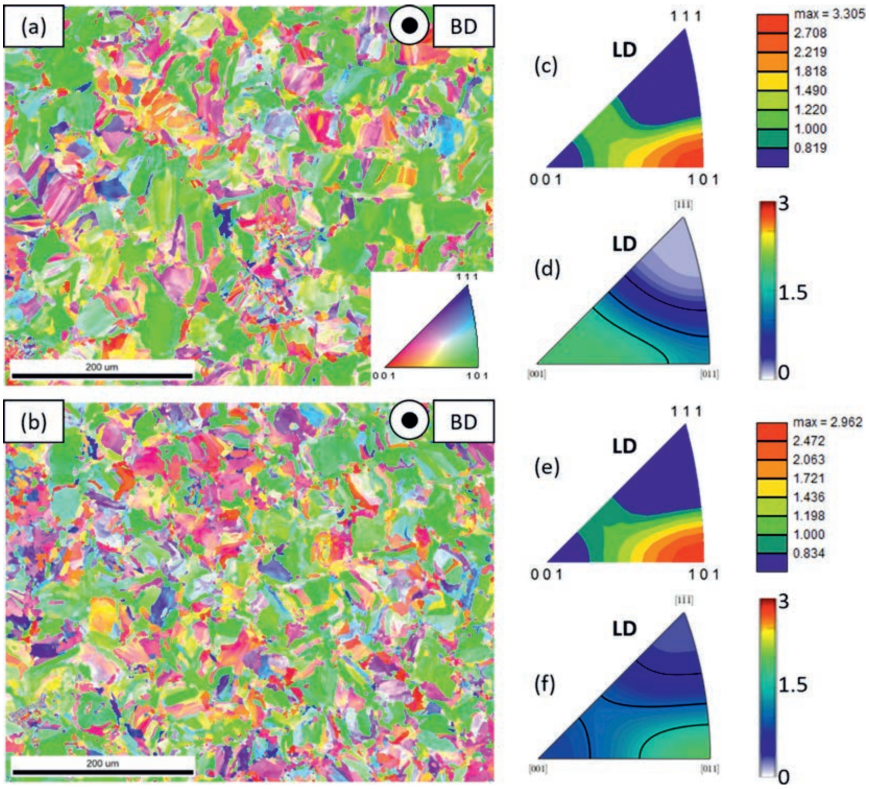


Fig. 5.16. Orientation maps with inverse pole figure (IPF) coloring of the as-fabricated samples in the direction parallel to the loading direction (LD), (a) sample C1, (b) sample C2. The building direction (BD) is indicated for each sample. (c) and (e) are IPFs along the LD obtained from EBSD analysis for samples C1 and C2, respectively. (d) and (f) are IPFs along the LD obtained from the neutron diffraction data and corresponding Rietveld analysis for samples C1 and C2, respectively. Sample C1 was manufactured at a laser power of 150 W and a scanning speed of 450 mm/s; sample C2 — 100 W and 300 mm/s. [Sofras et al., 2022].

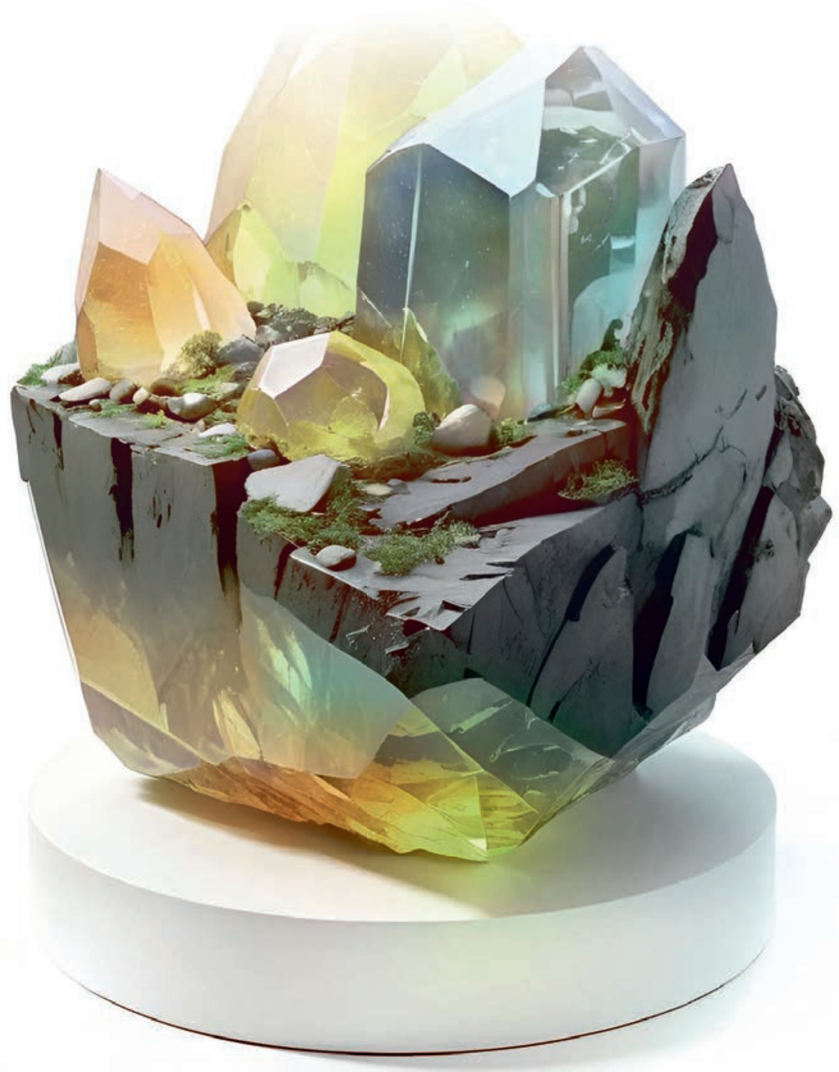
5.4. NEUTRON METHODS FOR STUDYING STRUCTURAL MATERIALS

Neutron scattering methods will make it possible to study new materials, for example, self-healing materials, high-entropy alloys, products produced using additive technologies, metamaterials, and will undoubtedly remain relevant for studying “traditional” materials: steels, alloys, ceramics that have undergone various thermomechanical treatments.

The presented data show that almost all neutron scattering techniques, including, for example, diffraction, small-angle scattering, inelastic scattering, spin-echo, energy-dispersive radiography and tomography, etc., are used to study all kinds of structural, functional, “smart”, meta-, bio- and nanomaterials and finished products, and an increase in the neutron flux at the instruments will provide additional opportunities for improving the accuracy of measurements, expanding scientific areas and attracting new users.

There is an ever-increasing number of tasks requiring measurements of large series of samples, *in situ* measurements, including those with good time resolution (for example, *in situ* tomography), reduction of the measured volume for "local" measurements in bulk samples, precision studies of microstructure, including materials that weakly scatter neutrons. **To solve these problems, it is necessary to increase the luminosity of scientific instruments. This can be realized by developing and constructing the advanced pulsed neutron source at FLNP JINR with optimization of all parameters of the source and beamline instruments.**

Earth sciences



In general, the objects of study of Earth sciences are the composition, structure and dynamics of the Earth, planets, meteorites. Rocks can be considered as specific materials that were formed under a rather limited set of conditions, which, however, are not always precisely known, but can be determined experimentally.

As in materials science, various neutron scattering methods are widely used in geophysical research, which often provide unique information about the structure of geomaterials.

6.1. ATOMIC STRUCTURE OF MINERALS

Thermal neutron diffraction makes it possible to determine the positions of hydrogen atoms in the structure of various minerals, such as fluorine-poor blue topaz $Al_2SiO_4(F,OH)_2$ from Padre Paraíso, Brazil [Precisvalle et al., 2021] or probertite $CaNa[B_5O_7(OH)_4]{\cdot}3H_2O$ from California, USA [Gatta et al., 2022].

The structure of blue topaz (space group *Pbnm*) consists of tetrahedral groups $(SiO_4)^{4-}$ linking octahedral chains of $Al[O_4(F,OH)_2]$. The tilted tetrahedral and octahedral chains are additionally linked by hydrogen bonds. Changes in the F/OH ratio, as well as potential ordering of fluorine and OH groups, can lead to changes in the symmetry of the topaz structure. The F/OH ratio is important not only for the formation of this particular crystal structure, but also to better understand the circulation of fluids (H_2O/F) in the rocks surrounding the mineral.

Probertite is an excellent mineral commodity of boron (with its ~50 wt% B_2O_3). It is considered a promising candidate as a B-rich aggregate in concretes used as radiation-shielding materials, however, the solubility of probertite in cement pastes as well as its effect on the properties of the resulting material are still unknown. The hydrogen-bonding network in probertite is very complex, with 11 over 14 oxygen sites involved in H-bonds as donor or acceptors (Figure 6.1). So, destabilization of the H-bonding scheme, for example in response to the applied temperature or pressure, can lead to a phase transition or even decomposition of the structure.

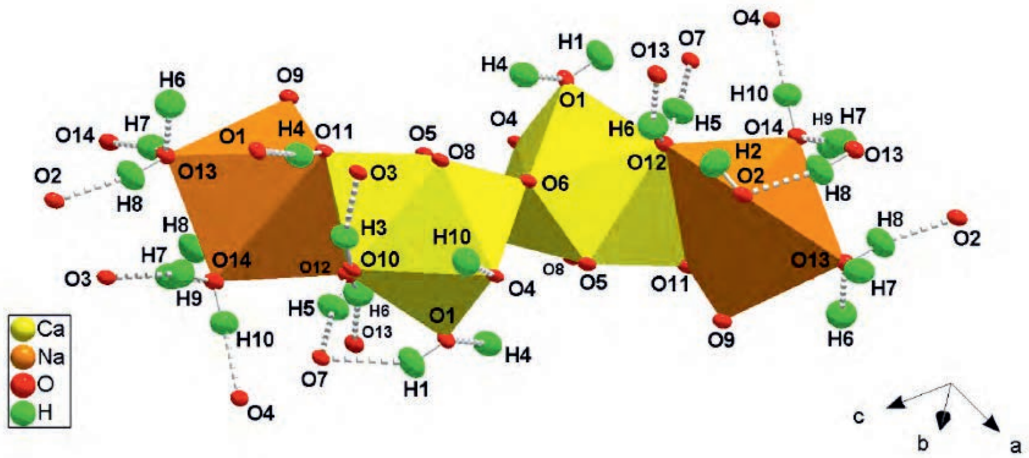


Fig. 6.1. Hydrogen-bonding network in the crystal structure of probertite (from neutron diffraction data collected at a temperature of 20 K). Displacement ellipsoid probability factor: 70%. [Gatta et al., 2022].

Neutron diffraction structural analysis is also applied, for example, to study trapped hydrogen in mantle rocks. The presence of hydroxyl groups in the structure of minerals can significantly change their melting behavior, phase relationships, transformation kinetics, rheology, and seismic wave velocities. Of great importance for the development of hydrogen energy are studies of natural sources of H_2 (e.g., processes of hydrothermal alteration of ultramafic rocks, radiolysis of water due to the radioactive decay of U, Th, K, the activity of certain anaerobic bacteria, the decomposition of methane in the upper mantle, oxidation of Fe(II)-bearing minerals in the presence of water, etc.), as well as processes of trapping of the formed H_2 in the lithosphere (absorption by microporous rocks, various reduction reactions, etc.) [Truche & Bazarkina, 2019].

It is quite obvious that neutron diffraction studies of the structure of minerals are of importance both for a better understanding of geodynamic processes and for the rational use of mineral raw materials.

6.2. MAGNETIC STRUCTURE OF MINERALS

Goethite is one of the most common minerals in nature and finds its use as a component of ferrofluids, as well as in the production of yellow pigment. Detailed neutron diffraction studies of goethite in [Zepeda-Alarcon et al., 2014] confirmed that the magnetic moments of iron are collinear and form two antiferromagnetically coupled sublattices located parallel to the *c* axis in the *Pb'nm* space group. The presence of the magnetic diffraction 100 peak and the absence of the 010 peak refute the model with magnetic moments of iron tilted relative to the *c* axis (Figure 6.2).

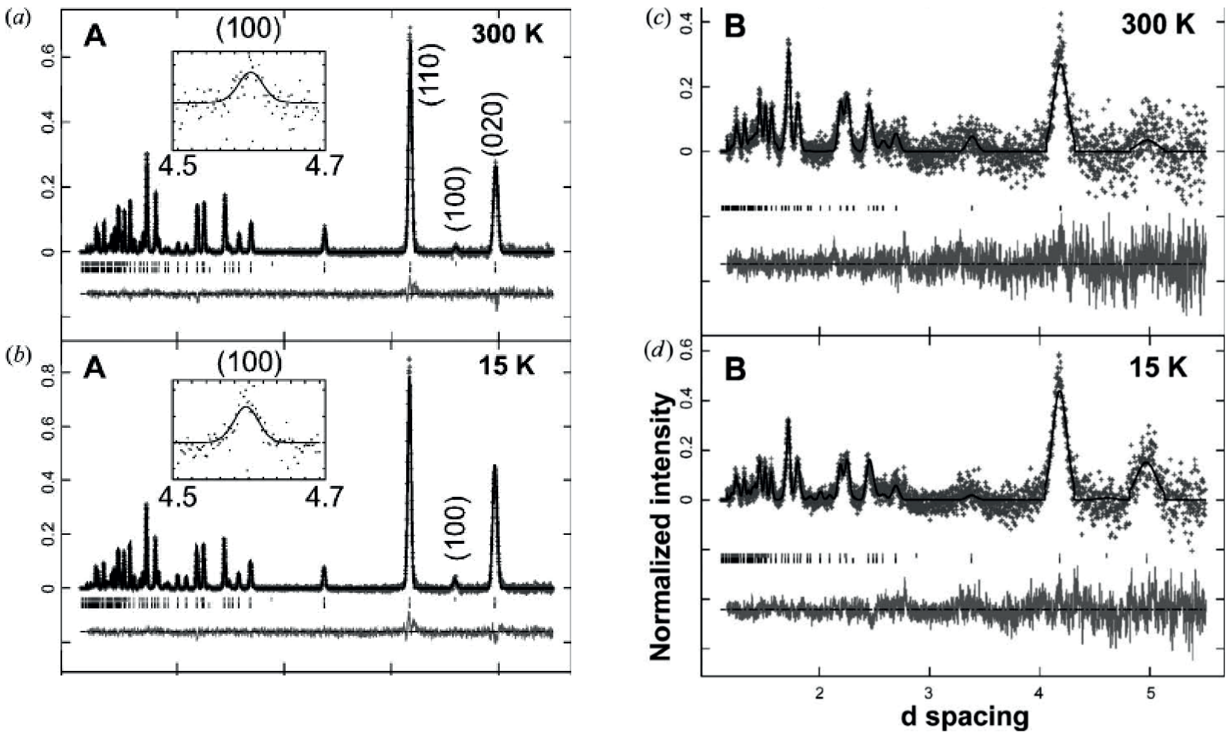


Fig. 6.2. Neutron diffraction patterns of goethite samples with grain sizes of ≈100 nm (a, b) and ≈12 nm (c, d) at 300 K (a, c) and 15 K (b, d). The peak (100) is magnetic. [Zepeda-Alarcon et al., 2014]

In nanocrystalline (grain size ≈ 12 nm) goethite, a significant decrease in the Néel temperature was found compared to well-crystallized (grain size ≈ 100 nm) goethite. Systematic neutron diffraction studies are needed to establish the relationship between the Néel temperature, water content and the size and shape of goethite crystallites. Such information is important not only for the use of this mineral in production, but also, for example, in paleomagnetic studies for the reconstruction of paleoclimate, since on the one hand, magnetic susceptibility during soil formation depends on the amount of precipitation, and on the other hand, the magnetic susceptibility of antiferromagnets rises with increasing temperature to the Néel point, and then lowers according to the Curie-Weiss law, and it is important to take into account the structural and microstructural dependence of the magnetic transition temperature.

6.3. CRYSTALLOGRAPHIC TEXTURES AND ANISOTROPY OF PHYSICAL PROPERTIES OF ROCKS

For many medium- and coarse-grained rocks (granite, granodiorite, sylvinite, etc.), neutron diffraction texture analysis is practically the only method for quantitative analysis of the preferred orientations (crystallographic textures) of minerals, since only measuring samples of ~10-100 cm^3 in size allows us to obtain sufficient grain statistics. Measurements of crystallographic textures in large series of samples collected in a particular region of the Earth make it possible to study local deformations and metamorphic processes in the lithosphere.

