Joint Institute for Nuclear Research
Frank Laboratory of Neutron Physics

Department of Neutron Investigations of Condensed Matter

Proposals for Development of a Suite of Instruments *for Condensed Matter Research* at the IBR-2 Reactor

DUBNA 2020

2021 2022 2023 2024 2025

CONTENTS

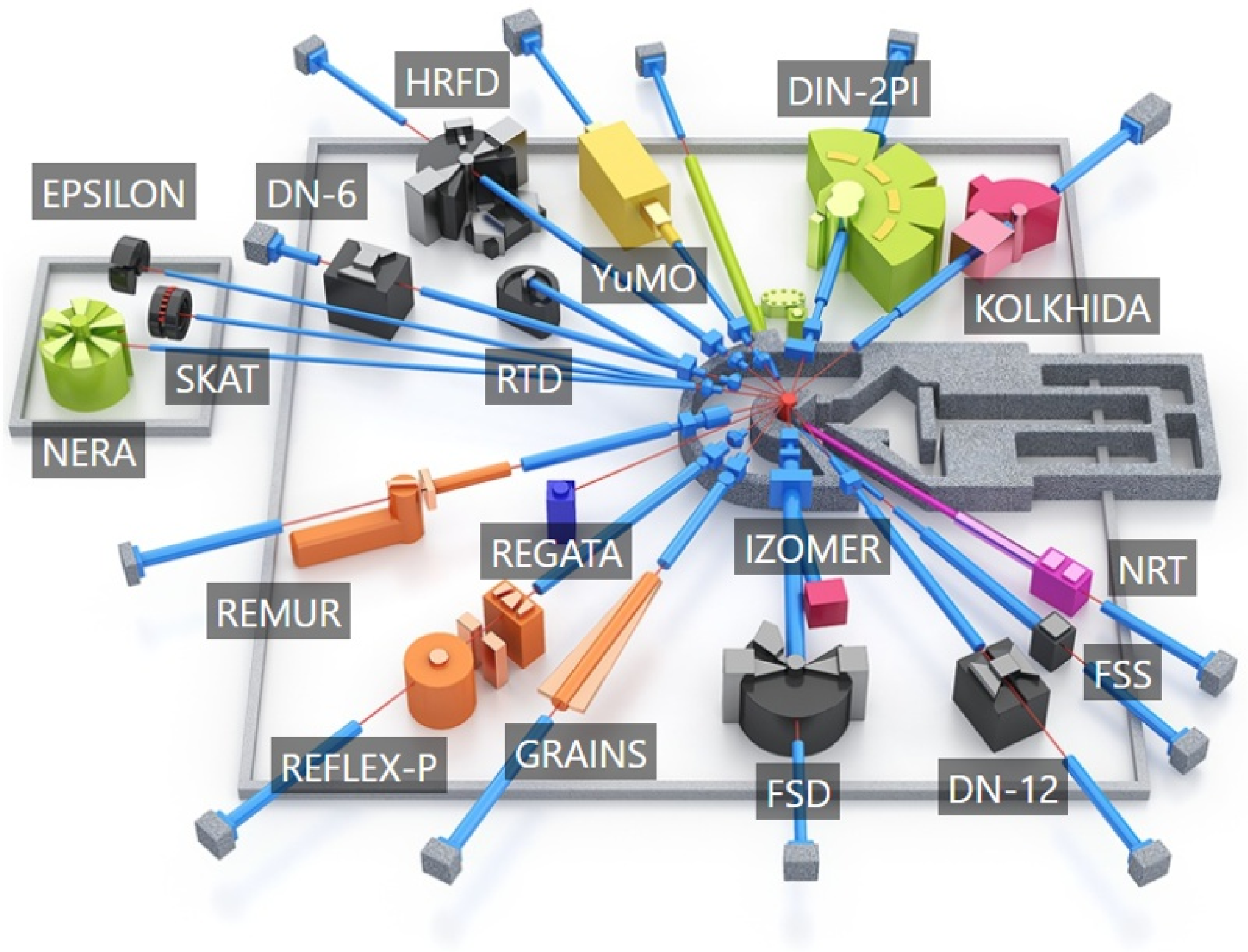
INTRODUCTION

The high-flux pulsed IBR-2 reactor was commissioned in 1984. The IBR-2 service life expired at the end of 2006 and in 2007-2010 a large-scale modernization was carried out involving the replacement of practically all reactor systems. After successful physical (December, 2010) and power (July-October, 2011) startup of the reactor, in 2012, the IBR-2 operation for physics experiments was resumed at a rated power of 2 MW. In general, the expected service life of the upgraded IBR-2 reactor is estimated to be around 20-25 years (taking into account the scheduled maintenance replacement of individual systems), which offers long-term prospects for conducting neutron investigations at the facility. The reactor technical parameters are presented in Table 1. In addition, since the autumn of 2012 the first cold pelletized moderator has started its operation providing an increase of up to 13 times in the flux density of cold neutrons for IBR-2 beamlines 7, 8, 10. In 2020, it is planned to install one more cold moderator for beamlines 4-6, and in the coming years, to develop and construct a cold moderator for IBR-2 beamline 2.

Technical parameters of the IBR-2 reactor before and after modernization

IBR-2 parameter	Before modernization	After modernization
Pulsed thermal neutron flux, $n/cm^2/s$	$5 \cdot 10^{15}$	$5 \cdot 10^{15}$
Average power, MW	2	2
Power in pulse, MW	1850	1850
Fuel	PuO_2	PuO_2
Number of fuel assemblies	78	69
Maximum burnup, %	6.5	9
Pulse repetition rate, Hz	5, 25	5, 10
Neutron pulse half-width: Fast neutrons, µs Thermal neutrons, µs	 215 320	 240 340

The IBR-2 reactor is equipped with a unique suite of neutron spectrometers that makes it possible to carry out a wide range of interdisciplinary investigations in the field of condensed matter physics, materials science, chemistry, biology, geophysics, pharmacology, medicine, nuclear physics, ecology, etc. At present, at the IBR-2 reactor, fifteen instruments for condensed matter research are in service or in the final stage of development and construction, including 8 diffractometers, 3 reflectometers, 1 small-angle neutron scattering spectrometer, 2 inelastic neutron scattering spectrometers, and 1 spectrometer for neutron radiography and tomography.



Layout of instruments in the IBR-2 experimental hall.

The existing prevalence of diffractometers has to some extent historical reasons, as well as is due to a number of objective factors – development of a new unique technique of Fourier diffractometry, which makes it possible to perform diffraction experiments with a very high resolution (up to $\Delta d/d \sim 0.1\text{-}0.2$ %), and a broad potential for application of diffraction techniques in interdisciplinary scientific investigations ranging from condensed matter physics to biophysics, geophysics and medicine.