In [Keppler et al., 2021], crystallographic preferred orientations (CPOs) of minerals in 30 samples of gneiss and two metabasites from the Adula nappe of the Central Alps were investigated. The CPOs of quartz in the gneisses differ significantly from those obtained for the Alpine quartzites. For example, the poles to (0001) either form a maximum between the foliation normal and the lineation direction (lying in the foliation plane), or form a wide belt with a peripheral maximum at an angle to the foliation normal. However, all samples show an asymmetry in the preferred orientations of quartz, indicating a top-to-the-north sense of shear.

To elucidate the deformation mode of quartz in detail, further studies are needed on large collections of samples, using both neutron diffraction and electron backscatter diffraction and mathematical modeling. In addition to describing the deformation history of the studied rocks, the data from neutron diffraction texture analysis were used to calculate the effective elastic properties of the rock bulk and their changes depending on depth as a result of the closure of pores and microcracks present in the rocks with increasing depth. The results of modeling are compared with the data from the elastic wave velocity measurements carried out at different pressures, thus making it possible to assess the closure of cracks and pores with pressure changes. The advantage of such studies is that complementary research methods, including ultrasonic measurements, neutron diffraction, and neutron tomography are used for the same macroscopic sample with linear dimensions of several centimeters. In gneiss from the Tambo nappe of the Central Alps, the experimental elastic wave velocities measured at a pressure of 100 MPa (Figure 6.3) were found to be consistent with the model of elastic properties with 0.1 vol.% of primary cracks, i.e. cracks parallel to mica platelets, and 0.6 vol.% of secondary cracks, which intersect the muscovite grains and indicate that the rock was subjected to extensional strain parallel to the foliation plane.

It should be noted that modeling of texture formation processes in rocks consisting of several low-symmetry minerals with anisotropic properties and non-trivial microstructure is very difficult both using the mean-field approximation and using the finite element method. However, neutron diffraction studies of large collections of rock samples can be used to create extended ODF databases for minerals, including also the mineral composition of rocks, grain sizes and shapes, thermodynamic conditions, strain rates, directions of the principal axes of the mechanical stress tensor, etc. These databases can then be used to train neural networks (AI), which can be used to quickly type ODFs and determine the most likely conditions for their formation. In its turn, it will be possible to use these data to model the anisotropic elastic properties of the lithosphere and their evolution over time. **A significant increase in the neutron flux for the beamlines of the new source**

of FLNP JINR will greatly shorten the measurement time for crystallographic textures of geological samples, which at present can take up to several days.

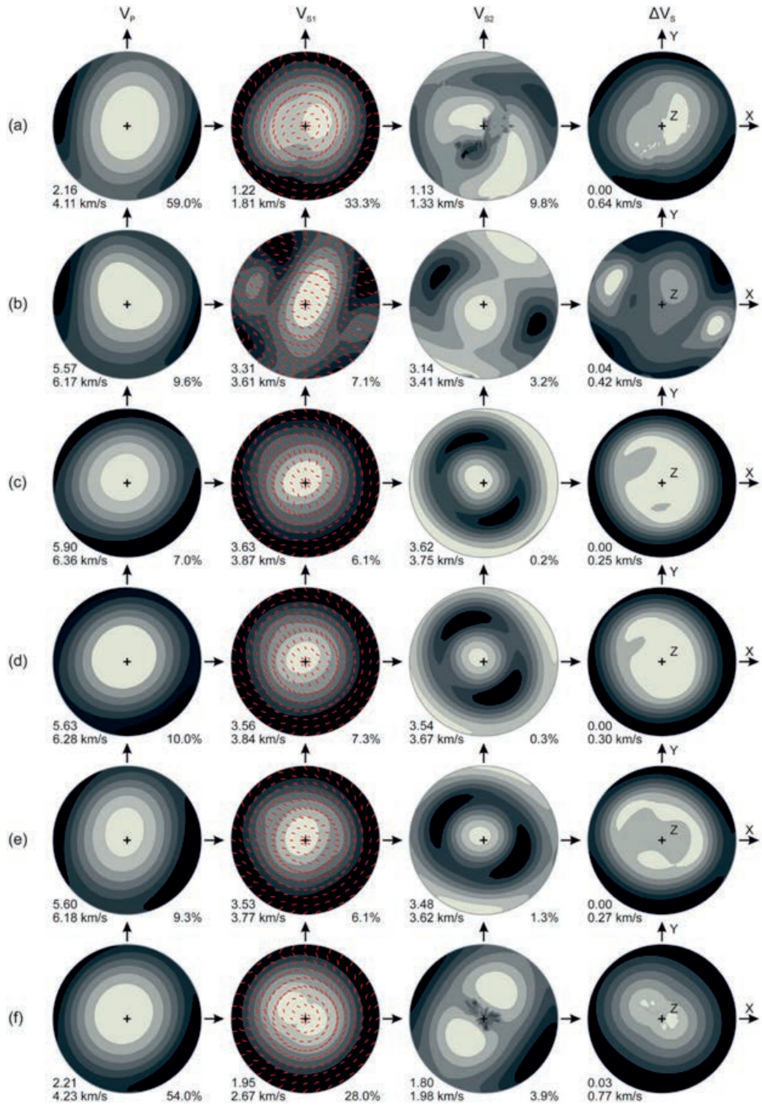


Fig. 6.3. Distributions of *P*- and *S*-wave group velocities (V_P, V_{S1}, V_{S2}) as well as shear wave splitting ΔV_S in gneiss: experimental measurements at 0.1 MPa (a); 100 MPa (b); different Tambo gneiss models ((c) — without pores and cracks; (d) — with 0.1 vol.% of primary cracks; (e) — with 0.1 vol.% of primary cracks and 0.6 vol.% of secondary cracks; (f) — with 2.6 vol.% of primary cracks and 1.0 vol.% of secondary cracks). Fast S-wave polarization projections for different wave propagation directions are shown as red dashes on corresponding projections. Z-axis is normal to foliation, X-axis is parallel to lineation. Equal-area projections, linear scale [Vasin et al., 2017].

6.4. MICROSTRUCTURE AND PERMEABILITY OF ROCKS

The movement of water and other fluids in fractures within rocks is important in a variety of contexts, including hazardous waste storage, enhanced oil recovery, shale gas extraction, geothermal energy, and seismic zone modeling. In [Cheng et al., 2015], it was shown that *in situ* neutron radiography can be used to study fluid movement in rock fractures. Spontaneous imbibition of water in fractured Berea sandstone cores was investigated (Figure 6.4). It was found that the rate of water uptake in the fracture damage zones is very rapid, with wetting fronts travelling between 2 and 3 cm per second. This rapid water uptake is due to a combination of capillary rise of water within the fracture and its spreading over the rough surface of the fracture. The rise of water along the rough surface is faster than along the smooth surface. In general, neutron radiography and tomography methods can be used not only for the analysis of the internal structure of rocks. **For example, energy-dispersive neutron imaging can be used to assess residual mechanical stresses in different parts of a sample. Conducting such studies *in situ* requires a pulsed neutron source with high-flux beamlines.**

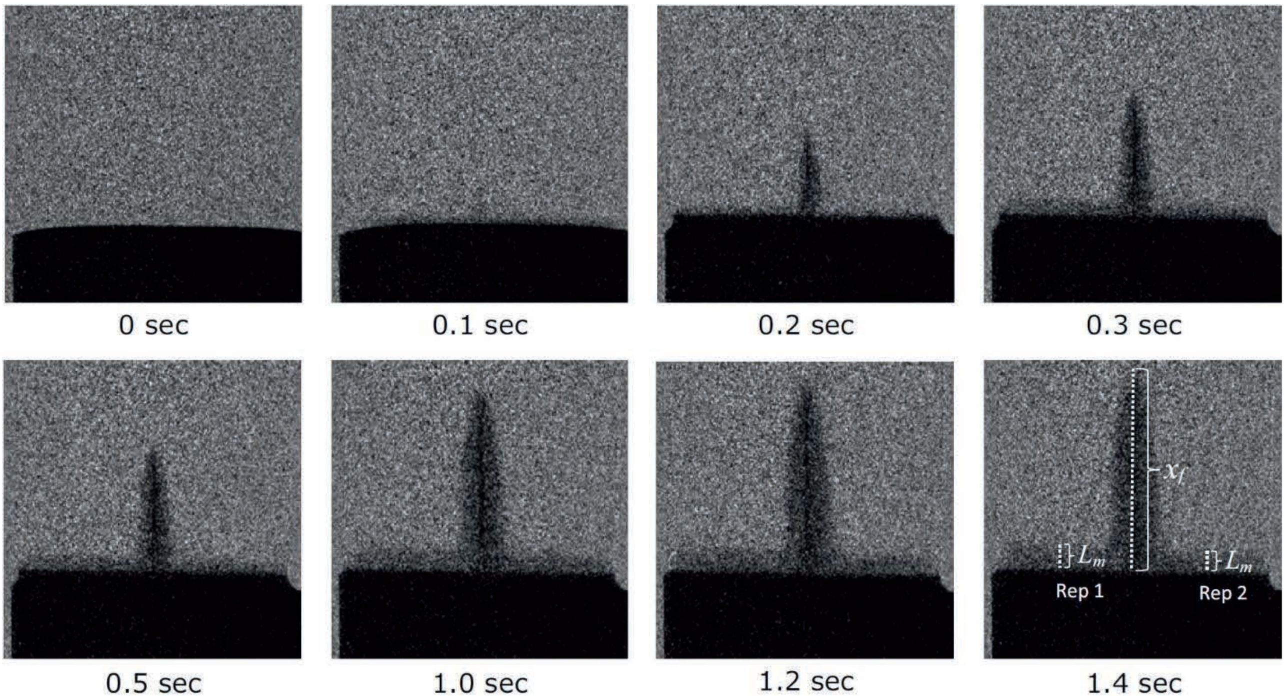


Fig. 6.4. Uptake of water into a longitudinal, air-filled fracture zone in Berea sandstone (permeability class ~ 50 mD). The images have been normalized with respect to the initial dry image, so that only water (black) is visible. Annotations on the 1.4-sec image indicate where the distances traveled by the wetting front in the matrix, L_m (2 replicate locations) and in the fracture zone, x_f, were measured. For scale, the width of each image is 26 mm. [Cheng et al., 2015].

Small-angle neutron scattering is also used to obtain valuable information on the internal structure of rocks. In recent years, there has been an increasing number of studies on the structure of pores and fractures in shales to improve processes of shale gas extraction. In [Zhan et al., 2022], shale samples from the Southern Sichuan Basin were studied. Their burial depths are more than 4000 m. The Sichuan Basin is one of the main gas producing regions in China. Tectonic evolution processes have led to the formation of various pores in the rocks in this region. Using small-angle neutron scattering (Figure 6.5) and the low-pressure nitrogen adsorption method, the fractal structure of pores in shale was analyzed, and a correlation was established between the fractal dimension and mineral composition, organic content, porosity, and permeability. For example, the permeability and the surface fractal dimension have a negative correlation: the higher the dimension, the more complex the surface of cracks and pores and the higher the resistance to gas flow.

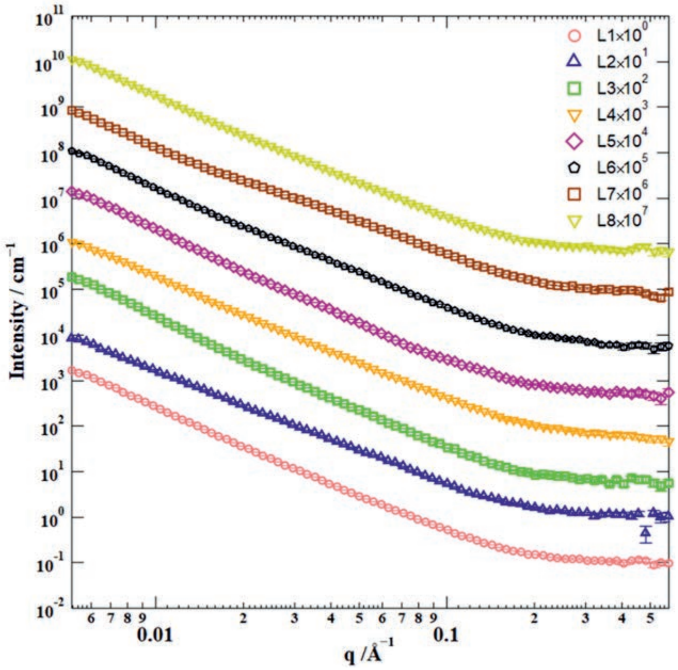


Fig. 6.5. Small-angle neutron scattering curves for deep shale samples from the Sichuan Basin [Zhan et al., 2022].

6.5. PROCESSES OF DEFORMATION AND FAILURE OF ROCKS

An interesting opportunity to investigate rock failure mechanisms is provided by the combined application of neutron diffraction, which allows studying the deformation behavior of the crystal structure of minerals, and acoustic emission for tracking the processes of formation and development of cracks [Nikitin & Vasin, 2010; Abe et al., 2014]. Such studies can also be carried out in the presence of a fluid, for example by pumping heavy water through a large permeable sample [Gudehus et al., 2023]. These experiments are of great interest for a better understanding of rock mechanics, rock bursts and earthquake physics.

In [Nikitin & Vasin, 2010], it was shown that quartzite, subjected to a slight uniaxial compression of 27 MPa, when heated above the temperature of the α–β transition in quartz, accumulates elastic strains of ~ 10^{-3}, which are comparable in magnitude to the hypothetical value for superplastic strain, theoretically calculated for this phase transformation (Figure 6.6). Such deformations can lead to local cracking of the rock due to the lowered ultimate strength in the temperature region of the phase transition. At temperatures above the phase transformation in quartzite, intense splashes of acoustic emission were observed, which corresponds to the occurrence of elastic vibrations in the rock. If such a process occurs in a potential earthquake focus, it can cause macroinstability of the earthquake source for at least three hypothetical reasons. First, the structure of the stress state changes and areas of increased stress appear. Second, the strength properties of the medium change and areas of lowered strength arise. Finally, the resulting vibration can serve as a trigger effect.

Conducting such experiments, which are valuable for the development of the physics of earthquake origin, is complicated by the fact that, as a rule, the collection of neutron diffraction data requires significantly more time than the generation and recording of acoustic emission events. **An increase in the luminosity of the instruments at the future advanced neutron source will make it possible to significantly reduce the time of diffraction experiments and conduct the above studies with better time resolution.**

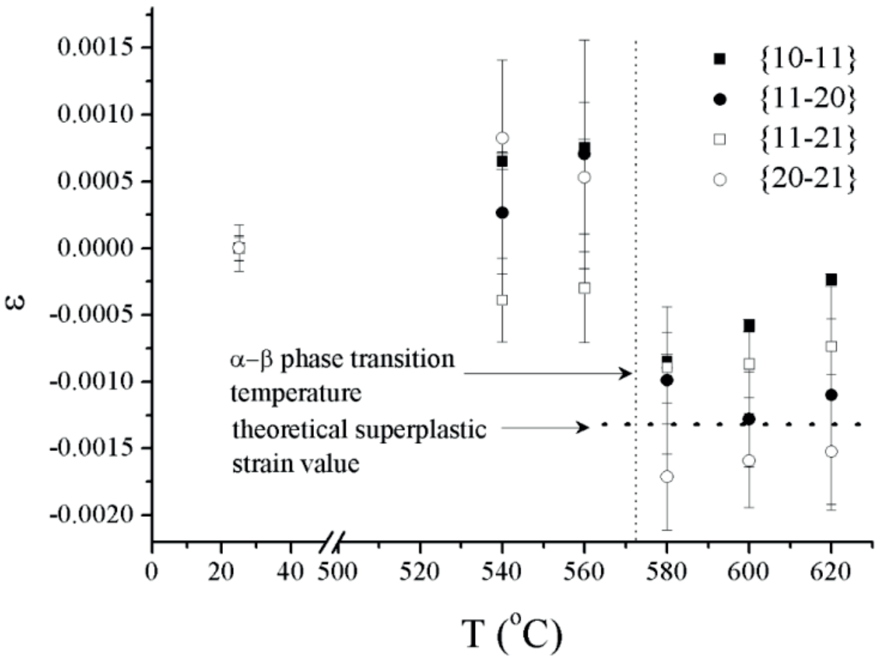


Fig. 6.6. Changes in relative elastic strains in the directions normal to different crystallographic planes of a sample of Shokshinskii quartzite experiencing a uniaxial compression of 27 MPa during its heating and the α→β phase transition in quartz (at 573°C). The dotted horizontal line shows the hypothetical superplastic strain value during this phase transition. [Nikitin & Vasin, 2010].