The User Program is efficiently realized for a suite of IBR-2 spectrometers. Calls for proposals are issued twice a year. The proposals are peer-reviewed and rated, and beam time for experiments is allocated on the basis of the reviews by Expert Committees. A total of more than 200 proposals are submitted annually from 15-18 countries, with the majority of them being from external organizations.

Among recently constructed instruments of special note are the DN-6 diffractometer for investigations of micro-samples, which allows experiments with record-breaking small volumes of studied materials of the order of 0.01 mm^3 under extreme conditions (at pressures of up to 50 GPa and temperatures in the range of 4 - 300 K); multifunctional reflectometer GRAINS with a horizontal sample plane, which opens up new possibilities for investigations of liquid and soft interfaces; spectrometer of neutron radiography and tomography, which makes it possible to perform nondestructive testing and studies of the internal structure of materials and products with a spatial resolution at a level of less than 200 µm. At beamline 13, experiments were started with the basic configuration of the FSS correlation diffractometer transported from GKSS (Germany). To improve the parameters of the diffractometer, a mirror curved neutron guide was replaced.

It should be noted that at the present time the situation with small-angle scattering instruments at IBR-2 is particularly acute. About 30% of the total number of submitted proposals for experimental time is for one existing SANS instrument and the available beam time is significantly less than required. To improve the situation, work is currently underway to construct a second small-angle instrument and a spin-echo small-angle spectrometer. In addition, it is planned to develop and construct two new inelastic scattering spectrometers, which will replace the existing NERA and DIN-2PI spectrometers and will significantly expand the possibilities for research of atomic and magnetic dynamics of materials.

The availability of a neutron source with a long service life and world-class parameters equipped with a cold moderator, the intensive development of neutron scattering methods and competing synchrotron radiation scattering techniques as well as the increasing demand in using neutron scattering for interdisciplinary investigations call for further development of the suite of IBR-2 spectrometers with due consideration of these factors aimed at expanding experimental possibilities and improving technical parameters.

In addition, due to the fact that the IBR-2 reactor will reach the end of its service life during the next 12-15 years, work is currently underway on the project for the development and construction of a new pulsed neutron source with neutron fluxes approximately an order of magnitude greater than those available at IBR-2, which is expected to be commissioned in 2032-2035. An important task is to develop the concept of a suite of advanced neutron spectrometers for equipping the new source, the prototypes of which can be the IBR-2 instruments.

This book contains proposals for the development and modernization of the available spectrometers and for the design and construction of new instruments at the IBR-2 reactor. It can be considered as a "road map" for the development of the suite of IBR-2 spectrometers in the long-term perspective until 2025.

1. LIST OF PROJECTS

№	INSTRUMENT	PROJECT TITLE
		DEVELOPMENT OF OPERATING INSTRUMENTS
1.	HRFD	HRFD - High-Resolution Fourier Diffractometer
2.	FSD	FSD - Fourier Stress Diffractometer
3.	FSS	FSS - Fourier Diffractometer
4.	RTD	RTD - Neutron Diffractometer (Real-Time Diffraction)
5.	DN-6	DN-6 - Neutron Diffractometer for Ultrahigh-Pressure Research
6.	DN-12	DN-12 - Neutron Diffractometer for Investigations of Microsamples at High Pressures
7.	EPSILON-MDS	EPSILON-MDS - Strain/Stress Diffractometer
8.	SKAT	SKAT - Texture Diffractometer (project 1) SKAT - Texture Diffractometer (project 2)
9.	YuMO	YuMO - Small-Angle Neutron Scattering Instrument
10.	GRAINS	GRAINS - Neutron Reflectometer with Horizontal Sample Plane
11.	REFLEX	REFLEX - Reflectometer with Polarized Neutrons
12.	REMUR	REMUR - Reflectometer with Polarized Neutrons
13.	NRT	NRT - Neutron Radiography and Tomography Station
		NEW INSTRUMENTS
14.	INS_NEW	New Inverse-Geometry Inelastic Neutron Scattering Spectrometer
15.	SANSARA	SANSARA - Small-Angle Neutron Scattering Instrument
16.	NRT_COLD	Neutron Radiography and Tomography Station with Cold Neutrons

2. PROJECTS ON DEVELOPMENT OF OPERATING INSTRUMENTS

HRFD - High-Resolution Fourier Diffractometer

Leaders: A.M. Balagurov, I.A. Bobrikov

Main participants: S.V. Sumnikov, V.G. Simkin, R.N. Vasin, T.N. Vershinina

Collaborating organizations: M.V. Lomonosov Moscow State University, National Research Technological University “MISiS”, St. Petersburg State University, Saratov State University, Institute of Physics and Technology of the Mongolian Academy of Sciences, Institutes of the Russian Academy of Sciences, Belarusian State University, Tsin Hua National University, China Institute of Atomic Energy.

1. Abstract

The High-Resolution Fourier Diffractometer (HRFD) constructed within the framework of the collaboration between FLNP JINR (Dubna), PNPI (Gatchina) and VTT (Espoo, Finland) has been in continuous operation at IBR-2 since 1995. Its initial design, principle of operation and rated parameters are described in detail in [1]. Examples of numerous studies carried out with HRFD as well as some ideas for possible development of the diffractometer are presented in [2, 3]. Over the past period, some components of the diffractometer including the neutron guide and Fourier chopper have been replaced, as well as there has been a complete replacement of data acquisition and experiment control electronics. In addition, the extensive experience gained in operating HRFD allowed us to reveal some technical problems in its operation and find ways to rectify them.

2. Scientific program, topicality and comparison with the world level

Over the past years, wide experience has been gained in operating HRFD and a scope of problems that can be studied most effectively using the diffractometer has been identified. The HRFD is mainly intended for precision structural analysis of polycrystalline substances with an average unit cell volume of up to ~500 Å^3. Among the most remarkable studies performed with HRFD are investigations of mercury-based high-temperature superconductors with different amounts of oxygen or fluorine [4, 5], origin of a giant isotope effect in manganites [6, 7], magnetic effects in ruthenates [8, 9], structural anomalies in cobaltites [10, 11]. The HRFD is also used to perform analysis of single crystals when its unique d_{hkl} resolution is required, e.g., to study phase separation in $La_2CuO_{4+\delta}$ crystals due to low-temperature diffusion of hyperstoichiometric oxygen [12].

The high resolution of HRFD enables us to reliably determine microstrains and characteristic sizes of coherent blocks of polycrystals under study using the d_{hkl} dependence of diffraction peak width (Williamson-Hall analysis). The practice of studying microstructural effects using HRFD has shown that its resolution allows microstrains in crystallites to be determined at a level of $\varepsilon \approx 0.0008$ and higher, and the average sizes of coherently scattering domains – at a level of $L_{coh} \approx 2500$ Å and smaller [13].