6.6. SPATIAL DISTRIBUTION OF MINERALS IN METEORITES

Since the last century, a fairly large number of theoretical models have been developed to describe the formation of different types of meteorites on the basis of experimental data on cooling rates of various constituent minerals of meteorites, petrologic data, chemical composition of major and minor phases, or their textural associations in meteorites. For example, for iron-stone meteorites (pallasites), a model has been developed that assumes primarily fractional melting of the asteroid upon collision through the mixing of previously separated metal core and olivine mantle. Studies of meteorite components and their dimensions, shapes, textures and spacing arrangement using neutron imaging and complementary methods can provide a better understanding of the petrography of meteorites.

As an example, let us consider pallasites, which are stony-iron meteorites consisting of olivine grains and FeNi metal alloy. The minor phases are troilite (FeS), schreibersite, pyroxene, and phosphates. A neutron tomography reconstruction of the internal structure of the Seymchan meteorite [Kichanov et al., 2018a] is presented in one of the neutron radiographic images of the studied pallasite (Figure 6.7). It should be noted that the neutron attenuation coefficients for a neutron beam with an average wavelength of ~2 Å of iron (Σ_{Fe} = 0.151 cm^{-1}) and nickel (Σ_{Ni} = 0.468 cm^{-1}) are larger than the corresponding parameters for olivine components. Therefore, in neutron radiography experiments, a complex network of metal veins contrasts well with olivine grains. Figure 6.7 (b-d) shows several images corresponding to different transverse slices of the studied meteorite. Here, the dark areas correspond to rounded olivine grains. It can be seen that olivine grains occupy most of the volume of the fragment under study, and large clusters of olivine are formed within its volume.

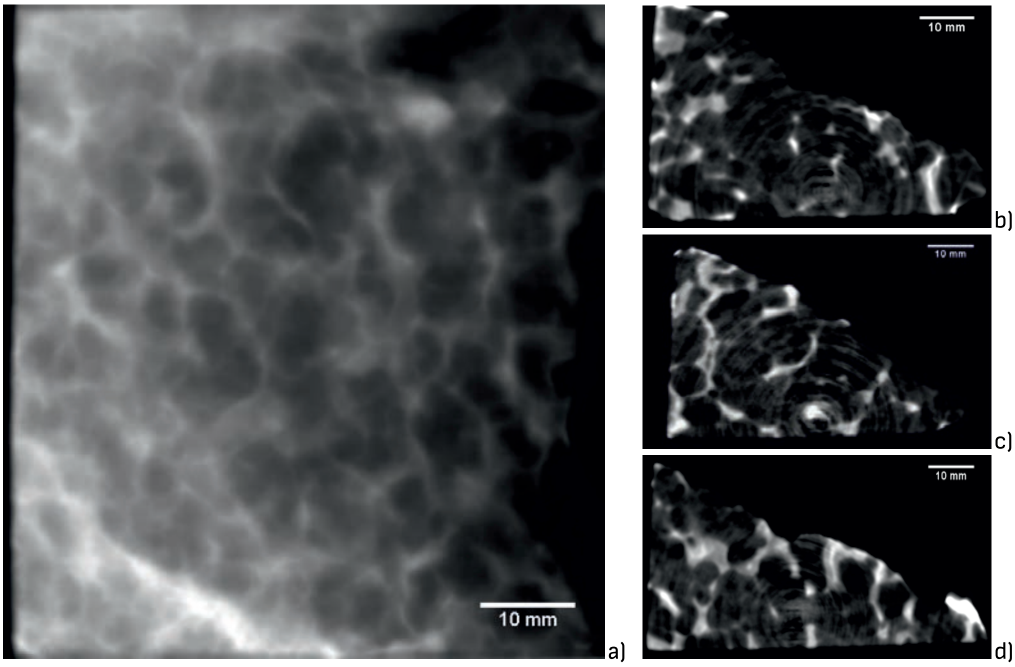


Fig. 6.7. a) Neutron radiography image of the fragment of the Seymchan meteorite. Bright regions correspond to high neutron attenuation in the metal component. Dark areas are low neutron attenuation regions of olivine grains. (b–d) Examples of virtual tomography slices of the pallasite under study, which illustrate the arrangement of metal and olivine components inside the meteorite body. The slices correspond to the bottom (b), middle (c), and upper (d) parts of the studied meteorite fragment.

As a result of the analysis of the obtained images, the volume fraction of olivine in the studied fragment of the Seymchan meteorite was estimated to be 60.4%. This result agrees well with the previously obtained data for other pallasites.

The reconstructed 3D model of the meteorite sample is presented in Figure 6.8.

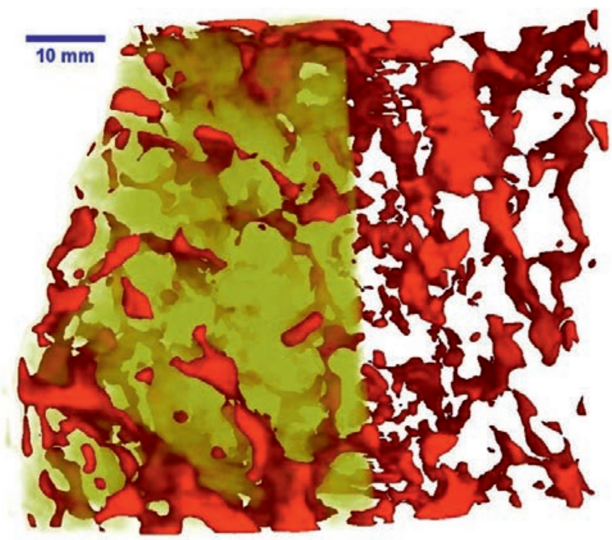


Fig. 6.8. Virtual 3D model of the studied fragment of the Seymchan meteorite after tomographic reconstruction. The metal regions are labeled in red, and the olivine component is yellow. The olivine fraction of the left part of the meteorite is made transparent for convenience.

6.7. NEUTRON METHODS IN GEOPHYSICAL RESEARCH

Neutron scattering has a wide range of applications in geophysical research, for which the main neutron scattering methods are diffraction, radiography/tomography, and small-angle scattering. From this point of view, of particular interest are the tasks of studying the anisotropic elastic properties of the lithosphere and their evolution over time, studying the properties of rocks in complex reservoirs in order to extract hard-to-recover hydrocarbon reserves, as well as experiments that contribute to the development of the physics of earthquake source.

As with solving problems in other fields of knowledge, in geophysical applications of neutron scattering there is a growing need for measurements of large collections of samples, conducting *in situ* studies under extreme conditions, including simultaneous measurements of some physical properties of the sample, and enhancing the accuracy of measurements. These requests will be possible to fulfill at the new pulsed neutron source at FLNP JINR.

Investigation of cultural heritage and paleontology

Using the neutron radiography method, due to different degrees of attenuation of the intensity of the neutron beam when passing through materials of different chemical composition, density and thickness of the components of the object being studied, it is possible to obtain information about the internal structure of the materials under study with spatial resolution at the micron level. This method of non-destructive testing is characterized by deeper penetration into the thickness of the material being examined compared to the complementary method of X-ray radiography and has advantages in the study of materials that simultaneously contain both light elements (for example, hydrogen or lithium) and heavy elements (for example, iron). Radiography provides a two-dimensional projection of the object. To obtain a three-dimensional image, the tomography method is applied, where a 3D reconstruction of the internal structure of the object under study is performed from a set of radiographic projections obtained at different angular positions of the sample relative to the direction of the neutron beam [Podurets et al., 2021].

7.1.RESEARCH OF OBJECTS OF CULTURAL HERITAGE

Investigations of cultural heritage objects using natural science methods are important for expanding and deepening knowledge about the historical and archaeological prerequisites for the appearance of these objects. These studies make it possible to determine the place where artifacts were created, the routes of their distribution, establish their age, manufacturing technology, original appearance and subsequent changes. This allows us to obtain new data on culture, science, crafts, technologies, trade relations, and the history of entire countries and peoples. It should be noted that a feature of cultural heritage objects is that they can often combine materials with different physical and chemical properties: metals, substances of mineral and organic origin [Lehmann & Mannes, 2021; Kozlenko et al., 2019], so the use of complementary methods for their study is very important [Kozlenko et al., 2016]. In particular, neutron imaging data can be supplemented by X-ray imaging, as well as studies of elemental, phase and texture analysis of materials [Sedyshev et al. 2020; Gorini et al., 2007; Luzin et al., 2020].

As noted earlier, neutron scattering methods are non-destructive, therefore they are actively used in archaeological and paleontological research, in the study of objects of cultural heritage. For example, data on the effect of high temperatures on the vibrational and rotational modes of motion of various groups of atoms in human bones can be used to analyze the funerary rituals of ancient people [Marques et al., 2021]. Neutron diffraction studies have shown changes in the preferred orientation of hydroxyapatite crystals in human tibia during evolution, the dependence of the crystallographic texture of the bone on the living conditions of ancient people, and significant anisotropy of the preferred orientations in modern humans [Bacon, 1990].

Neutron diffraction texture analysis is also used to determine the deformation history of materials. With its help, it became possible, for example, to obtain information about the conditions and temperatures of minting ancient Judaean “biblical” bronze coins from the first century BCE and CE [Nagler et al., 2019]. Information on structural phases obtained from the entire volume of the coin using neutron diffraction makes it possible to identify hidden traces of corrosion, for example, the presence of copper monochloride (nantokite) in the material, and to take measures to stop the "bronze disease" and prevent the complete destruction of the affected artifact.

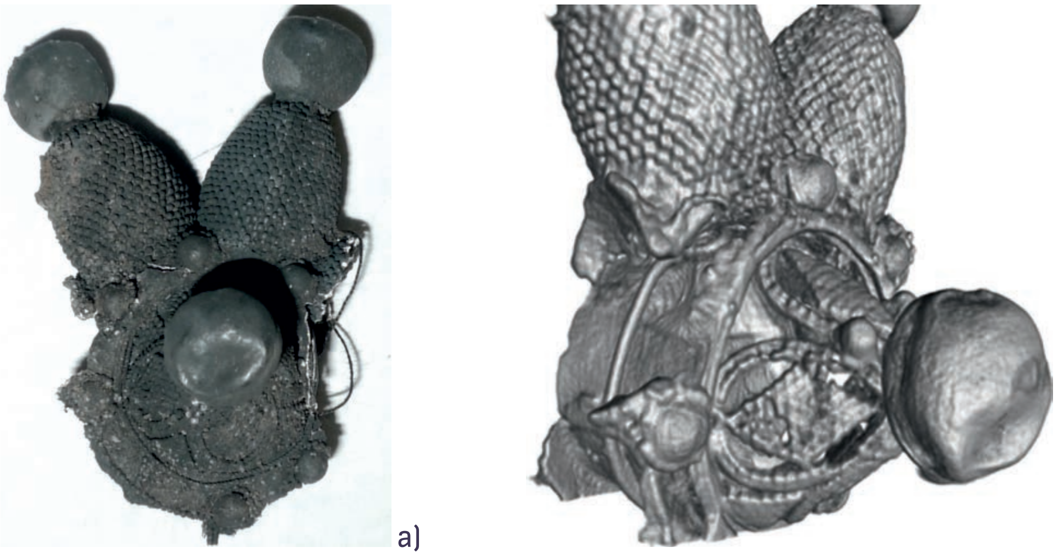
The active use of neutron tomography and radiography in the field of preservation of objects of cultural (archaeological) heritage in the last decade is largely due to research activities within the framework of specially oriented programs initiated by the IAEA (the "Ancient Charm" project) and the European Council (the "Authentico" project), focused on high-tech structural studies of cultural heritage objects and verification of their authenticity. So, for instance, within the framework of these programs, researchers have determined the authenticity of a number of artefacts and identify forgeries of antiquities from ancient Greek and Roman times, the Merovingian era, stored in European museums. Undoubtedly, similar programs in different countries will not lose their relevance for many decades to come, and neutron research techniques have a high potential to be applied within their framework.

Nowadays, scientific studies of art and archaeology present a necessary complement to the preservation, conservation and research of cultural heritage. As cultural heritage objects are frequently unique and non-replaceable, non-destructive techniques and approaches play a predominant role, simultaneously ensuring the physical integrity of the object under study and providing the most complete information about its chemical composition, internal defects, and structural features. In particular, successful cooperation has been established between the Joint Institute for Nuclear Research and the Institute of Archaeology of the Russian Academy of Sciences. Complementary archaeological and physics investigations make it possible to study a large number of valuable objects from various large-scale archaeological excavations on the territory of the Russian Federation. With the help of FLNP JINR, these research areas are being developed in the JINR Member States as well. For archaeological investigations and work in the sphere of preservation of cultural heritage objects, the method of neutron tomography and radiography is still among the rare ones. In this regard, all the more interesting are the results of the study of a number of archaeological objects, in particular, a miniature incense vial from the excavations of the Sarmatian burial of the Chebotarev-V burial ground (excavations by R.A. Mimokhod) and fragments of a bracelet and a kolt from the Tver hoard of 2014 (excavations by A.N. Khokhlov, S.A. Kungurtseva).

Old Russian jewelry has been the subject of numerous and long-term special studies since the first half of the 19th century, and items found in treasures hidden at the time of the tragic events of 1237–1238 are the objects of the closest attention of researchers as one of the reliable sources for the reconstruction of pre-Mongol period of Russian history and culture. In 2014, researchers of the Institute of Archaeology of the Russian Academy of Sciences, during excavations in the city of Tver on the territory of the Kremlin, in the building of the Real School, discovered a hoard of silver jewelry, the time of concealment of which, according to the experts, was the end of winter – beginning of spring 1238. The hoard contained at least 59 pieces of jewelry of various types, heavily fragmented: kolts, temporal pendants-ryasnas, three-bead temple rings, medallions and beads from a necklace, a two-leaved folding bracelet, made in the traditional techniques of granulation, filigree and niello, dating by analogy to the XII century — the first third of the XIII century. The objects were quite badly damaged both as a result of the subsequent life of the city in this area and, apparently, at the time of the events of 1238. Considering the fact that neutron radiography and tomography were successfully used to analyze relatively large objects of the Roman period, weapons, lead sculptures and urns, this method was used in the study of objects from the Old Russian hoard [Saprykina et al., 2018; Kichanov et al., 2018b].

One of these objects is a fragment of a ray kolt. The ray or star-shaped kolt (Figure 7.1) differs from those in the hoard both in size (the authors of the find give reconstructed dimensions of 52×56 mm) and in its state of preservation [Saprykina et al., 2019]. The kolt belongs to the jewelry of group

1; in terms of the shape of the rays and stylistic features of the design, it is close to the paired kolts manufactured by craftsmen from the Kiev school of jewelry in the first half of the XII century from the Terekhov hoard of 1876.



a) b)

Fig. 7.1. Photograph (a) and three-dimensional model (b) of an Old Russian kolt reconstructed from neutron tomography data. The model is presented after analysis of 3D data and the procedure of virtual segmentation of the outer corrosion layer.

A preliminary examination with a binocular microscope showed that most of the objects had lost their gilding and niello inlay, and that sections of the engraved ornament had not been preserved either. In addition, some jewelry items have visual signs of prolonged but indirect exposure to high temperatures (deformation, dents, the character of silver on the fracture; no traces of "flow" of metal were detected). A three-dimensional model of the object under study, reconstructed using neutron tomography, makes it possible to visualize both the assembly sites of individual parts and the internal fastening elements of the structure of the kolt.

The neutron tomography method, as well as algorithms for analyzing three-dimensional data, can be successfully applied for segmentation of reconstructed 3D data, which opens up wide opportunities for virtual non-destructive reconstruction of corroded cultural heritage objects. As an example, following is a non-destructive reconstruction of decorative elements on a bronze bracelet.

The fragment of a wide two-leaved cuff bracelet, which, before the start of restoration work, was a poorly preserved plane between the wired arches, with traces that can be interpreted both as markings for engraving and as the remains of heavily damaged engraved decoration. On its surface, neither microscope examination nor X-ray fluorescence analysis revealed any traces of gilding or areas with niello inlay. Neutron tomography experiments provided evidence of the presence of gilded areas on the arches and grooved wires running along the edge of the bracelet, and also, probably, on the clasps (Figure 7.2). The remains of niello inlay are located in all ornamental zones of the bracelet: in the lower and upper fields, in the space between the arches [Kichanov et al., 2017]. It is clearly visible that the engraved ornament is completely finished and does not require any additional finishing. The obtained results provide additional opportunities for identifying the ancient workshops in which the artifacts were manufactured.