Starting from 2012, the HRFD has been used for experiments to study structural processes in electrodes of Li-ion batteries during charge-discharge processes [14]. The possibility to switch between two different modes of operation (high-intensity and high-resolution) without changing the experiment geometry has significantly added to the success of these investigations. The high-intensity mode was used for acquiring data in real time with reasonable statistics collection time (1-10 min). The high-resolution mode was applied to obtain data on batteries in a steady state, which allowed us to reliably identify emerging structural phases. Since 2016, this approach has been successfully applied to the study of phase transitions in functional iron-based alloys with giant magnetostriction [15, 16]: upon real-time heating or cooling, phase transitions were monitored in the high-intensity mode, while the high-resolution mode was used to determine the phase composition of samples in a steady state at a given temperature and to study the features of their microstructural state.

The greater part of experiments conducted with HRFD are carried out in cooperation with Russian and foreign scientific organizations for condensed matter, crystallography and materials science research. Thus, it can be stated that HRFD is a successfully operating spectrometer with a well-established research program and a broad community of users.

3. Scientific and methodological groundwork laid in FLNP JINR

FLNP JINR is currently the only research center in the world with operating neutron Fourier diffractometers. The main specialists and engineers specializing in this technique work in the Frank Laboratory of Neutron Physics. Over the past time, some components of the diffractometer including the neutron guide, position-sensitive detector and Fourier chopper have been replaced, as well as there has been a complete replacement of data acquisition and experiment control electronics. In addition, the vast experience gained during the operation of HRFD allowed us to identify some technical problems in it and propose algorithms for their elimination.

4. Current status of the instrument and proposals for its modernization

The HRFD diffractometer is operated with the application of the correlation method of data collection using a fast Fourier chopper and reverse time-of-flight electronics. The layout of the diffractometer is shown in Fig. 1.

At present, the design of HRFD allows one to obtain high-resolution diffraction patterns using back-scattering detectors ($2\theta = 152°$) in the d_{hkl} range of 0.6 - 4 Å and a detector at $2\theta = 90°$ in the d_{hkl} range of 0.8 - 5 Å. In the low-resolution mode ($\Delta d/d \approx 0.01 - 0.02$) the same detectors provide spectra in the range of up to 4.5 and 6.0 Å, respectively. And finally, the position-sensitive detector (2D PSD) placed at $2\theta = 30°$ makes it possible to observe diffraction up to $d_{max} = 16$ Å.

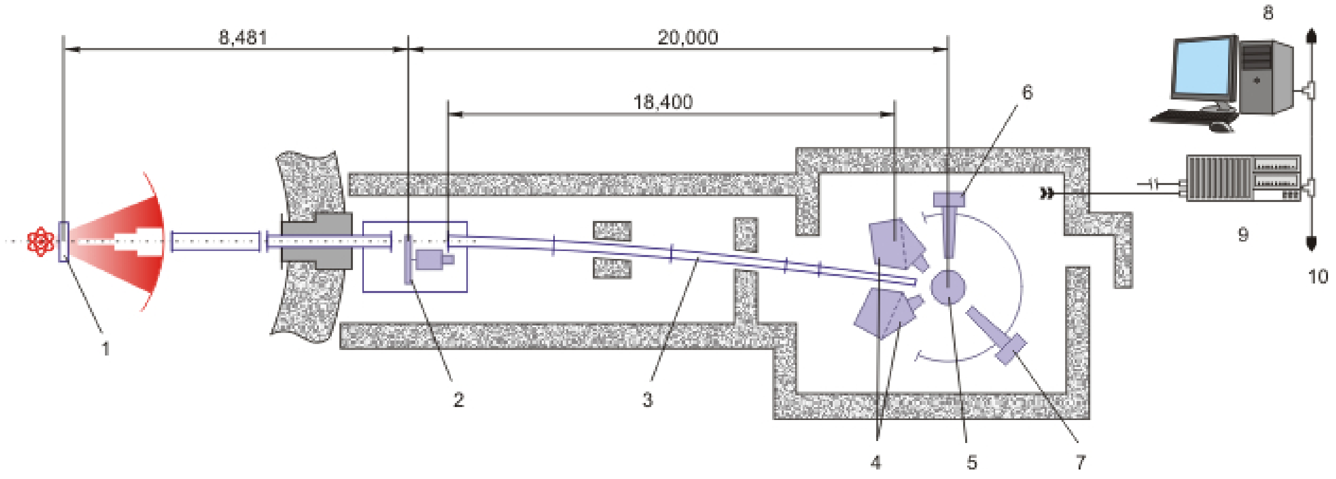


Fig. 1. *Layout of HRFD. The fast Fourier chopper (2) is located immediately behind the wall of the ring corridor. The neutron beam at the sample position is formed by a curved focusing neutron guide. (3). The main detectors (4, 6) and PSD (7) operating in the low resolution mode are placed around the sample position (5). Signals from the detectors are sent to correlation electronics (9). The flight path lengths are given in millimeters.*

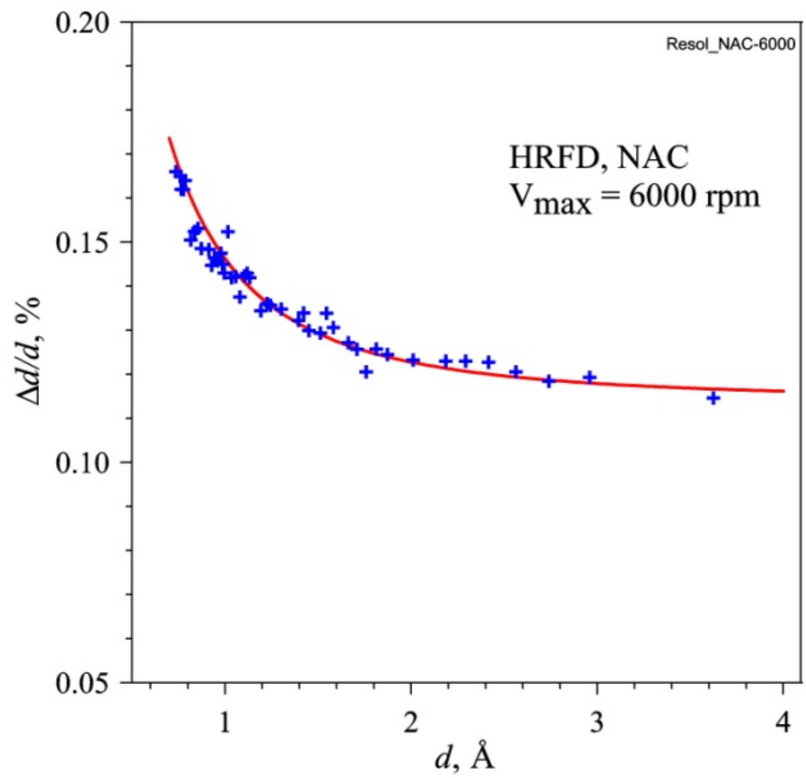


Fig. 2*. The HRFD resolution function measured with a standard sample of $Na_2Al_2Ca_3F_{14}$ (NAC) at the maximum rotational speed of the chopper of 6000 rpm. The figure shows the experimental points and the calculated curve.*

The main methodological feature of HRFD is exceptionally high resolution ($\Delta d/d \approx 0.001$) at a rather short flight path from the chopper to the sample position ($L = 20$ m). The HRFD resolution is determined by the maximum rotational speed of the fast Fourier chopper, poorly depends on interplanar spacing and enhances with increasing d_{hkl} (Fig. 2).

Main parameters of HRFD

Direct neutron guide	
- length, m	3.5
Curved neutron guide	mirror, Ni/Ti coating
- length, m	18.8
- radius of curvature, m	2120
Moderator-to-sample distance, m	29.65
Chopper-to-sample distance, m	21.14
Fourier chopper (disk)	high-strength Al alloy
- outer diameter, mm	540
- slit width, mm	0.7
- slit number	1024
- maximum rotational speed, rpm.	6000
- maximum beam modulation frequency, kHz	100
Pulse width for thermal neutrons:	
- low-resolution mode, μs	340
- high-resolution mode, μs	9.8
Neutron flux at sample position:	
- without Fourier chopper, $n/cm^2 \cdot s^{-1}$	$1 \cdot 10^7$
- with Fourier chopper, $n/cm^2 \cdot s^{-1}$	$2.5 \cdot 10^6$
Wavelength range, Å	0.9 ÷ 8
Detectors:	
- 2θ=152° (back scattering)	^{6}Li, time focusing
- 2θ=90°	^{6}Li, time focusing
- 2θ=30°	2D PSD, ^{3}He
Detector resolution $\Delta d/d$ (d = 2 Å):	
- 2θ=152° (back scattering)	$1.2 \cdot 10^{-3}$
- 2θ=90°	$3.0 \cdot 10^{-3}$
Detector resolution $\Delta d/d$ (d=2 Å) in high-intensity mode:	
- 2θ=152° (back scattering)	
- 2θ=90°	$1.5 \cdot 10^{-2}$
- 2θ=30°	$2.5 \cdot 10^{-2}$
	$5 \cdot 10^{-2}$
d_{hkl}-range, Å	
- 2θ=152° (back scattering)	0.6 – 4
- 2θ=90°	0.8 – 5
d_{hkl}-range in high-intensity mode, Å	
- 2θ=152° (back scattering)	0.6 – 6
- 2θ=90°	0.8 – 7
- 2θ=30°	1.5 - 15

The modernization of HRFD should be aimed at enhancing the luminosity of the diffractometer, reducing the background level, developing sample environment equipment, and improving Fourier analysis parameters. According to the estimates this will make it possible to double the number of conducted experiments, noticeably increase the precision of the obtained structural information, and essentially enhance the diffractometer capabilities for carrying out experiments in a wide range of temperatures and other external conditions.

4.1. Operation of HRFD at a cold neutron source

The HRFD is located at IBR-2 beamline 5 where it is planned to install a cold moderator. Test experiments with a cold methane moderator conducted in 1999 showed that it offers more favourable working conditions than a regular water moderator. In addition, it was found that the moderator temperature in the range of 60-100 K is optimal for analysis of relatively complex structures (with a unit cell volume of over 200 $Å^3$). This makes it possible to detect diffraction peaks at large d_{hkl}, which is often a principal factor in the study of magnetic structures.

A specific feature of HRFD is the operation in the scanning mode by sweeping the chopper rotation frequency (frequency sweep). The HRFD operation experience has shown that sweeps with a duration of 1 or 2 hours are optimal and the number of them is usually from 1 to 10, i.e., the experiment lasts from 1 to 100 hours. This means that the operation of HRFD on a cold source will be possible only if the time of stable operation of the source is no less than four days.

4.2. Enhancement of diffractometer luminosity and reduction of background level

At present, the total solid angle of the main backscattering detectors is 0.16 sr, and in this respect HRFD is far inferior to state-of-the-art high-resolution diffractometers with their detector solid angles being, as a rule, about 2 sr and larger. The detecting element is Li-glass-based scintillators with a high sensitivity to γ-background.

These disadvantages can be avoided by using ZnS(Ag)-based scintillators and combined electronic-geometric focusing. Figure 3 shows a schematic drawing of a large-area backscattering detector consisting of individual scintillator plates assembled into 8 rings with approximately the same geometrical contribution to the resolution function. The effective solid angle of the detector is close to 1.5 sr, which will provide a 10-fold gain in the luminosity of the diffractometer. The change-over to ZnS-scintillators will allow the γ-background level to be drastically reduced.

By the middle of 2020, the first section (out of 12) of the large-area detector is expected to be manufactured, and by the end of 2020, it will be tested directly at HRFD. At the estimated rate of manufacturing and commissioning of the detector sections (~ 4-5 sections per year), its commissioning is expected by the end of 2023.

4.3. Sample environment system

At present, HRFD is equipped with a helium refrigerator ($T \geq 4.0$ K) and a high-temperature vacuum furnace ($T \leq 1200$°C). Recently, the number of experimental proposals has significantly increased, which involve careful studies of structural and magnetic phase transitions in the temperature range close to room temperature or in a wide temperature range from helium temperatures to the boiling point of water and above, as well as with the application of a magnetic field. The proportion of proposals without the application of external conditions is only 20%. To expand the range of experiments conducted continuously in a wide temperature range, it is necessary to purchase a refrigerator with $T_{min} \leq 2$ K and sample heating option of up to 500°C. To conduct research in a magnetic field and low temperatures, it is planned to manufacture an electromagnet (5 T) with superconductors with its own system for cooling and heating the sample ($4\ K \leq T_{min} \leq 500\ K$). For precise positioning of the new equipment at the sample place, it is planned to purchase a multifunctional motorized platform.

4.4. Modernization of Fourier chopper

The available Fourier chopper was produced in Hungary in 2016. The chopper disk is made of Al-based alloy and has 1024 slits filled with Gd_2O_3. The maximum chopper rotational speed is V_{max} = 6000 rpm. A magnetic rotational speed sensor is fixed on the motor shaft. A stator with a similar set of slits non-transparent to thermal neutrons is located near the disk. Due to the poor stability of magnetic sensors, auxiliary sensors and a digital control device under radiation, they need to be replaced frequently, which negatively affects the stability of HRFD. One more disadvantage of the available Fourier chopper is an indirect method of acquiring information about the position of the disk relative to the stator. To overcome this disadvantage is possible with the help of a design developed by G.D.Bokuchava and realized by the Airbus company, in which the disk and the stator of the chopper have real slits, which allows one to control the parameters of rotation and signals of the "open-closed" type using conventional optical sensors. At present, a chopper of this type is being manufactured and planned to be installed at FSD. If this project is successfully implemented, it is planned to manufacture a similar chopper for HRFD.