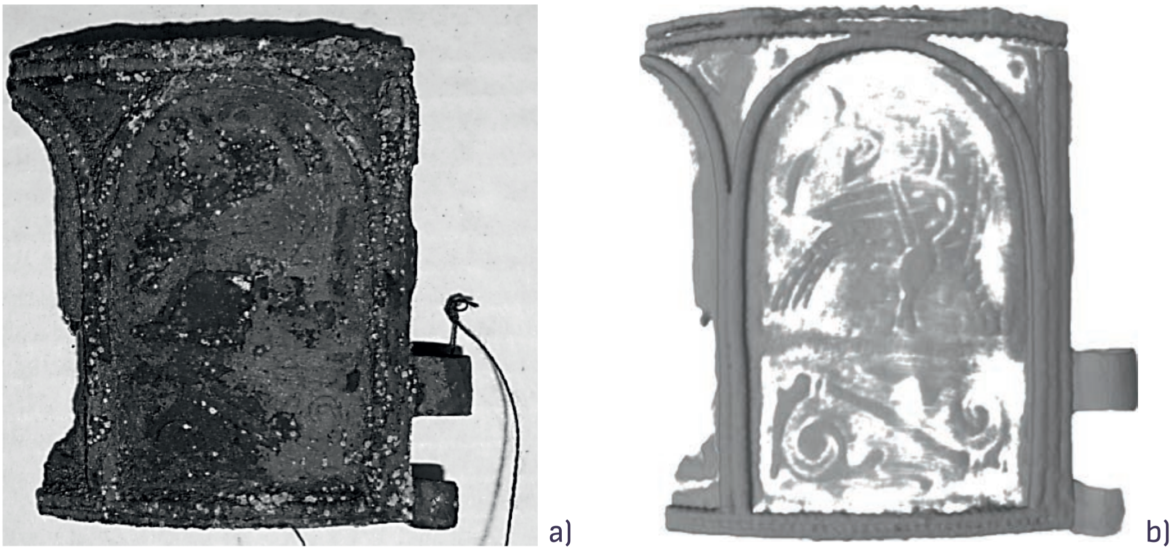


Fig. 7.2. Photograph (a) and 3D model of a fragment of a three-leaved bracelet reconstructed from neutron tomography data (b). The reconstructed model is presented after analysis of the 3D data and the procedure of virtual segmentation of the outer corrosion layer.

Another example of interest for research is an object found in the Sochi expedition of the Institute of Archaeology of the Russian Academy of Sciences, which explored an intact Sarmatian burial in the Rostov region. It dates back to the 1st century AD and, judging by the finds (gold and silver jewelry), belonged to a noble woman. A golden vial of an ancient Sarmatian woman (Figure 7.3) from the Chebotarev-5 burial ground serves as a convenient model object demonstrating the possibilities of various algorithms for analyzing three-dimensional data. The photo clearly shows the preserved handles of the vial and the decorations on the top of the lid. However, the internal volume of the closed bottle remains hidden.

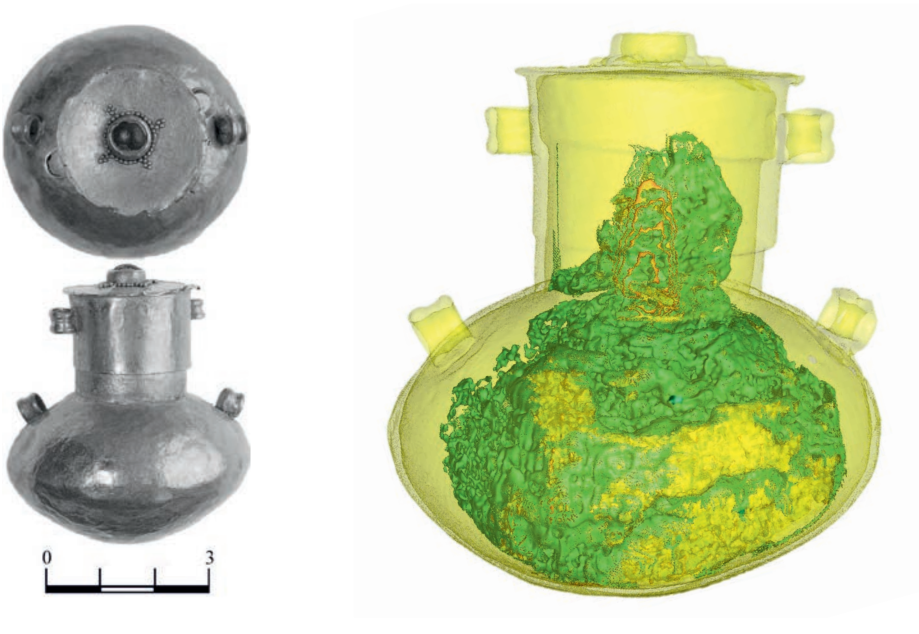


Fig. 7.3. Photo and 3D model of a golden vial reconstructed from neutron tomography data. The study revealed the presence of residues of some substance inside the vial, presumably incense.

After the procedure of reconstruction of the neutron tomography data, a 3D model of the vial was obtained (Figure 7.3). The reconstructed model clearly shows areas corresponding to the material of the internal filling. The substance is a sintered ("petrified") mass. Judging by the volume of the remains, it can be assumed that when the miniature vial was placed in the burial, the material occupied a rather large part of the volume of the vial, a fact suggesting a fairly high social and economic status of the buried person. The material residues as a whole have a homogeneous composition. The obtained data are expected to be useful in further studies of the chemical composition of incense residues.

The presented examples clearly demonstrate the possibilities that neutron research methods open up for studying cultural heritage and, of course, this direction will be actively developed at the future advanced neutron source at FLNP JINR. With its even higher neutron fluxes on the scientific instruments, it will be possible to obtain higher-quality results with better resolution and in shorter measurement times.

7.2. INVESTIGATION OF PALEONTOLOGICAL MATERIALS

Paleontology is a unique combination of all scientific disciplines that study the evolutionary history of life on Earth, including the history of mankind. Paleontological sciences include such areas of scientific knowledge as paleoanthropology, archaeology and related disciplines. This highly complex science involves many layers of knowledge about what happened in the past and what role it plays in the history and present-day existence of animals and plants. Fossils are the remains of animals, plants or hominids that form a kind of matrix, such as sedimentary rocks, preserving ancient material over thousands and millions of years. It is not surprising that fossils are discovered after millions of years, either through human activity (limestone mining or special exploration of caves) or as a result of natural phenomena (soil erosion, earthquakes).

Fossils and fossilized materials are unique and quite rare expensive objects. Countries with extensive collections of natural fossils are particularly concerned about the preservation of their natural heritage, so the role of non-destructive testing and related data analysis procedures is gradually increasing. In recent years, X-ray tomography and microtomography have become an important method for studying the internal structure of paleontological objects. These techniques are of great importance for studying rare and fragile specimens, as well as type specimens, the destruction of which is unacceptable. During studies, limitations of the method were identified, which are caused, firstly, by insufficient contrast, since the composition of fossil objects of extinct flora and fauna often contains minerals that are close to each other in terms of the level of absorption of X-ray radiation, and secondly, by the size and thickness of the object being studied due to insufficient penetration depth of X-rays.

Neutron tomography, as a representative of non-destructive testing methods, is characterized by deeper penetration into the thickness of the material under study, compared to X-ray radiation, which makes it possible to study fairly large objects of both scientific and applied interest. The high incoherent neutron scattering cross section for hydrogen determines the high neutron radiographic contrast in studies of samples containing even low concentrations of hydrogen-containing components. One of the tasks is the reconstruction of remnants or derivatives of organic substances in the fossilized remains of fossil animals or plants, which is precisely the subject of interest of paleontology.

The idea of searching for organic matter in stromatolites (colonies of cyanobacteria) is not new. However, it has not received development in this area of paleontology. Compared to X-ray methods, neutron tomography has advantages in studying such materials [Пахневич и др., 2013], which simultaneously contain both light elements, such as hydrogen or lithium, and heavy metals. It is also used to study paleontological and geological objects to determine the localization of hydrogen-containing substances that may be represented by organic matter.

The studied stromatolite consists of several mineral phases, which are clearly visible on virtual sections of X-ray microtomography. It has a fuzzy layered structure, which is expressed in the absence of clear boundaries between the layers. One of the layers is a sandy or quartz layer. Sand grains form a loose layer, rich in voids and cracks between them. Figure 7.4 presents a photograph and a reconstructed three-dimensional model of the stromatolite. Using neutron radiography data, it was possible to reveal contrasting areas that most likely correspond to the localization of a hydrogen-containing substance, which is distributed unevenly in the sample: both small and large clusters are observed [Pakhnevich et al., 2020]. The former are more often localized inside the sample. Large clusters of matter with a high neutron beam attenuation coefficient are located in the near-surface parts of the stromatolite. In rare cases, they are located near large cavities and cracks inside the sample. By origin, hydrogen-containing substances detected by neutrons may be minerals with a hydroxyl group, which are the result of the decomposition of organic matter.

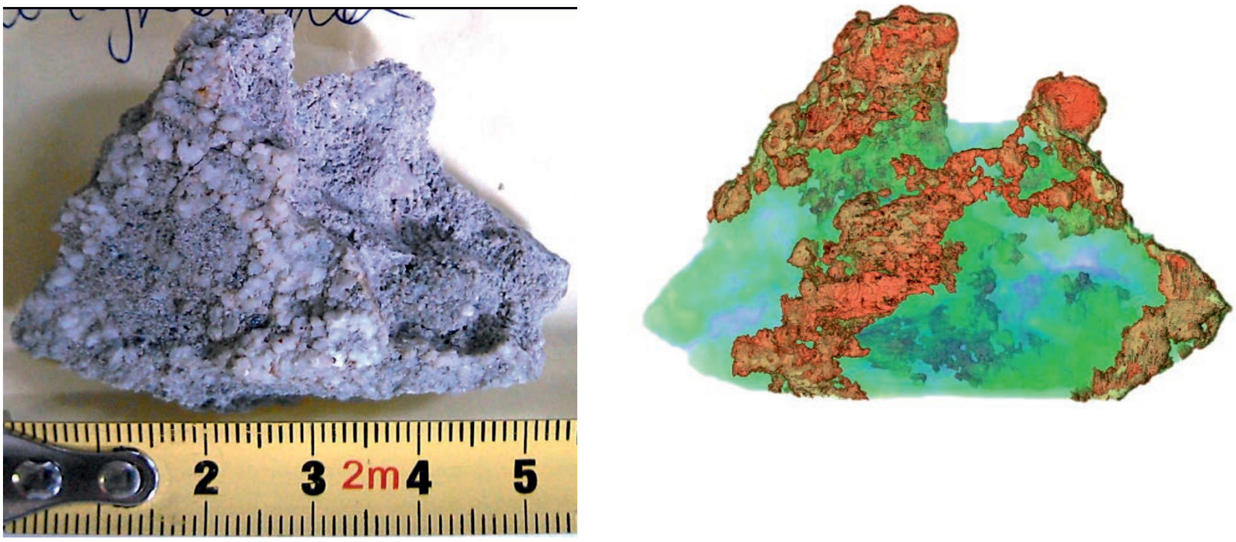


Fig. 7.4. Photograph (a) and three-dimensional model (b) of the stromatolite under study reconstructed from neutron tomography data. In the reconstructed model, the darker areas correspond to the remains of a stromatolite colony rich in hydrogen-containing components.

Due to the high penetrating power of thermal neutrons, it is possible to study the preferred orientations of grains in the shells of fossil mollusks [Pakhnevich et al., 2022]. In combination with X-ray studies, electron microscopy methods, etc., such studies help, for example, to discover related species of fossil mollusks and trace their evolution [Chaterigner et al., 2002].

7.3. NEUTRONS IN THE STUDY OF CULTURAL HERITAGE AND PALEONTOLOGY

The high information value of neutron imaging in the study of cultural heritage objects and paleontological specimens allows the use of neutron radiography and tomography methods for their study. Neutron imaging data can be supplemented by elemental, phase and texture analysis of artifacts, in particular using neutron diffractometers. The combination of neutron scattering techniques in the study of historical heritage objects, together with other non-destructive methods, opens up new possibilities for their study, as well as for the analysis and interpretation of data in the context of historical events, technologies existing at that time, trade routes, etc. Undoubtedly, at the advanced neutron source at FLNP JINR, neutron imaging instruments will be in high demand not only by scientists from the physics community, but also by scientists from other fields of knowledge.

Fundamental low-energy nuclear physics

Despite the shift in the focus of neutron research towards condensed matter physics, neutrons remain a unique research tool in the area of fundamental interactions, cosmology and nuclear physics. Examples of this type of investigations are experiments to refine the neutron lifetime, search for the electric dipole moment of the neutron, search for neutron-antineutron oscillations, measurement of the gravitational mass of the neutron, study of fundamental symmetries in processes involving neutrons, search for new types of interactions.

All these studies, one way or another, are aimed at the experimental detection of phenomena beyond the Standard Model (SM), which may provide a clue to solving the questions facing theorists today: why are there so many free parameters in the SM, why does matter dominate over antimatter, what are "dark matter" and "dark energy"?

Along with it, neutron experiments belong to the class of studies at the "intensity limit" — precision experiments that use highly sensitive detectors registering subtlest effects associated, for example, with the exchange of heavy virtual particles. They complement studies at the "energy limit" at new high-energy accelerators that can produce heavier particles than those previously observed. Progress in investigations at the "intensity limit" is important because it is determined by the intensity of the particles being studied (in our case, by an increase in the number of neutrons available in experiments), as well as by new original approaches to the design of experiments, development of the methods and unique equipment.

The study of nuclear reactions induced by neutrons is a tool for investigating fundamental symmetries at the nuclear level, as well as for studying deep restructuring of nuclear systems, for example, in the process of fission, which in turn is a source of rare nuclei located far beyond the boundaries of stability. Data on the structures of nuclei that can be obtained from the reactions with neutrons, energy dependences of neutron reaction cross-sections are still relevant and require further clarification. The corresponding requests are formulated by International Atomic Energy Agency (IAEA) expert groups.

Taking into account the experience of JINR in international cooperation, it is proposed to equip the new neutron source with the most universal beam infrastructure possible, providing ample opportunities for modification and modernization of nuclear physics instruments, which may be of interest to the widest possible range of researchers from different countries.

In terms of research directions, the tasks proposed to be solved at the advanced neutron source at JINR can be conditionally divided into three areas:

- fundamental interactions, properties of the neutron, ultra-cold neutron (UCN) physics, neutrino;
- neutron-nuclear interactions;
- nuclear-physics methods for determining the isotopic composition of matter.

To meet these challenges, the following infrastructure is required:

- source of ultra-cold (UCN) and very cold neutrons (VCN);
- beam of cold neutrons with maximum intensity and a minimum of fast neutrons and gamma-rays;
- beam of cold polarized neutrons with maximum intensity and a minimum of fast neutrons and gamma-rays;
- "hot source" with a chopper to reduce the duration of the neutron pulse and a polarizer;
- channels for activation analysis with a laboratory for working with open sources.

8.1. PHYSICS BEYOND THE STANDARD MODEL AND PROPERTIES OF THE NEUTRON

At present, the SM is a highly successful theory, with no significant deviations from its predictions or deviations that can be eliminated. However, the specific features of the SM (a large number of parameters, the complication of the theory with the addition of new effects), as well as the need to solve the problem of dark matter and the matter/antimatter ratio, require new experiments both to determine the limits of applicability of the SM and to search for and study phenomena lying beyond the SM.

8.1.1. Neutron lifetime

Lifetime is a fundamental characteristic of any elementary particle. In high-energy physics experiments, the lifetime can be measured in different ways, for example, from the widths of resonance peaks in the invariant mass spectra [CMS collaboration, 2015], using the well-known relation $\tau=\hbar/\Gamma$. Another option is to extract the lifetime of a particle from the characteristics of its tracks (the path traveled by the particle from birth to decay, and its velocity), measured using track detectors. In this regard, the neutron is unique: on the one hand, it lives a very long time by the standards of elementary particles, on the other hand, high neutron fluxes can be obtained relatively easily. These circumstances allow measuring the neutron lifetime in two different ways: using the beam method and the method of storing UCNs in a trap. Interestingly, these two approaches have so far given consistently different results:

1. The 'bottle method' measures the neutron lifetime by storing UCNs in a material or magnetic bottle (trap) and counting their remaining number after some time, with the latest results being τ=878.3±0.3 s [Strumia, 2022] and τ=877.75 ± 0.28 s [Gonzalez et al., 2021].
2. The 'beam method' measures the β-decay rate of neutrons in the beam, by counting the number of protons produced in the decay from a beam of cold neutrons, with the results being 888±2 s [Strumia, 2022] and 887.7 ± 1.2 [stat] ± 1.9 [syst] s [Yue et al., 2013].