Since the new reactor currently being designed will have generally similar characteristics to those of the IBR-2 reactor, with minor changes in the configuration of the neutron guide and the location of the chopper, the upgraded HRFD diffractometer can be used at the new neutron source.

5. Expected scientific results, comparison with the world level

Since the luminosity of the HRFD diffractometer will be significantly enhanced after its modernization, taking into account the already existing level of resolution, the HRFD will be one of the best high-resolution diffractometers in the world, not inferior, for example, to the POWGEN diffractometer (solid-state detector area – 12 m^2. SNS, USA). So, the experiment time at a medium resolution ($\Delta d/d$ = 0.01) with the preservation of data statistics will be decreased by more than a factor of 10, and at a high resolution by a factor of 5 ($\Delta d/d$ = 0.001). The modernization of the diffractometer will make it possible to efficiently conduct high-resolution experiments with a small amount of sample (less than 1 g), which is currently almost impossible; obtain unique characteristics with high accuracy in determining the crystal structure parameters of substances and study processes with a time resolution of hundredths of a second. The increase in the covered range of interplanar spacing due to the operation of HRFD at a cold moderator will allow us to effectively study complex magnetic structures, as well as organic crystals. The use of a cryofurnace will make it possible to efficiently study phase transitions not only in a large temperature range, but also in the region of room temperatures. The application of an electromagnet with sample temperature control will significantly expand the range of problems in crystal physics, which can be studied using high-resolution neutron diffraction. Information on the structure, magnetic structure, and microstructure at different temperatures and/or magnetic fields is of great significance in the study of various phenomena and effects in crystals.

6. Requested resources, costs and time frames of instrument modernization

The units to be upgraded are the backscattering detector, cryofurnace, cryomagnet, precision motorized platform and Fourier chopper. Their costs are given in **Table 1 (Section 4)**. Work on the project is to be carried out by the specialists of the HRFD Group of the Diffraction Sector with the assistance of the personnel of the Spectrometers' Complex Department.

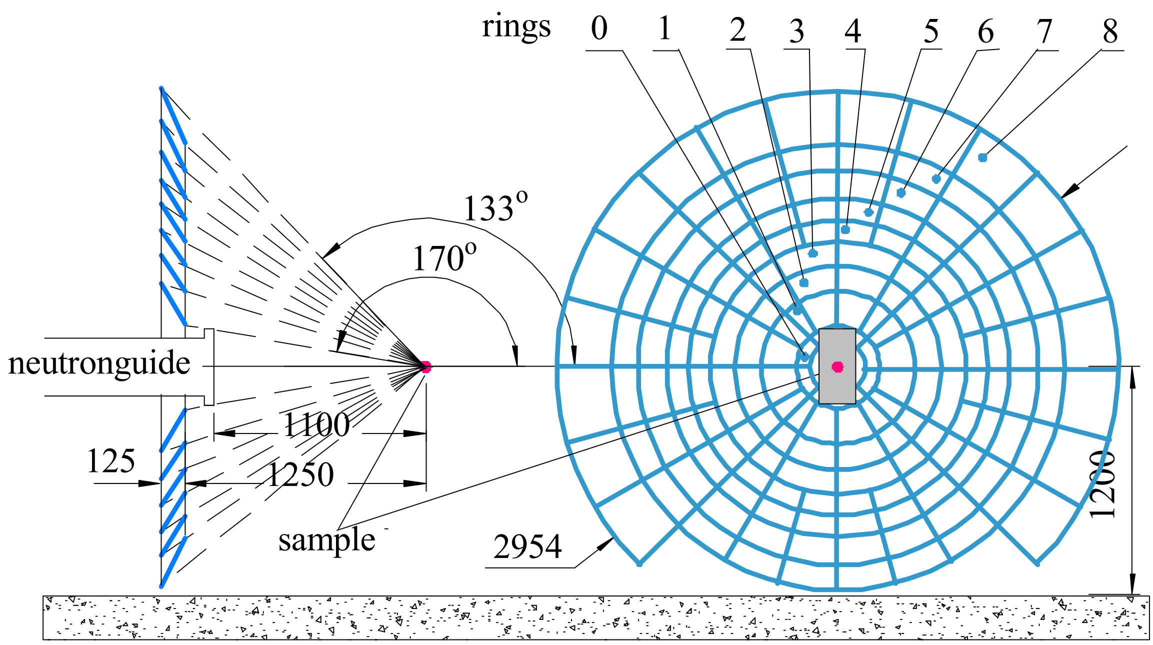


Fig. 3. *Schematic drawing of a wide-aperture detector at large scattering angles. Side view (at the left) and view from the sample side (at the right). The detector consists of individual plates (a total of about 200 elements) of ZnS(Ag)/^{6}LiF scintillator, each of which meets the time focusing conditions. The plates are assembled into 8 rings with an equal geometrical contribution to the resolution function, which varies within (3.7 – 8.8)·10^{-4}. The detector area is about 13.5 m^2; the effective solid angle is 1.5 sr.*

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FSD - Fourier Stress Diffractometer

Leader: G.D. Bokuchava

Main participants: I.V. Papushkin, A.A. Kruglov, T.N. Vershinina

Collaborating organizations: Studies conducted with the FSD diffractometer are of interest both to various research organizations and universities in Russia (NIKIET, Gidropress, VNIINM, IMET RAS, BelSU) and abroad (BAM, CENIM, IE BAS, AGH University), as well as such organizations as the IAEA, ROSATOM and a number of industrial enterprises (Tulamashzavod, JSC “KBP”, Gazprom, etc.).

1. Abstract

The special-purpose Fourier diffractometer FSD is located at beamline 11a of the IBR-2 reactor in FLNP JINR and intended for measurements of residual stresses in bulk products and novel advanced materials. Regular experiments to measure residual stresses in various industrial products and to study elastic properties of advanced materials, as well as methodological investigations have been conducted with FSD since 2001.

To further upgrade the FSD diffractometer, extend its possibilities and improve its technical characteristics, it is necessary to complete the construction of the detector system and carry out the modernization of a number of its units.

2. Scientific program, topicality and comparison with the world level

The investigation of internal mechanical stresses in materials is of fundamental as well as of applied importance. The neutron diffraction technique for stress investigations came into use in the mid-1980s and since then it has become widely applied due to a number of significant advantages over conventional methods. The most important advantage is that neutrons can penetrate matter to a depth of 2-3 cm in steels and up to 10 cm in aluminium. The advantages of neutron diffraction are so great that in recent years, diffractometers for internal stress investigations have been built in almost all advanced neutron centers in the world.

The FSD belongs to a class of high-resolution diffractometers. The high-resolution neutron diffractometer is a complex and expensive instrument, that is why precision neutron diffraction experiments with a very high resolution (at a level of $\Delta d/d \approx 0.002$ or higher) are conducted only in a few most advanced neutron laboratories in the world. At present, JINR is the only scientific center in Russia where regular world-class neutron diffraction investigations of residual stresses are conducted. The technical characteristics and description of FSD are given in [1, 2]. During the period of the FSD operation, the real potential of the diffractometer in solving various problems has been revealed and the main directions of research have been identified and formed. They are connected with the achieved resolution and luminosity as well as the accessible range of interplanar spacings d_{hkl}.

The greater part of the studies are concerned with the determination of residual stresses in industrial products and structures. The most common source of stresses is various technological processes. These studies are of interest for manufacturers from the viewpoint of creating optimum properties of materials and optimization of technological production processes. The results of these studies help to create optimum residual stress states in different cross sections of the component part and consequently, improve its performance characteristics and service life [3, 4].

Another important direction of research activity is investigations of residual stresses and mechanical properties of advanced materials, such as composite or gradient materials as well as different steel grades. Within the framework of these tasks, the coexistence of different phases in one material and their combined effect on the elastic properties and residual stresses in the material are studied. These investigations are important for the creation of materials with tailored physical, chemical and elastic properties. The results of these studies make it possible to create novel materials with targeted properties and behaviour. Typical examples are studies of residual stresses and elastic properties in steels, advanced composite and gradient materials [5, 6].

3. Scientific and methodological groundwork laid in FLNP JINR

First studies on the determination of residual stresses in bulk products and novel materials started in FLNP JINR in 1993 on the basis of the neutron high-resolution Fourier diffractometer at beamline 5 of the IBR-2 reactor. For this purpose, a new method for analysis of internal mechanical stresses in materials using neutron correlation Fourier diffraction technique on a long-pulse neutron source (IBR-2) has been developed, the necessary equipment has been designed and constructed, test experiments to study stresses in specific materials have been conducted in order to trial the developed technique and determine the potential scope of studies.

A few years later the accumulated operating experience allowed us to start the implementation of a new project aimed at constructing a special-purpose Fourier diffractometer FSD at beamline 11a of the IBR-2 reactor for internal stress studies, which started to operate in 2001. During the period of its operation the FSD diffractometer was used to carry out numerous experiments characterizing the main directions of research in this area: studies of mechanical properties of materials under different loading modes, of various welded joints, structural components of various industrial products, novel advanced materials, gradient structures and composites. The results of these experiments have demonstrated a high efficiency of the Fourier diffractometer in addressing the challenges.

4. Current status of the instrument and proposals for its modernization

4.1. Current status and main units of FSD

The FSD diffractometer is located at beamline 11a of the IBR-2 reactor at FLNP JINR. The instrument was developed taking into account the world experience in conducting internal mechanical stress studies in bulk samples and products [7]. The experience of the Petersburg Nuclear Physics Institute, Gatchina (mini-SFINKS diffractometer [8]), GKSS, Geesthacht (FSS diffractometer [9]), and the Frank Laboratory of Neutron Physics, JINR, Dubna (HRFD diffractometer [10]) in the application of the correlation Fourier technique in neutron diffraction was taken into account. All three above-listed instruments are TOF diffractometers using a fast Fourier chopper for primary beam intensity modulation and the RTOF method [11] for data acquisition.

Main parameters of FSD

Curved neutron guide	mirror, Ni-coated
- length, m	19
- radius of curvature, m	2864.8
Straight neutron guide	mirror, Ni-coated
- length, m	5.01
Moderator-to-sample distance, m	28.14
Chopper-to-sample distance, m	5.55
Fourier chopper (disk)	High-strength Al-based alloy
- outer diameter, mm	540
- slit width, mm	0.7
- number of slits	1024
- maximum rotational speed, rpm	6000
- maximum beam modulation frequency, kHz	100
Thermal neutron pulse width:	
- in low-resolution mode, μs	320
- in high-resolution mode, μs	9.8
Flux at sample position:	
- without Fourier chopper, $n/cm^2 \cdot s^{-1}$	$1.8 \cdot 10^6$
- with Fourier chopper, $n/cm^2 \cdot s^{-1}$	$3.7 \cdot 10^5$
Wavelength range, Å	0.9 ÷ 8
Detectors:	
- 2θ=140° (backscattering)	^6Li, with time focusing
- 2θ=±90°	ZnS, with combined electronic and geometric focusing
Detector resolution Δ*d*/*d* (*d*=2 Å):	
- 2θ=140° (backscattering)	$2.3 \cdot 10^{-3}$
- 2θ=±90°	$4.0 \cdot 10^{-3}$
d_{hkl} range, Å	
- 2θ=140° (backscattering)	0.51 – 5.39
- 2θ=±90°	0.63 – 6.71

The main functional units of the FSD diffractometer (Fig. 4) are:

1) neutron source (IBR-2 reactor with grooved water moderator) producing thermal neutron pulses of ~340 μs long at a repetition rate of 5 Hz;
2) long mirror neutron guide separating the beam from fast neutrons and γ-rays;
3) fast Fourier chopper providing neutron beam intensity modulation;
4) straight mirror neutron guide shaping the thermal neutron beam on the sample;
5) detector system comprising detectors at scattering angles of ±90° and a backscattering detector;
6) collimation devices (diaphragms and radial collimator) setting primary beam divergence and defining a gauge volume in the sample;
7) HUBER goniometer (up to 300 kg) which can accommodate bulk samples and additional equipment (testing machine, furnace, etc.);
8) Software package SONIX+ enabling local and remote control of experiments.

Detector system

Progress in the development of relatively low-cost correlation electronics based on digital signal processors made it possible to propose a new principle for the development of the FSD detector system, namely, a multi-element detector with combined electronic and geometric focusing [12]. In the final version, the FSD detector system will consist of two ASTRA detectors at scattering angles $2\theta = \pm 90°$ each comprising seven independent (i.e. with independent outputs of electronic signals) elements [13] (Fig. 5). These elements are made on the basis of ZnS (Ag) scintillator with wavelength-shifting optical fibers. The combined use of electronic and time focusing of the scattered neutron beam allows an increase in the solid angle up to ~0.16 sr for each ASTRA detector. This sharply increases the detector solid angle while retaining high resolution for the interplanar spacing of $\Delta d/d \approx 4{\cdot}10^{-3}$.

At present, eight elements (out of 14 planned) of ASTRA detectors have been installed at FSD at scattering angles of $2\theta = \pm 90°$, as well as one backscattering detector with time focusing, which consists of 16 scintillation ^{6}Li-elements at a scattering angle $2\theta = 140°$. At the end of 2020, it is planned to perform a complete upgrade of the ASTRA detectors with the replacement of old elements and install all 14 elements of the ASTRA detectors according to the project. In 2021, it is planned to carry out the final geometric alignment of the ASTRA detectors at FSD and the adjustment of operating parameters. Thus, the continuation of the work to expand the FSD multi-element detector system will significantly improve the instrument luminosity.