These results differ by more than 4.6σ (Figure 8.1), which contradicts the SM, according to which the lifetime is independent of the measurement method. One explanation for this phenomenon may be the existence of other neutron decay channels besides beta-decay. Since the products of these decays have not yet been observed, it is assumed that they may be dark matter particles. The possibility of such processes could lead to the loss of mass by neutron stars due to the transition of neutrons into dark matter, which would limit the mass of these objects to two solar masses [Strumia, 2022].

Direct observation of neutron decays only into dark matter particles (the so-called invisible decay, $n\to\chi\chi\chi$), or $n\to\chi\chi\chi\gamma$ (decay into dark matter particles and matter particles) is possible with neutrino detectors.

To date, the following results have been obtained: for invisible decay in the Sudbury Neutrino Observatory (SNO) experiment [SNO Collaboration, 2019]: $\tau>2.5*10^{29}$ years, while for the 'visible' decay the Super-Kamiokande result is more than $5.5*10^{32}$ years [Takhistov et al., 2015].

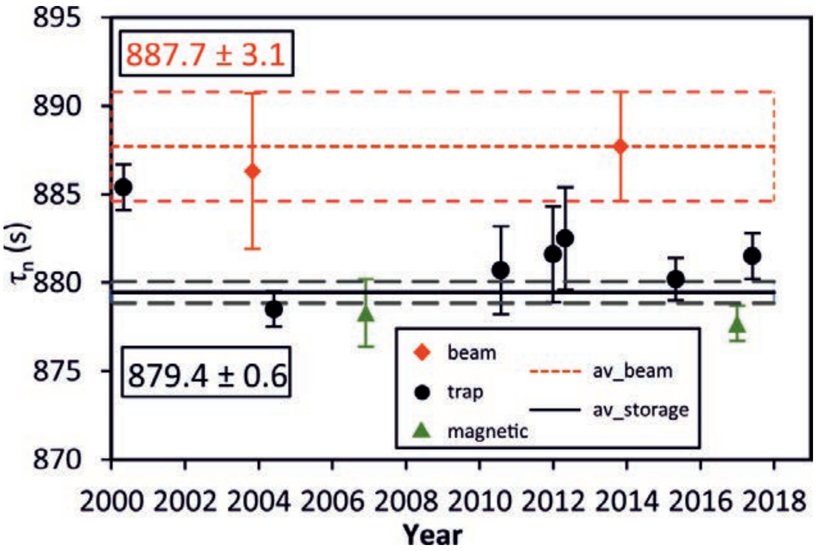


Fig. 8.1. Current status of experiments on measuring the neutron lifetime. The systematic discrepancy between the results of the beam measurements and experiments with UCN storage is clearly visible. [Serebrov, 2018]

To sum up, it can be concluded that the problem of discrepancies in neutron lifetimes obtained using different measurement methods is still far from being solved, but at the same time, the occurrence of unaccounted systematic experimental errors cannot be ruled out. **It should be noted that significantly fewer beam experiments have been conducted to date as compared to neutron storage experiments. The construction of a new high-flux pulsed neutron source at JINR will contribute to filling this gap.** In preparation for these experiments, FLNP specialists are developing a technique for direct measurements of the neutron flux in high-intensity beams, which will make it possible to conduct a beam experiment ideologically close to a neutron storage experiment. The possibility of creating a vacuum neutron guide in which it will be possible to place equipment for detecting protons in order to conduct a "traditional" beam experiment is also under consideration.

8.1.2. Violation of P and T invariance

It was long assumed that the equations describing physical processes are invariant under inversion of spatial coordinates, replacement of particles by antiparticles, or time reversal. However, in the 1950s, evidence for non-conservation of P-parity was discovered in studies of decays of charged K-mesons.

A clear experiment demonstrating the non-conservation of P-parity was reported in [Wu et al., 1957], in which anisotropy of electron emission in beta-decay relative to the spin direction of decaying 60Co was observed. The scale of this effect is quite large, and it does not present great difficulties in observation. The situation is different with nuclear processes, in which P-parity violation also occurs, but on a much smaller scale and caused by the weak component of the nuclear forces. However, in some nuclei the P-odd effect is enhanced due to the fact that:

- the main transition between states is suppressed and is mixed with another transition due to P-odd forces (the so-called structural enhancement);
- the transition occurs from a highly excited state of the nucleus, in which the S ($J^P=1/2^+$) and P ($J^P=1/2^-$; $3/2^-$) states are mixed by means of weak forces.

P-odd effects can be observed in a wide variety of phenomena including:

- circular polarization of gamma-rays emitted by nuclei after neutron capture [Alberi et al., 1972], arising from mixing a gamma-transition of allowed multipolarity (for example, a transition with momentum 1, and not changing parity, M1) with a transition changing parity and taking away the same value of the momentum (E1);
- asymmetry in the direction of gamma quantum emission "along spin – against spin" relative to the direction of the spin of the neutron causing radiative capture;
- asymmetry in the direction of emission of one of the fragments (light or heavy) relative to the direction of the spin of the neutron causing nuclear fission;
- dependence of the transmission of longitudinally polarized neutrons passing through an unpolarized target on the helicity of incident neutrons.

The investigation of the P-odd effects has a long history. The experimental confirmation of the existence of the enhancement phenomenon was the results obtained at FLNP JINR for resonances in ^{117}Sn, ^{139}La, ^{81}Br [Alfimenkov, 1983]; the magnitude of the observed P-odd effects was 10%.

Currently, these studies continue to be of great interest and can be carried out at the advanced neutron source at JINR at a new level of accuracy using state-of-the-art electronics. When studying P-odd effects in the angular distributions of γ-rays, it is critically important to isolate individual γ-transitions upon excitation of specific states. Examples of related studies that are currently underway are experiments at the J-PARC accelerator complex. From the obtained angular distributions of γ-rays, partial neutron widths of the studied resonances were extracted, which are necessary for estimating the value of the matrix element of the weak interaction violating spatial parity [Okudaira, 2018; Okudaira, 2023; Koga 2022]. The layout of the experimental setup used in these studies is shown in Figure 8.2. Gamma-rays were detected by a spectrometric system consisting of 25 high-purity germanium detectors, which made it possible to observe the studied effect in a selected γ-line.

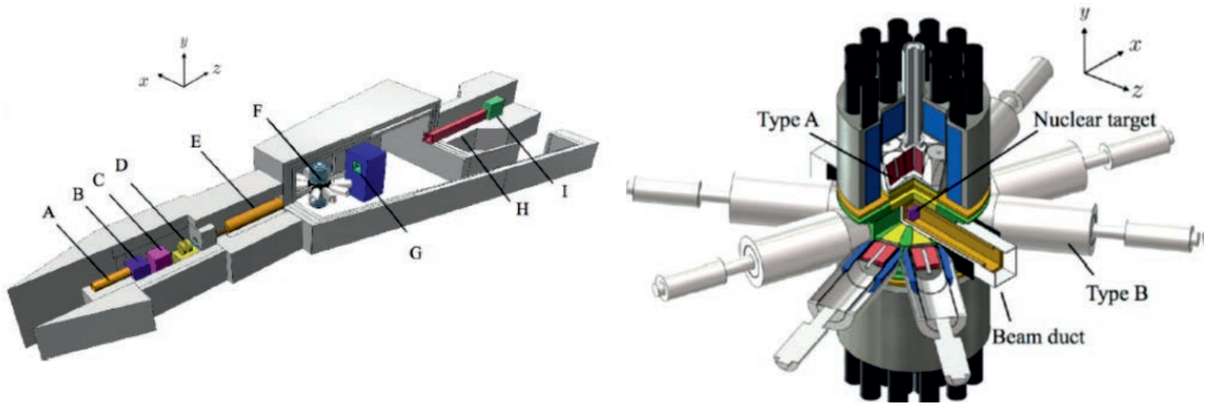


Fig. 8.2. Layout of the spectrometer based on germanium detectors at the ANNRI (Accurate Neutron-Nucleus Reaction Measurement Instrument), J-PARC, for measuring angular distributions of γ-rays. A, E, G – collimators, B, D – choppers, F – assembly of germanium detectors, H, I – beam stop.

The presented experimental setup is quite universal for studying γ-radiation emitted in neutron-nuclear reactions. The use of a similar setup at the new neutron source may be useful not only for studying the parameters of low-lying resonance states, but also, for example, for studying the yields of fission products similar to [Michelagnoli, 2018].

Of particular interest is the search for T-violation in neutron-nuclear reactions, which, according to the CPT-theorem, is equivalent to the CP-violation. To date, this effect has been observed only in the decays of K^0 and B^0-mesons. Detection of T-violation in nuclear reactions will be an important step for confirming the universality of the weak interaction. In [Okudaira, 2018], an estimate was made of a possible enhancement of the T-violation in the vicinity of the p-wave resonance. The same mechanisms of the space and time parity violation were assumed in [Gudkov, 1992], therefore a detailed study of P-even and -odd effects opens up the possibility of observing the effects of the time parity violation in neutron-nuclear interactions.

One of the possible experiments for testing the violation of T-invariance is the "polarization-asymmetry" type experiment, discussed in detail in [Беда, 2007], the schematic of which is shown in Figure 8.3.

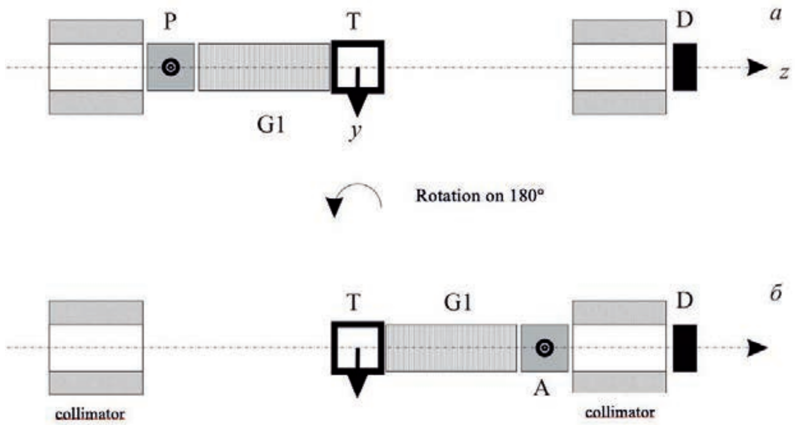


Fig. 8.3. Schematic of the polarization-asymmetry experiment. A-analyzer, P-polarizer, G1-transport system, maintaining neutron polarization. T-polarized target, D-neutron detector. [Беда, 2007].

The idea of the proposed experiment is as follows: an unpolarized neutron beam with a constant intensity *I* passes through a polarizer and a polarized target and falls onto a neutron detector. In this case, the detector count rate will be N_1. The application of the time reversal operation to this experiment should result in that neutrons moving in the direction "from the detector" successively pass through the target and the polarizer. This effect can be achieved by rotating the setup by 180° around the axis perpendicular to the direction of the neutron beam. In the absence of the T-invariance violation, the neutron detector count rate N_2 will be equal to N_1. The expected magnitude of the effect is currently undetermined.

The organization of investigations on the search and study of violation of P- and T- invariance is possible at the new neutron source, provided that special beamlines with polarized neutrons are created.

8.2. NEUTRON OPTICS

8.2.1. Non-stationary quantum mechanics and neutron optics at large accelerations

Neutrons are rather convenient for studying non-stationary quantum phenomena, when the parameters describing the interaction of a neutron wave with an object vary in time. A non-stationary action on the neutron wave allows one to significantly change the intensity, wavelength, and direction of its propagation. FLNP researchers have extensive experience in both theoretical and experimental investigations in this area (Figure 8.4) [Frank et al., 2016; Кулин и др., 2019].

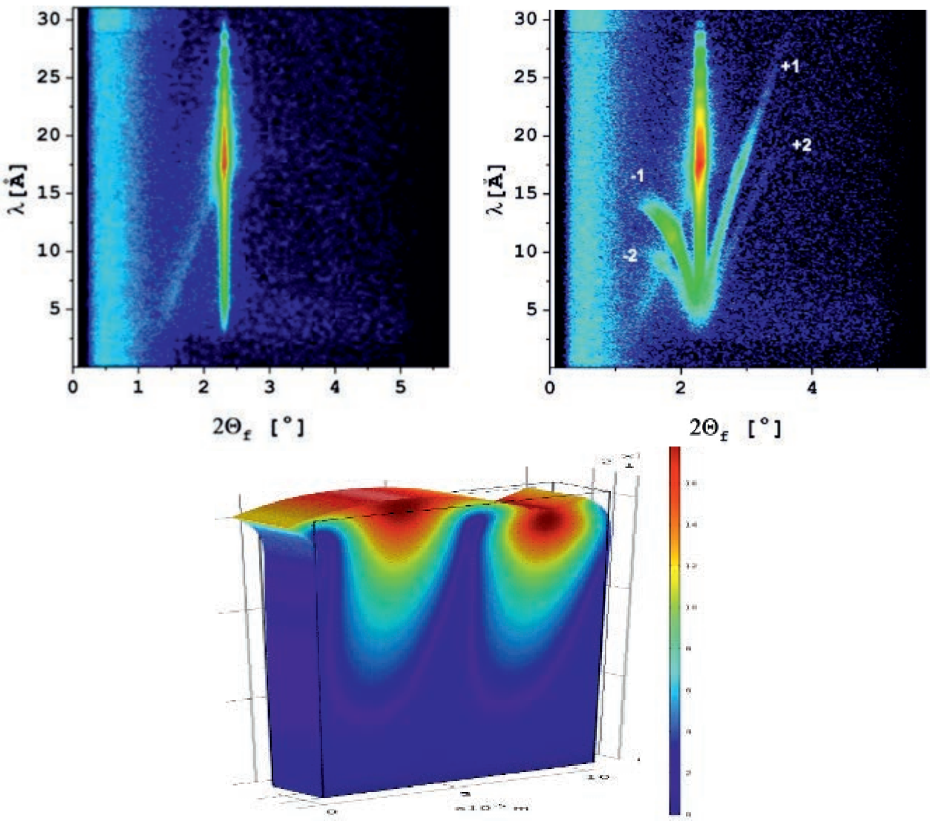


Fig. 8.4. 2D scattering pattern for cold neutrons from $LiNbO_3$ single crystal sample in the absence of SAW (left); 2D pattern of scattering during diffraction of cold neutrons from a running SAW (middle), numbers of diffraction orders are shown; a typical calculated pattern of surface deformation upon excitation of SAW (right), the color shows the magnitude of the displacement of atoms from the equilibrium position.

Of great interest is the study of inelastic scattering of neutrons, in particular UCNs, on surface acoustic waves (SAWs). SAWs arise due to periodic oscillations of a near-surface layer of matter, which moves with variable velocity and acceleration. For SAWs with a frequency of tens of MHz, this acceleration reaches a value of 10^7 g. Therefore, experimental studies of this phenomenon can be considered not only as a visual demonstration of the non-stationary quantum effect, but also as a sensitive test for verifying the validity of the generally accepted laws of neutron optics in the case of high accelerations. The very fact of observing the effect of the non-stationary diffraction in the reflection geometry suggests that the time of formation of the reflected wave in the matter is at least less than the period of surface oscillations. At the same time, the question of the reflection time of neutron and X-ray waves when the grazing angle exceeds the critical angle of the total external reflection still remains open [Бушуев и Франк, 2018]. Any experimental information shedding light on this problem is very important. An experiment with extremely high (no less than 1 GHz) frequencies of matter oscillations will provide answers to this question. The advanced pulsed neutron source at FLNP JINR is the most suitable for solving such kind of problems.

There is a substantial groundwork in the theoretical study of the problems of neutron transmission and reflection from oscillating resonance structures [Захаров и др., 2020; Zakharov et al., 2021]. From these studies it follows that it is not so much the long interaction time that has a significant effect on the final picture, but rather its combination with the fact of accelerated motion of the sample. Experimental confirmation of these results is of great interest and can be performed at the advanced neutron source at JINR.

8.2.2. Neutron microscopy

The fundamental possibility of creating a neutron microscope was demonstrated experimentally using UCNs [Франк, 1987] back in the late 80s of the last century. In the last decade, the active development of non-destructive methods for analyzing the structure of samples using neutrons such as neutron radiography, as well as the improvement of elements of neutron optics, have revived interest in neutron microscopy. This led to the development of a cold neutron microscope by a research group at MIT in collaboration with NIST [Khaykovich et al., 2011; Liu et al., 2013; Hussey et al., 2021]. Almost simultaneously, a cold neutron microscope was also developed at PSI [Trtik et al., 2015], which has already entered the stage of inclusion of the instrument into the PSI user program.