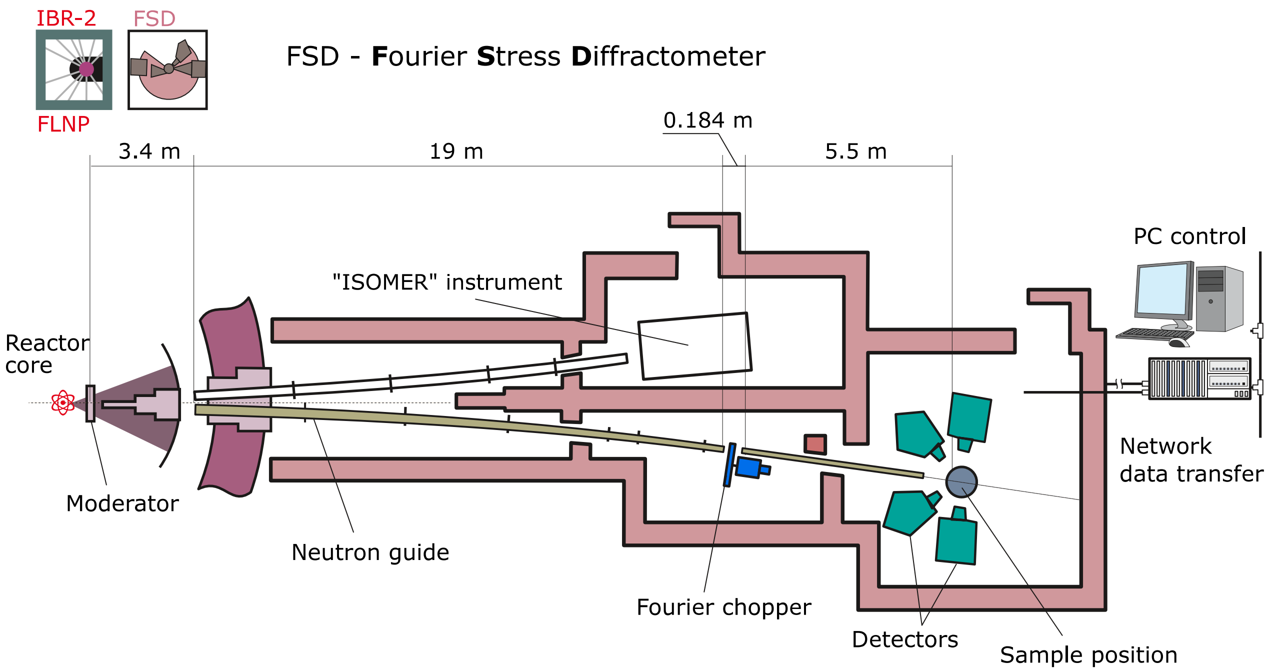
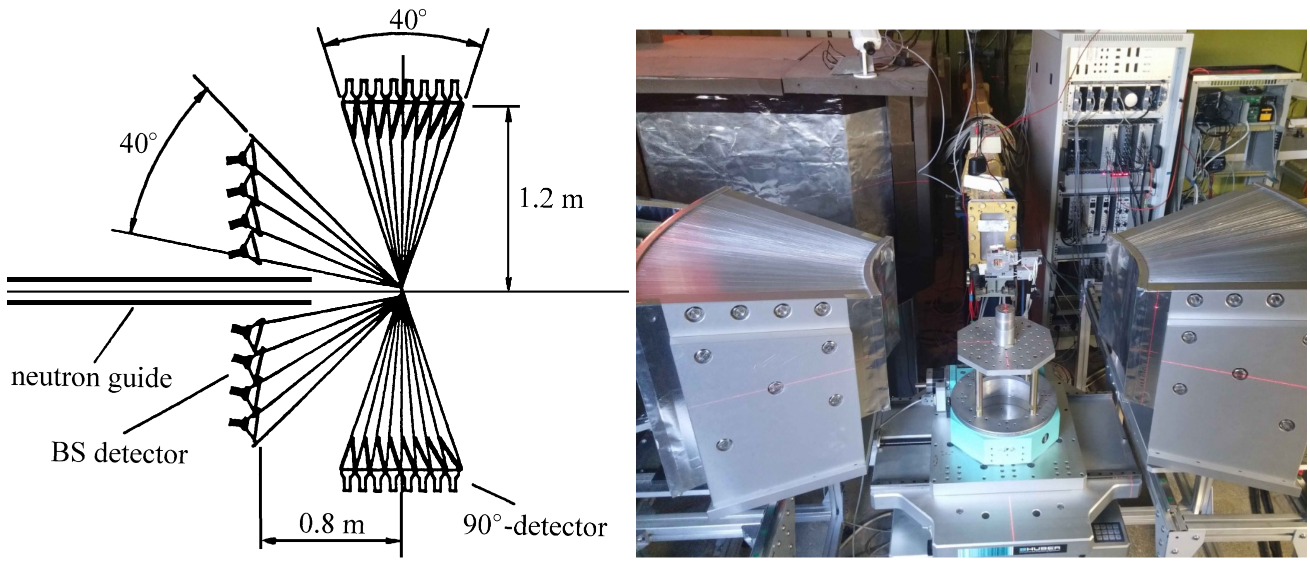


Fig. 4. *Layout of the FSD diffractometer at the IBR-2 reactor.*



a) b)

Fig. 5. *a) Schematic drawing of the detector system of FSD. BS – backscattering detectors at 2θ=140°, 90°-detector – ASTRA detector system (left and right wings) at 2θ=±90°. b) Sample position at FSD. One can see a HUBER goniometer with a sample, radial collimators in front of ±90°-detectors, BS detector, end part of the neutron guide with a diaphragm for the incident beam.*

Fourier chopper

The quality of the correlation Fourier analysis is influenced by a number of factors. One of the main factors is the degree to which the Fourier chopper follows the specified rotation frequency distribution law, which depends on the accuracy and stability of the control system operation. Among other important factors are also the intensity modulation depth of the neutron beam passing through the chopper and the operation stability of the system generating pick-up signals.

In the framework of the development of the experimental base of the FSD diffractometer, work is underway to manufacture a new Fourier chopper with an advanced design and improved characteristics. The new chopper is a rotor-stator system in a vacuum housing. A distinctive feature of the chopper is a number of real radial slits cut in the material of the stator plate and rotor disk with an absorbing ^{10}B coating. This design of the chopper will provide more accurate PID control, the absence of phase error (phase shift of the pick-up signal with respect to the neutron signal), the absence of absorption and scattering from the material of the stator disk, less vibration and a low level of gamma-background. Thus, all this will make it possible to significantly improve the quality of diffraction patterns, i.e. reduce the background, increase the intensity of the spectrum and improve the profile and symmetry of the diffraction peak.