Neutrons have a set of unique properties that make them more suitable than light, electrons or X-rays for studying physical and chemical properties, as well as processes occurring inside the object of investigation. The absence of a monotonic dependence of the scattering length on the atomic number or charge of the nuclei, as is the case, for example, for X-rays, leads to a significant difference in the refractive indices not only for chemical elements close in masses, but also for isotopes of the same element. The refractive index value is related to the coefficients of reflection and transmission of neutrons. Therefore, substances with different but similar chemical compositions can differ significantly in their neutron-optical properties. The negative scattering length of protons distinguishes hydrogen from most other elements that make up organic substances. Due to the different hydrogen content, substances that are quite similar in composition can differ significantly in neutron-optical properties. In this regard, a neutron microscope can be especially useful in biological research.

Due to the magnetic moment of the neutron, neutron microscopy can be useful for obtaining information about the magnetic structure of the object under study. The use of beams of polarized neutrons will allow measuring magnetic properties of materials.

The resulting contrast in the images from cold neutron microscopes is based on a change in the beam intensity due to absorption or scattering in the sample. The use of UCNs in this case has a number of advantages. In particular, this is an increase in contrast due to the growth of the cross-section of all processes as 1/v, where v is the neutron velocity. In [Masalovich et al., 1996], an approach was proposed that combines a neutron microscope using UCNs with the phase contrast method, which opens up the possibility of studying objects that are sufficiently transparent to neutrons.

8.2.3. Spin-echo for UCNs

The problem of the interaction time in quantum mechanics has been the subject of discussions for quite a long time. The approach to measuring the time that a particle spends in a potential region by using the Larmor precession of the neutron spin in a magnetic field, proposed in [Базь, 1966], was successfully applied in a number of experiments with neutron spin-echo of cold neutrons, in particular, for measuring the time of tunneling through a resonance potential structure (neutron interference filter), as well as the time of reflection from a Bragg structure [Франк и др., 2002].

The development of a spin-echo spectrometer for UCNs, as well as the methodology developed by FLNP scientists, will make it possible to continue studies of the interaction time at a new level of sensitivity at the advanced neutron source.

8.2.4. Gravitational spectroscopy and verification of the weak equivalence principle

Neutrons are among the most suitable objects for studying the gravitational interaction of elementary particles. Although gravitational experiments with neutrons have a history of more than half a century, the available experimental data are rather scarce and significantly inferior in accuracy to the results obtained using atomic interferometers. The most accurate estimates for the equivalence factor were obtained from processing the Maier-Leibnitz and Koester experiment on measuring the coherent scattering length of neutrons by nuclei [Maier-Leibnitz et al., 1962; Koester, L., 1976]. The latest analysis of these results was performed by Schmiedmayer [Schmiedmayer, 1989], who obtained the equivalence factor with an accuracy at a level of 3×10^{-4}.

In quantum gravity experiments with a neutron interferometer, in which the gravity-induced phase shift of the neutron wave function was observed, a discrepancy [Littrell et al., 1997] between the experimental and theoretical phase shifts was obtained at the level of 1% with an error smaller than an order of magnitude. The results of a later experiment [Zouw et.al., 2000], the accuracy of which was 0.9%, did not eliminate this problem. In the experiment with a neutron spin-echo spectrometer, the measured value of the gravity-induced phase shift agrees with the estimate at the level of 0.1%, while the overall measurement accuracy was 0.25%.

In the experiment [Франк и др., 2007], in which the change in the energy of the neutron falling to a known height in the Earth's gravitational field was compensated by a quantum of energy $\hbar\Omega$, that was transferred to the neutron via a nonstationary interaction with a moving diffraction grating, the FLNP researchers succeeded in achieving an accuracy of verification of the validity of the weak equivalence principle at a level of 2×10^{-3}.

In experiments investigating transitions between quantum states arising from the quantization of the energy of vertical motion of ultracold neutrons, the group from TU Wien [Cronenberg et al., 2015] achieved an accuracy of 4×10^{-3}, comparable to the result obtained by the FLNP group.

A new approach to the free-fall experiment with UCN has been proposed [Zakharov et al., 2016]. The idea is to measure time-of-flight values of neutrons from different equidistant lines of a discrete energy spectrum with a precisely known distance between the lines (Figure 8.5). This method does not require knowledge of either the initial neutron energy or the geometric parameters of the setup. Such kind of experiments at the new UCN source could well provide the opportunity to achieve greater accuracy.

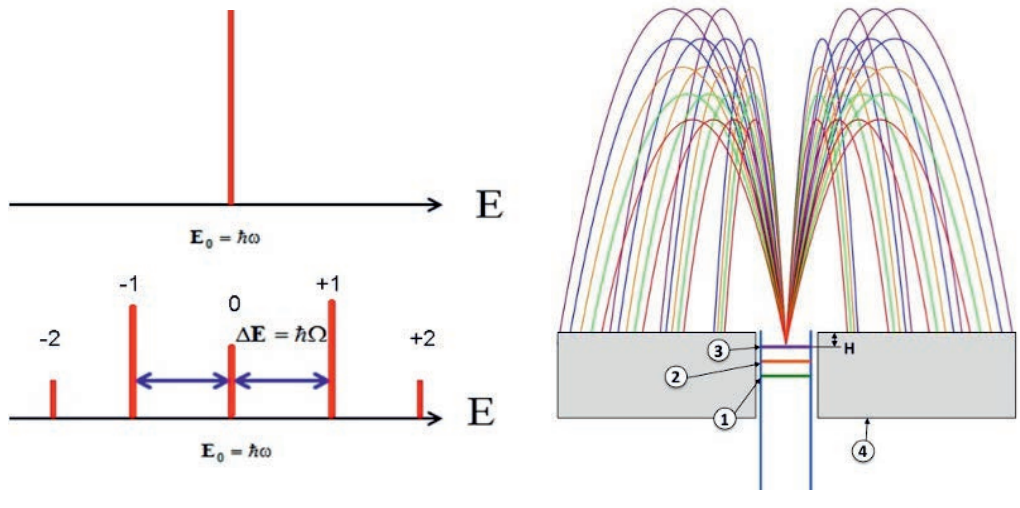


Fig. 8.5. Splitting of the energy spectrum by a nonstationary quantum device (left); Schematic of the UCN experiment with a free fall of the neutron (right): 1 — neutron interference filter (monochromator), 2 — nonstationary quantum device, 3 — Fourier chopper, 4 — ring detector.

8.3. PHYSICS OF FISSION

8.3.1. Investigation of T-odd effects in fission

Fission of heavy nuclei is a process with a huge (about 200 MeV) energy release, which makes possible the occurrence of various exotic processes (production of mesons, fission with the emission of three or more fragments). Also, among fission products, it is possible to search for bound states of neutrons dineutrons, tetraneutrons, etc. The study of TRI and ROT effects, leading to the asymmetry of the emission of fission fragments and secondary particles (light charged particles, gamma-rays and neutrons) with the change in the polarization of incident neutrons, allows studying the fission mechanism in more detail.

Induced fission of nuclei $^{Z}A(n,f)$ occurs with the formation of a highly excited and strongly deformed intermediate state of the nucleus $^{Z}(A+1)$, which often has a rotational nature. In this case, the fission products acquire a tangential component of velocity at the initial moment of rupture of the neck of the deformed nucleus, directed perpendicular to the axis of deformation. The trajectory of the fragment, instead of being rectilinear, due to the Coulomb repulsion of the fragments, becomes hyperbolic and deviates from the initial position of the axis of deformation by a certain small angle $\Delta\theta$. Measurements of this angle give information about the rotation speed of the nucleus.

The effect of rotation of the nucleus, the so-called ROT effect, was first discovered in the angular distributions of α-particles from the ternary fission of the ^{235}U nucleus induced by cold polarized neutrons [Goennenwein, 2007]. However, the trajectories of motion of α-particles from ternary fission at the moment of nuclear scission partially rotate together with the fission axis, since their motion is significantly affected by the Coulomb field of the moving fragments (Figure 8.6). Therefore, to determine the rotation angle of the fission axis (the magnitude of the ROT effect) in ternary fission, detailed trajectory calculations are necessary [Guseva, 2007].

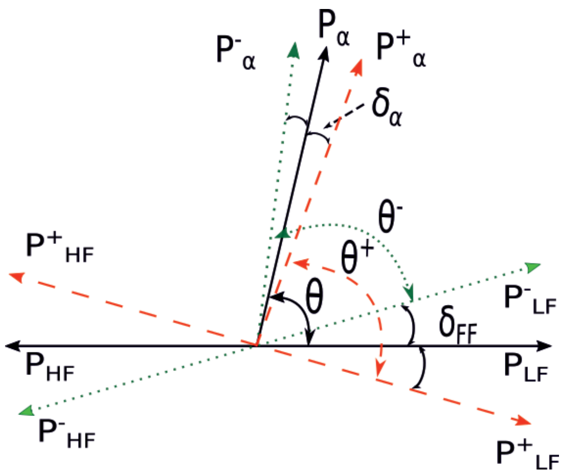


Fig. 8.6. Schematic representation of the developed shift in the angular distribution of α-particles in ternary fission. PLF, PHF are the initial directions of light and heavy fragments, respectively; Pα is the motion of the α-particle at the moment of scission. "+" and "—" denote the final directions of the object for opposite directions of neutron polarization.

The so-called prompt γ-rays emitted by excited fission fragments can serve as a marker of the orientation of the deformation axis before the nucleus fission. At the moment of the neck rupture of the fissioning nucleus, the spins of the excited fission fragments are aligned in a plane orthogonal to the axis connecting the centers of mass of two fragments, and their orientations do not change when the trajectory of the fragments deviates from the initial direction of the deformation axis. It is important to note that for γ-quanta, unlike for α-particles, the determination of the rotation angle does not require trajectory calculations, being in this sense model-independent. This fact significantly simplifies the study of the ROT effect.

An example of the design of an experimental setup for detecting correlations of γ-rays and directions of fragment emission is shown in Figure 8.7.

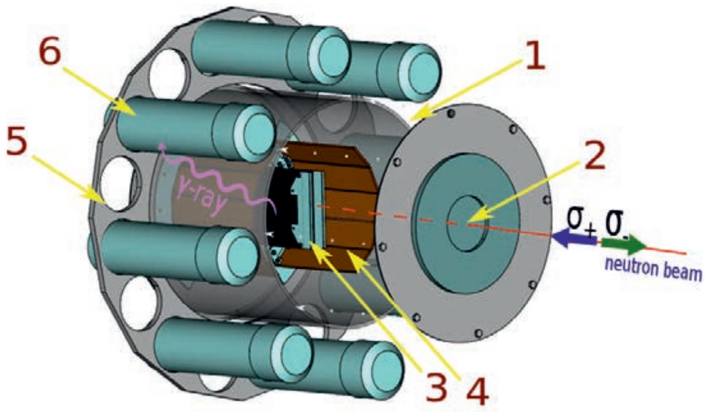


Fig. 8.7. Schematic of the experimental setup for studying the ROT effect using correlations of γ-rays and fission fragments. 1 — fission chamber, 2 — input Al window of the chamber, 3, 4 — detectors of fission fragments based on position-sensitive multi-wire proportional low-pressure counters (start and stop detectors), 5 — holder, 6 — scintillation plastic detectors of γ-rays and neutrons. The fissioning target is located in the center between the start detectors.

Of particular interest is the study of the ROT effect in the resonance region, since it is the resonance states that allow us to isolate individual channels characterized by a clearly defined (and known) set of quantum numbers. In particular, the observed TRI and ROT effects in fission are currently the only sources of reliable information on the quantum number K characterizing the fission channels. The study of the lowest resonance states can be performed on a pulsed source, despite the long duration of the pulse (Figure 8.8).

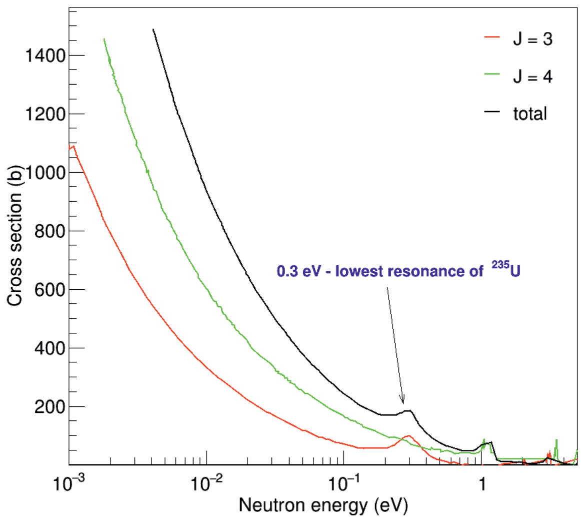


Fig. 8.8. Spin-separated fission cross sections for ^{235}U. The red line corresponds to spin J = 3, the green line corresponds to spin J = 4, the black line corresponds to the total cross section.

In 2018, for the first time, it was possible to measure the ROT effect for gamma-rays in the fission of ^{235}U in the low-lying resonance of 0.3 eV. The results obtained are consistent with theory, but for further investigation of the quantum-mechanical properties of the fission process it is advisable to continue these studies in order to obtain data for higher-lying resonances, as well as for other nuclei. In particular, the nuclei ^{241}Am and ^{245}Cm are proposed as candidates.

8.3.2. Investigation and search for rare fission modes

Another possible line of research, successfully developing both at FLNP and FLNR of JINR is the study of rare fission modes. Usually, two fragments are formed as a result of fission, but sometimes, instead of the usual "binary fission", a process of higher multiplicity is observed with the emission of one or more additional fragments, which are lighter than the main fission fragments (Figure 8.9). The reason for this process is clustering — the formation of stable groups of nucleons inside nuclei. The probability of such processes rapidly decreases with increasing multiplicity of products. A challenging task is to determine the nature of fission with the emission of three or more fragments by answering the question whether they are emitted directly at the moment of scission simultaneously with heavy fragments or they are products of the following decay of the fragments. In particular, in the case of the quaternary fission, in addition to two heavy fragments, two light fragments are produced, which can be emitted at the moment of scission of the nucleus ("true quaternary fission"), or during the decay of an unstable light product of ternary fission, for example $^{7}Li^{*}$, ^{8}Be, $^{9}Be^{*}$ ("pseudo-quaternary" fission). These processes can be separated kinematically.

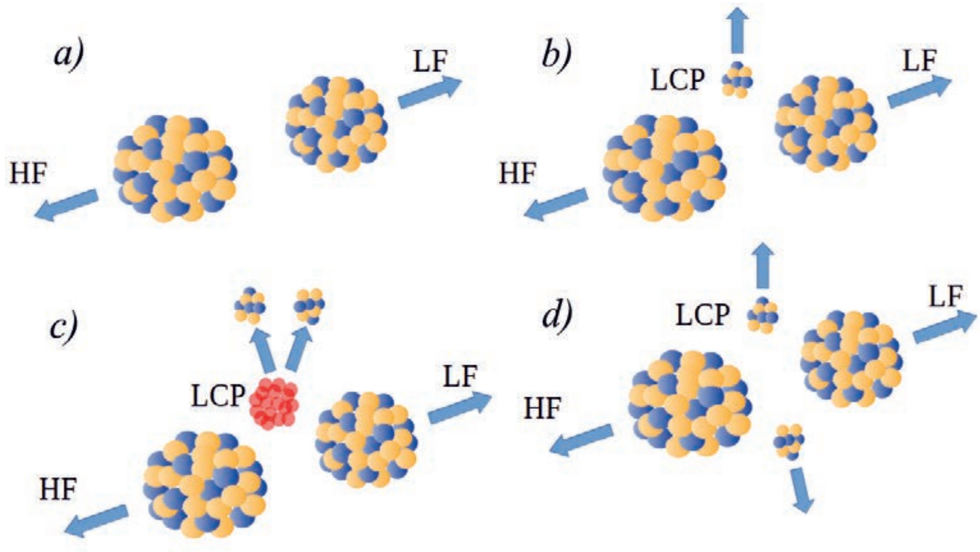


Fig. 8.9. Schematics of different types of fission processes: *a)* most common binary fission, *b)* ternary fission, *c)* "pseudo" quaternary fission, *d)* "true" quaternary fission.

The rare fission modes can be studied using modern achievements in experimental techniques. The layout of the experimental setup and the principle of the experiment are shown in Figure 8.10.

Identification of fission products is performed using position-sensitive *E*-*ΔE* telescopes. Detectors of this type can provide multi-parameter event-by-event spectroscopic information (position, energy and time, type) for almost any charged particle. In addition, the combination with the event tracking analysis provides better signal-to-noise ratio with high suppression of background and unwanted events. Examples of identification of light fission products are shown in Figure 8.11.

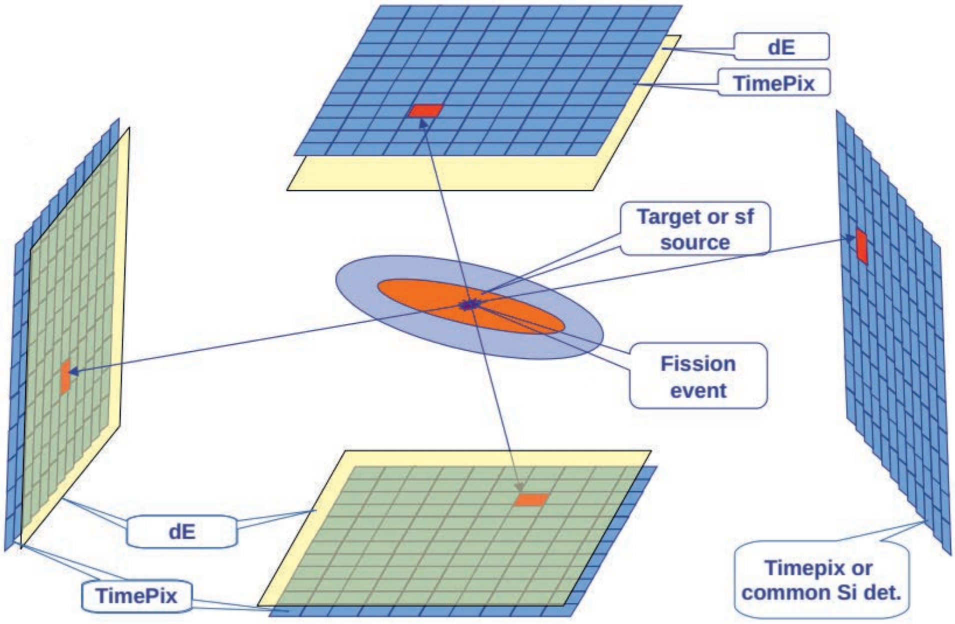


Fig. 8.10. Scheme of the experimental setup and the principle of the experiment for studying rare fission modes.

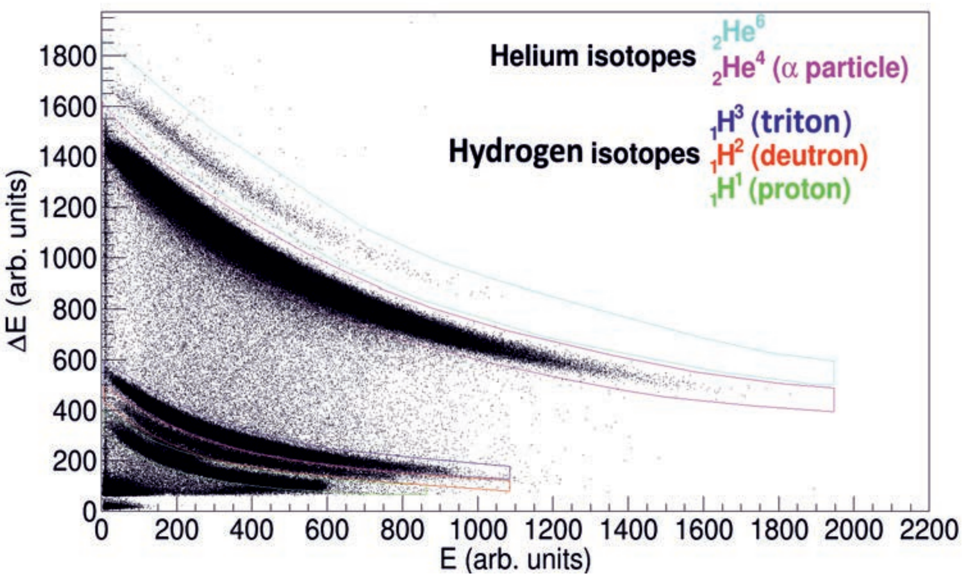


Fig. 8.11. *ΔE–E* spectrum of light ternary and quaternary particles.

The study of fission physics is a promising research area that will be developed at the new neutron source. To conduct such kind of experiments, an intense beam of polarized neutrons in the low-energy resonance region is required.

8.4. OBTAINING OF NUCLEAR DATA

Obtaining and updating nuclear data is an important component of the scientific program at the advanced neutron source at FLNP. Accurate information on the cross-sections of neutron-nuclear reactions is necessary for the design of new-generation power and research reactors, the development of technology for the production of isotopes for industrial and medical applications, the development of new radioisotope energy sources, elemental analysis and other areas of human activity [Bernstein L., 2015].

The main areas of research activities on obtaining nuclear data that will be carried out at the advanced neutron source at JINR are as follows:

- Activation cross-sections for dosimetric purposes.
- Fission cross-sections and yields of fission products for a wide range of incident neutron energies.
- Data on the decay of radioactive isotopes, including short-lived isotopes.

8.4.1. Activation cross-sections for dosimetric purposes

In dosimetry, the use of standards is one of the most common techniques. Their application is often much simpler than direct measurements of particle fluxes. The accuracy of the results obtained in this method is limited from above by the existing uncertainties of the reaction cross-sections for the reference elements. The choice of these reference or "standard" samples is mainly determined by practical considerations (for example, a smooth energy dependence and a large cross-section are desirable; the process should be easily observable in common types of detectors, etc.).

In particular, the reactions H(*n,n*), ^{3}He(*n,p*), ^{6}Li(*n,t*), ^{10}B(*n,α*), ^{10}B(*n,α1γ*), Au(*n,γ*) and ^{235}U(*n,f*) are recommended for measuring neutron fluxes. However, this list can be extended. One of the possible areas of activities at the new neutron source could be testing the suitability of some capture reactions for use as new standards and high-precision measurement of capture cross-sections at the request of teams involved in creating databases of evaluated data.

8.4.2. Fission cross-sections and yields of fission products for a wide range of energies of incident neutrons

Correct information about the process of fission of heavy nuclei is necessary for many applications: optimization of theoretical models, modeling of new-generation nuclear reactors and ADS systems. Accurate estimates of the yields of fission products are important for the development of methods for the production of isotopes for industrial and medical applications.

At present, the bulk of information on fission cross-sections, neutron multiplicity and yields of fission products is available for processes induced by thermal neutrons, while there is some shortage of information for the resonance region and fast neutrons up to 14 MeV. There is a great need for data for reactions induced by high-energy neutrons.

The yields of fission products, which are required for monitoring neutron fields and assessing the U/Pu ratio in nuclear fuel, are known with insufficient accuracy. For the development of theoretical models, data on the total kinetic energies of fission products as a function of the energy of incident neutrons corresponding to the formation of specific product nuclei are needed. Accurate measurements of spectra of gamma-rays emitted by decaying radioactive fragments are necessary to more easily determine the yields of fission products for further analysis of the irradiation conditions of fissile materials. The data on the yields of prompt gamma-rays are in demand for the development of elemental analysis techniques. The most complete collection of this type of data to date was created based on the results of measurements in the 1970s [Demidov, 1978]; high demand for this information is emphasized in [Bernsein, 2015] and [Hurst, 2021].

For such kind of studies, it makes sense to achieve the highest possible neutron flux (especially for measurements of the total kinetic energies of fission products depending on the energy of incident neutrons with reference to the yields of individual fission products) and a minimum background.

To measure the characteristics of gamma-radiation, it is advisable to create spectrometric systems similar to those described in section 8.1.2.

8.4.3. Data on the decay of radioactive isotopes, including short-lived isotopes

Information on lifetimes and decay channels of radioactive nuclei is of great importance. Isotopic sources of ionizing radiation are widely used for medical purposes, for flaw detection and disinfection, and can be used as markers in the study of flows of various liquids. Data on the decay of neutron-rich fission products are required for planning reactor operating modes and the frequency of fuel reloads.

Fission reactions are a unique source of neutron-rich nuclei. Among the fission products of ^{238}U, more than 800 different nuclides have been observed, during the decay of which electrons, antineutrinos, and in the case of a large neutron excess, delayed neutrons are emitted. Charged particles emitted by radioactive nuclei can cause defects in the cladding of fuel elements and containers for storing radioactive materials, and they also contribute to heat generation in the reactor. Information on the lifetimes of nuclei emitting delayed neutrons and the spectra of these neutrons, as well as dependences of the yields of fission fragments in the decay chain of which there are nuclides emitting delayed neutrons on the energy of the particles that induced the fission, are of great importance for modeling new-generation reactors.

The IAEA Nuclear Data Section has compiled lists of the most in-demand data on the decay of fission products [INDC(NDS)-0499, 2006; INDC(NDS)-0676, 2014; INDC(NDC)-0643, 2016], which include nuclei with expected lifetimes from fractions of a second (^{97}Sr) to tens of days (^{89}Sr); most of the isotopes proposed for study live for tens of seconds.

Measurements of the decay characteristics of radioactive nuclei produced by fission and fission product decay are one of possible directions of activities on nuclear data at the new neutron source. The pulsed operation of the source is a significant advantage in studying short-lived (~microseconds) radioactive nuclei.

8.5. SOURCE OF EXOTIC NUCLEI AND STUDIES USING RADIOACTIVE BEAMS

The investigation of neutron-rich nuclei is of great interest for understanding the isospin symmetry of nuclear forces, searching for new magic numbers and proving the correctness of parameters of nuclear models obtained for stable and long-lived nuclei.

Neutron-rich nuclei are produced in the well-studied process of fission of heavy nuclei because the N/Z ratio in heavy long-lived nuclei is greater than in average stable nuclei. In a fission induced by neutrons, the distribution of fragments by charge and mass is concentrated in the region of magic numbers, which is smoothed out with increasing energy of incident neutrons.

The feasibility of a factory of exotic nuclei at the new neutron source was discussed in

[Аксенов, 2021]. The fission of heavy nuclei can be used as a source of exotic nuclides, which has already been implemented in a number of projects: SPIRAL [Lewitowicz, 2008], FIPPS [Michelagnoli, 2018], PARRNe [Lau, 2003].

The PITRAP facility is planned to be built at the PIK reactor [Novikov, 2019]. In this project, a ^{235}U target (foil weighing 1.5 g, 10 μm thick, 150 cm^2 in area) will be placed in the reactor core. Fission products will be delivered to the ion source by helium flow through a capillary with inner diameter equal to about 1 mm (pressure 0.2–0.3 MPa). The resulting ions then pass through a mass separator and are collected in Penning traps for further study.

The expected neutron flux at the target location is 3×10^{13} $cm^{-2}\cdot s^{-1}$. It is assumed that the use of this source will allow obtaining a significant number of exotic nuclei in the traps, including those currently unknown.

According to the diagram presented in Figure 8.12, the PITRAP facility allows obtaining for study a sufficient number of previously unknown nuclei with 96<N<124 and 56<Z<72.

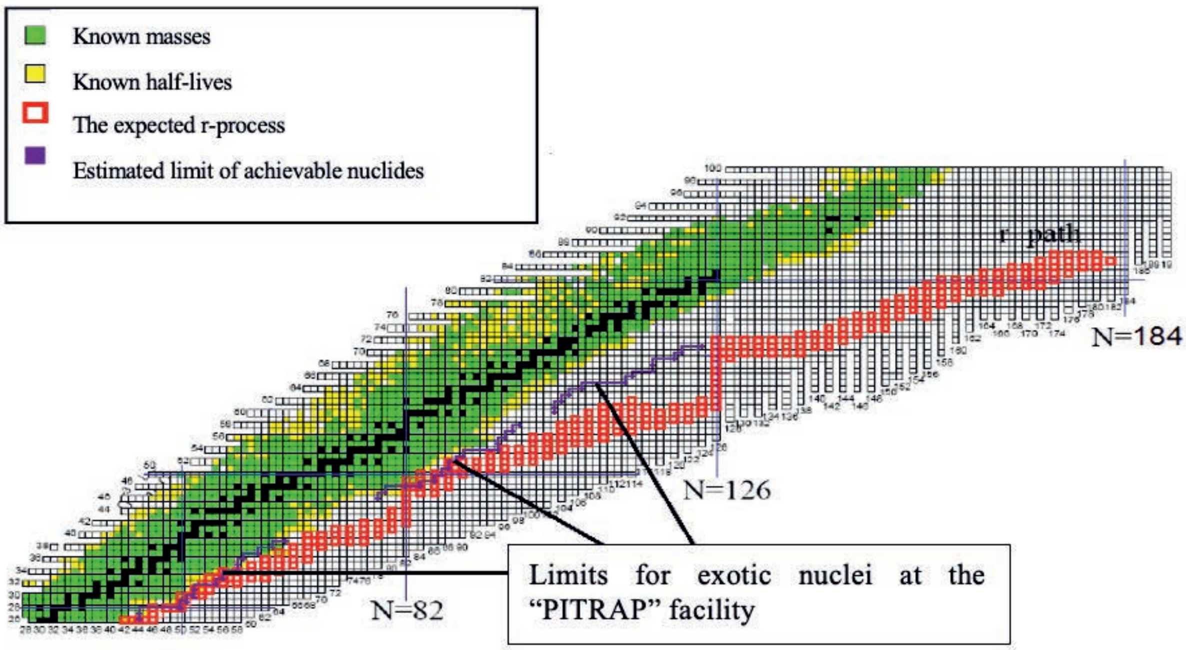


Fig. 8.12. Fragment of the N-Z diagram with the indicated.

At the new neutron source at FLNP JINR, the investigation of exotic nuclei can be developed in two directions:

1. Study of fission products coming directly from the fissile target (similar to the PITRAP project).

2. Use of fission products to create radioactive beams and further synthesis of superheavy nuclei and/or study of nuclear reactions with exotic nuclei (in inverse geometry).

The relevance of research on exotic neutron-rich nuclei can be evidenced by a significant number of similar projects in leading research centers: HIRFL [Yang, 2013], SPIRAL2 [Dolegieviez, 2019], ISOLDE [Catherall, 2018].

8.6. STUDY OF NEUTRINOS AND OTHER RARE EVENTS

8.6.1. Evaluation of antineutrino spectra for reactor monitoring

Nuclear reactors are powerful sources of antineutrinos (order of 10^{21} per second per GW) emitted during β-decay of neutron-rich fission products. Such an intense antineutrino flux allows the use of relatively compact neutrino detectors. Monitoring of the neutrino flux from a reactor is one of the promising methods for controlling reactor operating modes and makes it possible to evaluate the accumulation of β-radioactive nuclei. Information about the spectra of antineutrinos emitted during β-decay can be obtained by spectrometry of accompanying electrons. At present, there are two ways to calculate the "reference" spectra of reactor antineutrinos. The first way is to model the total spectrum based on the known data on the yields of fission products, their decay chains, and spectra of β-electrons [Fallot, 2012]. The second technique involves direct measurements of the spectra of electrons emitted by a fissile target and subsequent conversion into antineutrino spectra using the "effective" charges of the fission products [F. von Feilitzsch, 1972]. The first approach requires precise information on the yields and spectra of β-electrons for a large (about 800) number of fission products and daughter isotopes, which is available not for all possible fission products. The second method also requires information on the yields (about 30) of fission products for the correct calculation of the effective charge of the resulting radioactive nuclei, but the number of these nuclei is significantly less.

The relevance of a comprehensive study of β-electron spectra and precise determination of the yields of fission products is also supported by the discovery of the so-called short-range anomaly, which manifests itself in a deficiency of observed electron neutrinos at short distances from the source compared to model representations [Mention, 2011]. At present, the existence of this effect has not been confirmed with sufficient significance. One of the possible explanations for this effect is the hypothesis of a sterile neutrino.

8.6.2. Direct investigation of reactor neutrinos

The high flux of antineutrinos from nuclear reactors makes it promising to study their properties using relatively compact detectors placed near the reactor core. The energy spectrum of reactor antineutrinos fully satisfies the condition of complete coherence of elastic scattering from the nucleus. JINR is well known for its reactor neutrino program, which includes such experiments as DANSS [Skrobova, 2023], GEMMA [Beda, 2013], nuGeN [Alekseev, 2022], etc. So, the creation of a new site for neutrino studies (Neutrino Study New Site — NSNS) at the advanced pulsed source at JINR is considered to be very promising and relevant.

The list of potential studies that can be conducted at NSNS includes:

- Development and tests of new types of neutrino detectors. JINR has extensive experience in developing various types of neutrino detectors. In particular, neutrino studies are carried out at the Dzhelepov Laboratory of Nuclear Problems (DLNP) [Skrobova, 2023; Beda, 2013; Alekseev, 2022]. DLNP specialists developing new neutrino detectors taking into account various approaches to identifying neutrino events. Such detectors can be used at the new neutrino research site at JINR for investigations in the area of neutrino detection techniques, as well as for the studies described above.
- Measurement of electron antineutrino spectrum. Obtaining of the spectrum at high energies and study of short-lived fission products. Some short-lived isotopes may have high-energy β-decay channels, which produce high-energy antineutrinos (which, in turn, can lead to the formation of high-energy antineutrinos). In fact, there is a lack of information on short-lived isotopes with decay times of less than a fraction of a second that are produced in nuclear fission. At the same time, high-energy decay can result in

significantly higher recoil energies in the process of coherent elastic neutrino-nuclear scattering (CEvNS) than is usually assumed. For example, the maximum elastic scattering of 10-MeV antineutrinos from germanium leads to a maximum recoil energy of about 500 eV. Measurements of such energies are possible only with a special unique HPGe detector. In contrast, a 20-MeV neutrino can generate a signal with an energy of 2-2.5 keV, which exceeds the energy threshold for almost all conventional large-size HPGe detectors. The number of detectable interactions of such high-energy neutrinos will increase dramatically. Detection of high-energy antineutrinos in coincidence with the pulse of the source may be the only way to obtain information about the existence of such high-energy β-transitions in nature. It could also be a critically important contribution to the experiments aimed at precision studies of neutrinos, such as RICOCHET [Augier, 2023], JUNO [JUNO, 2022] and others (with the participation of JINR).

- Search for high-mass axion-like particles [Krasznahorkay, 2019]. High-energy - transitions in fission products may be an indicator of the existence of some other exotic phenomena, such as a new high-mass scalar boson [Krasznahorkay, 2016; Feng, 2016; Cartlidge, 2016; Krasznahorkay, 2019]. Thus, the detection of unexpected gamma-radiation (the result of the decay of the boson-gamma conversion inside the detector) in coincidence with the reactor pulse may indicate its detection and will be a manifestation of such a widely sought new scalar boson. A search for sterile neutrinos is also possible.

CONCLUSION

The main challenges of modern civilization that humanity faces are related to population growth, concern for health and the environment, availability of clean water, food and energy, means of communication, storage and processing of large amounts of data, solving transport problems, ensuring comfort and safety of life, and much more. As the scale and relevance of these and other problems of society become more and more obvious, new challenges arise for researchers in condensed matter physics and soft matter research, which are posed to scientists from the JINR Member States by industry, economics, society and scientific community. The experimental base of the Joint Institute for Nuclear Research must be at the highest cutting-edge level to be able to respond to these challenges. Obviously, this will be facilitated by expanding the possibilities of using collective access to facilities at the advanced pulsed neutron source in the Frank Laboratory of Neutron Physics — the only pulsed high-flux neutron source in the JINR Member States.

Condensed matter physics encompasses investigations of fundamental properties of matter that arise from the interaction of large numbers of atoms and electrons. The complex nature of these interactions leads to structural features of different materials that are of interest in various areas of physics, chemistry, biology, geology and astronomy, as well as in almost all technical fields. A number of tasks in studying the structure and dynamics of condensed matter and soft matter in life sciences and in the field of Earth sciences, in the study of nanosystems, in materials science, including the study of functional and magnetic materials that are used in information systems, chemistry, energy, research and preservation of cultural heritage, ecology, etc., can be accomplished either only by neutron scattering methods or in combination with other methods complementary to neutron techniques [Belushkin et al., 2011; Lebedev et al., 2021].

The concentration at the advanced pulsed neutron source at JINR of beamline facilities operating in a wide range of wavelengths and momentum transfer, specialized for conducting research on solving a wide range of scientific and applied problems in the field of condensed matter, soft matter and nuclear physics, will provide unique opportunities for researchers from JINR Member States to solve the tasks set.

Interest in understanding the architecture of living systems and the processes occurring in them is growing every year. This information will help to synthesize new biomaterials and develop biotechnologies, control biosystems and organisms, create systems with specified characteristics and develop nature-like technologies. Here is just a small fraction of biological objects that have great potential for research and will receive increased attention in the coming decades:

- macromolecules (proteins, DNA, RNA, lipids);
- biological membranes and membrane proteins;
- disordered proteins;
- complex biocomplexes (enzymatic systems, protein-lipid, protein-nucleic acid complexes, etc.);
- signaling systems (receptors, photosystems);
- biohybrid materials;
- tissues;
- organelles and living cells, etc.

Their research requires the application and development of a number of neutron scattering methods, such as small-angle neutron scattering; diffraction of macromolecular crystals; reflectometry; neutron spectroscopy (inelastic scattering, inelastic spin echo, quasi-elastic scattering); neutron tomography and neutron activation analysis. Facilities for the implementation of these methods should undoubtedly be provided on the beamlines of the advanced neutron source in the Frank Laboratory of Neutron Physics of the Joint Institute for Nuclear Research. Neutron scattering methods will continue to be widely used in medicine and pharmaceuticals, for example, to study new advanced drugs. A separate major area of investigations at the new neutron source could be research in the field of radiobiology.

The implementation of the scientific program at the new neutron source at FLNP JINR in the field of soft condensed matter and nanosystems will make a major contribution to this area of scientific research and will have a significant impact on our understanding of these materials and their potential applications. The program will bring together a diverse community of researchers from a variety of fields, including materials science, chemistry, physics and biotechnology. With the support of the international scientific community of users and advances in neutron scattering techniques, the program will open new horizons in research in the field of materials science, contribute to the achievement of new breakthrough results and the development of new systems relevant for practical applications. One of the key factors here will be the high flux density at the beamline facilities of the new neutron source.

It is worth noting the observed trends in the fields of nanosystems and soft condensed matter, which can be expected to evolve over the next 20 years. First, there is an ongoing complication of the structure of systems towards complexity, heterogeneity and hierarchy. Second, the dynamics of the systems being studied and applied is becoming more complex. To obtain functional materials, new systems must respond to changing external parameters and, therefore, be in a nonequilibrium state. It is necessary to study nonequilibrium processes, rearrangements, dynamics in flows and hierarchical phenomena in time. At the same time, fundamental research will continue to be relevant (until a deep understanding of interactions and processes in nano- and meso-systems is achieved).

One of the major objectives for neutron scattering will be the detailed characterization of the structure and dynamics of materials on scales from ~1 nm to ~10 µm. The key neutron methods for these tasks are: small-angle scattering, reflectometry and neutron spectroscopy (inelastic scattering). The high neutron flux density on the sample will make it possible to obtain new information about the systems under study, which will open up opportunities for developing new advanced systems and gaining a fundamental understanding of interactions and nonequilibrium processes in complex structures.

To effectively address these challenges, high-luminosity small-angle and ultra-small-angle instruments with fast 2D position-sensitive detectors will be required. In the case of the small-angle instrument, among other things, it is also important that a wide q-range is covered. In the field of reflectometry, studies in the above-mentioned scientific areas will require the use of high-resolution low-background instruments in both geometries (vertical and horizontal scattering planes), as well as a medium- or low-resolution reflectometer with a horizontal plane for kinetic studies). There will also be a demand for additional instruments for efficient measurements of nonspecular scattering (characteristic structure sizes ~$10-10^5$ nm) and grazing-incidence small-angle neutron scattering (GISANS) on scales from several angstroms to hundreds of nanometers.

To study the relaxation and energy spectra of nanosystems and soft matter, it will be necessary to build a suite of neutron spectrometers, including spin-echo spectrometers.

It is also worth noting the continuous growth in the quality of computer simulation techniques. It can be expected that in 20 years the use of computer simulation in neutron research will become “not an advantage, but a requirement” at all stages of the experiment: preparation, measurement and processing of results. At present, the development of investigations of nanosystems and soft condensed matter is happening very quickly and is largely directed "in breadth" (a large number of hybrid materials, complex systems based on existing materials). This trend will continue, and in the future it is inevitable that "libraries" (possibly driven by artificial intelligence systems) will be created to automate the development of new materials. One of the main general tasks here is the continuous development of self-assembling structures to solve complex problems in medicine, technology, food industry, etc. This task requires the development of a comprehensive understanding of the structure and dynamics of the constituent components at all scales of size and time with high resolution. The solution of these problems will be greatly facilitated by the results obtained in studies using neutron scattering methods.

The study of magnetism in magnetic layers and thin films using polarized neutron reflectometry will undoubtedly attract increasing attention. With miniaturization, the effects will manifest themselves on smaller scales with an increasing role of interfaces and influence on the state of the electronic system. Understanding the role of new interaction mechanisms will not only lead to an understanding of the fundamental laws of low-dimensional magnetism, but will also make it possible to use them to design systems with specified magnetic and transport properties, for example, for magnetic memory devices, polarized electron injectors, etc. Another important and promising area of research is the study of systems with non-trivial magnetic ordering.

To study superconducting and magnetic multi-layer heterostructures at the advanced neutron source at JINR, it is necessary to have several reflectometers. The intense neutron flux at beamline instruments will make it possible to determine with high accuracy the correlation between the distribution of element concentrations and magnetization for a wide range of elements, and to study subtle magnetic phenomena associated with changes in magnetization <1%.

At the advanced neutron source at JINR, it is also necessary to build inelastic neutron scattering spectrometers covering a large Q-ω space and with a high neutron flux density on the sample, which will allow measurements of the four-dimensional scattering function $S(Q_x, Q_y, Q_z, \omega)$. In the foreseeable future, this technology for measuring inelastic neutron scattering (INS) will undoubtedly continue to improve and enjoy increasing demand from the user community.

Interest in inelastic neutron scattering research will remain high, among other things, due to three circumstances:

- The neutron has a magnetic moment. Magnetic inelastic neutron scattering is unrivaled compared to inelastic scattering at synchrotron sources.
- Magnetic INS allows obtaining detailed, spectroscopic information about the dynamics of the studied material at the microscopic level, which cannot be achieved by any other method.
- Synthesis of new materials containing magnetically active atoms yields many new interesting systems that require detailed study of magnetic dynamics both for the purpose of understanding their fundamental physical properties and for their use in applied problems.

Almost all neutron scattering techniques, such as diffractometry (including engineering and texture analysis), inelastic scattering, small-angle scattering, spin-echo, energy-dispersive radiography and tomography and others will be used to study all kinds of structural, functional, "smart", meta-, bio- and nanomaterials and finished products. Neutron scattering makes it possible to solve a huge number of problems in various areas of materials science and energy, including those that will be of interest in the coming decades: the study of new materials for promising power sources, such as K-ion batteries, multivalent metal-ion batteries, hydrogen fuel cells and materials for nuclear power plants and nuclear fusion energy sources, self-healing materials, high-entropy alloys, products obtained using additive technologies, metamaterials, etc. The study of "traditional" materials, such as steels, alloys, ceramics, subjected to various thermomechanical treatments, will continue to be highly relevant. There is also a wide range of geophysical applications for which the main neutron scattering methods are diffraction, radiography/tomography and small-angle scattering. Among the most exciting challenges are the study of anisotropic elastic properties of the lithosphere and their evolution over time, the study of the properties of rocks for the purpose of extracting hard-to-recover hydrocarbon reserves, and experiments that contribute to the development of physics of earthquake sources.

The construction of the advanced neutron source will also make it possible to increase the intensity of the neutron flux on microsamples for conducting experiments to study the atomic and magnetic structure and properties of functional materials under extreme external conditions (external high pressure and low temperature), which will be an important factor for carrying out these studies at a new, higher quality level. And, of course, the suite of beamline instruments at the new neutron source will necessarily include diffractometers for studying microsamples under extreme external conditions (high pressure, low temperatures, etc.).

Neutron radiography and tomography methods are of great interest to the scientific community from various fields of knowledge. Their use on a pulsed neutron source, including in combination with other methods, provides additional opportunities and has prospects for development, as well as an expansion of the areas of application from cultural heritage studies to engineering sciences and geophysics.

To perform experimental studies with high accuracy and optimal measurement time, it is necessary to increase the luminosity of beamline instruments. This can be realized on the new pulsed high-flux neutron source with optimization of all parameters of the source and beamline instruments: diffractometers, inelastic scattering spectrometers, reflectometers, small-angle scattering instruments, etc.

It is also necessary to highlight a number of tasks, the fulfillment of which is necessary for a more comprehensive realization of scientific research using neutron scattering methods:

- Provision should be made for the development of complex sample environment systems, for example, for generating a magnetic field on the sample, with the possibility of changing the sample temperature and its uni- or triaxial compression/extension with optimization of measurements with multi-detector configurations on spectrometers, fuel cells, systems that simultaneously produce ultra-high pressures and low temperatures, etc.
- The new neutron source requires several types of moderators. For example, cold neutrons are necessary for studies of magnetic structures of materials, while epithermal neutrons are needed for experiments on total scattering or deep inelastic neutron scattering.
- For some studies, it is necessary to consider the possibility of combining neutron scattering methods (for example, diffraction and small-angle scattering, diffraction and tomography/radiography, diffraction and inelastic neutron scattering) on one beamline instrument.
- Since the duration of some experiments is fixed and can be quite significant (tens of hours), such as *in situ* studies with heating/cooling, cycling of mechanical load or magnetic field at a constant rate, studies of kinetics of long-term processes, it will be useful to have some "duplication" of the functions of neutron instruments, so that some experiments can be carried out on another instrument while the "main" one is busy. In some cases, it is advisable to provide for the combined use of several methods complementary to neutrons (X-ray scattering and tomography, nuclear magnetic resonance, electron and cryo-

electron microscopy, molecular modeling, dynamic light scattering, acoustic emission monitoring, positron annihilation spectroscopy, etc.). It is necessary to provide the possibility and space for organizing such experiments at beamline instruments.

- It is obvious that improvement of data acquisition and processing techniques will be required. It is also necessary to provide for computing power for modeling complex multicomponent systems and to develop systems with artificial intelligence.
- It is necessary to create a laboratory for the production of deuterated compounds and deuteration and crystallization of biological objects.
- It is necessary to develop possibilities for time-resolved experiments (triggering processes with light, chemical signaling molecules, ionic strength, pressure, temperature, etc.).

Neutron activation analysis has found wide application as a powerful analytical method in ecological, biological research and archeology. There is no doubt that due to its high sensitivity and extensive experience in its use, this method will be in great demand among the scientific community at the advanced neutron source at FLNP.

The neutron is a unique object of research in the field of fundamental interactions and cosmology. Examples of this type of investigations are experiments to refine the neutron lifetime, search for the electric dipole moment of the neutron, search for neutron-antineutron oscillations, measurement of the gravitational mass of the neutron, study of fundamental symmetries in processes involving neutrons, search for new types of interactions. All these studies are aimed in one way or another at searching for the so-called "new physics" — the experimental discovery of phenomena beyond the Standard Model (SM), which may provide a clue to solving the questions facing by theorists today: why are there so many free parameters in the SM, why does matter dominate over antimatter, what are "dark matter" and "dark energy"? Along with it, neutron experiments belong to the class of studies at the "intensity limit" — high-precision experiments that use highly sensitive detectors registering subtlest effects associated, for example, with the exchange of heavy virtual particles. They complement studies at the "energy limit" at new high-energy accelerators that can produce heavier particles than those previously observed. Undoubtedly, an important area of research at the new neutron source will be investigations in the field of fission physics, neutron optics, the study of neutron-rich nuclei, etc. Since its emergence, neutron nuclear physics has demonstrated its effectiveness, becoming the basis of nuclear power engineering and a tool for studying the nuclear structure and properties of fundamental interactions. The challenges facing this area of research at the beginning of the 21st century are in many ways still relevant today [Аксёнов, 2000]. They echo the questions that were formulated by the international scientific community when discussing the prospects for the development of nuclear physics [NuPECC, 2024].

At FLNP there has always been a wide range of research directions in the field of nuclear physics. Its scientific program was always open to new topics, which made it possible to perform pioneering experiments on the detection of ultracold neutrons (UCNs) [Shapiro, 1968], which later turned out to be a very effective tool for studying fundamental interactions. The last decade has shown that investigations with UCN are extremely promising. Ultracold neutrons began to be used to study quantum systems and search for "new physics" beyond the Standard Model (search for new types of interactions, mirror worlds, etc.). The new intense UCN source at the advanced neutron source at FLNP JINR will bring these studies to a new level.

Neutrino physics may also become a separate promising direction of research at the new neutron source at FLNP.

Thus, investigations in the interests of the JINR Member States in the proposed scientific directions, which, as preliminary analysis shows, will not lose their relevance over the next 20 years, can be carried out at the projected new advanced pulsed research neutron source with cutting-edge beamline instruments at FLNP JINR, with due account of the detailed elaboration of methods, components of instruments and their optimization in combination with the parameters of the source, as well as the development of auxiliary laboratory and computing facilities.

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