The contract for the production of a new Fourier chopper for the FSD diffractometer was concluded with Airbus Defense and Space (Germany). At present, the Fourier chopper has been manufactured and is being tested by Airbus. In 2020, the new chopper is planned to be installed and adjusted at FSD. The chopper will be mounted on the high-precision positioner (purchased and delivered), which will allow one to remotely move the Fourier chopper into the beam and remove it if necessary. This will make it possible to flexibly form the program of experiments for FSD, quickly switching between the TOF (high luminosity) and RTOF (high resolution) operation modes.

Beam-forming system

To conduct experiments on the study of internal stresses, it is necessary to shape the incident and scattered neutron beams, and thereby to define a gauge volume in the sample bulk with characteristic sizes of several cubic millimeters. For this purpose, in 2016, two new wide-aperture radial collimators by JJ X-ray (Denmark) with a spatial resolution of 1.8 mm were installed at FSD in front of 90°-detectors. The collimators are mounted on mobile platforms with stepper motors and can be remotely introduced to and withdrawn from the working position. In addition, in 2018, a new automated diaphragm for the incident beam (JJ X-ray, Denmark) made of boron carbide with an adjustable aperture (0÷30)×(0÷80) mm was installed.

Mirror neutron guide

The mirror neutron guide for FSD was produced in PNPI (Gatchina) in 1998 from high-quality 19-mm-thick boron glass K8 with a Ni coating (natural isotopic composition). The neutron guide consists of two sections: curved section with a radius of curvature R = 2864.8 m, 19 m long; and straight section 5.01 m long. The characteristic wavelength of the neutron guide is $\lambda_C = 1.554$ Å. The mirror sections of the neutron guide are installed in a steel housing that provides the necessary level of vacuum and stability of the construction. The neutron guide is made conical in a vertical plane with cross sections: at the entrance of the curved section – 10 × 155 mm, at the exit of the curved and at the entrance of the straight sections – 10 × 91.8 mm, at the exit of the straight section – 10 × 75 mm.

Data acquisition system

Since 2014, for data acquisition at the FSD diffractometer, an RTOF analyzer (MPD-32 module) has been used. It operates in the mode of recording all events in a list-mode and has 32 detector inputs [14]. To extract diffraction spectra from the recorded list-mode data, a version of the algorithm for multidetector systems has been developed that allows one to simultaneously obtain high-resolution spectra from all connected detectors/detector elements with individual parameters of the time-of-flight scale. This made it possible to provide separate spectrum acqusition and high-precision electronic focusing both for the elements of the ASTRA detectors and for individual elements of the BS backscattering detector. In addition, it became possible to analyze reactor starts and the correctness of opening of frequency windows in the Fourier chopper on the basis of pick-up signals.

Sample environment system

The available supplementary equipment integrated into the experiment control system makes it possible to create various conditions at the sample. It includes:

1) 4-axis (x, y, z, ω) HUBER goniometer for positioning samples with an accuracy of ~0.1 mm and better. The maximum load on the goniometer axis is 300 kg;
2) HUBER goniometer rotation module with $\Delta\varphi=\pm15°$;
3) LM-29 testing machine (NPI, Řež, Czech Republic) with a maximum load of up to ±29 kN for uniaxial tension/compression of samples 30-100 mm long with a screwed cylindrical head in the neutron beam at temperatures ranging from room temperature to 800°C. The main advantage of this machine is almost backlash-free load transmission to the sample. The sample elongation is measured by extensometers from Epsilon Technology (USA);

4) MF2000 mirror furnace with halogen lamps (maximum temperature is up to 1000°C) with temperature control by a Lakeshore controller.

4.2. Proposals for FSD modernization

The development of FSD is aimed at enhancing the diffractometer luminosity, reducing the background, improving the Fourier analysis parameters and equipping the diffractometer with supplementary sample environment devices. According to the estimates, the accomplishment of these tasks will make it possible to increase the number of conducted experiments severalfold, significantly improve the accuracy of the obtained data, and substantially expand the capabilities of the diffractometer in performing experiments in a wide range of temperatures and external conditions.

1) Detector system

For experiments that require maximum resolving power of the diffractometer, it is necessary to use backscattering detectors. The available backscattering ^{6}Li-glass detector has a small solid angle and high sensitivity to γ-background. Therefore, it should be replaced with two new wide-aperture (~ 0.4 sr each) backscattering ZnS(Ag) detectors with combined electronic and geometric focusing.

2) Neutron guide

To increase the neutron flux at the sample, it is necessary to install a new mirror neutron guide with an advanced multilayer coating of mirrors ($m = 1.75 \div 2$), which will provide a significantly higher reflection coefficient, lower surface roughness and waviness. To significantly enhance the neutron flux, the optimal parameters of the neutron guide including the curvature and the degree of vertical convergence (taper), and the size of the aperture of the outcoming beam will be chosen. It is also planned to solve a number of technical problems associated with the tracing of beamlines 11a and 11b.

3) Data acquisition system

In view of the plans to install a new Fourier chopper and upgrade the FSD detector system, it is necessary to develop a new version of list-mode correlation analysis electronics (MPD modules) with higher speed, larger number of detector inputs and additional options.

4.3. Operation of the instrument and a cold moderator

The FSD diffractometer is located at beamline 11a of the IBR-2 reactor, where the cold moderator is not supposed to be placed. The experiments are carried out using a thermal neutron beam.

4.4. Expected technical parameters after modernization

As a result of modernization, a significant increase in the diffractometer luminosity is expected due to an increase in the solid angle of the detectors: up to ~ 0.32 sr for the ASTRA detectors and up to ~ 0.8 sr for the BS detectors. The use of the ZnS (Ag) scintillator will drastically reduce the background level. The commissioning of the new Fourier chopper will improve the quality of diffraction spectra (i.e. signal/background ratio and peak profile) while maintaining the current resolution level of the diffractometer ($\Delta d/d \approx 2 \div 4 \cdot 10^{-3}$). The installation of the new neutron guide will result in a 2-3-fold increase in the neutron flux at the sample.

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

For long-pulse neutron sources, the only practical way to achieve high resolution is to use the reverse time-of-flight method in combination with a Fourier chopper (RTOF method) [15], which provides an optimal balance between resolution and luminosity. The experience of upgrading the FSD will be extremely useful for the development of spectrometers on the new neutron source of FLNP.

5. Expected scientific results, comparison with the world level

It is expected that after modernization, the FSD diffractometer will be equipped with an advanced wide-aperture detector system with a high resolving power. The gain in the luminosity will make it possible to significantly reduce the spectrum accumulation time and increase the number of experiments performed in the framework of the user program. In addition, it will become possible to study in detail the distribution (2D map) of residual stresses in thick industrial samples for a reasonable measurement time. The planned improvements in the resolution and peak shape will enhance the accuracy in determining residual stresses in advanced structural materials and allow reliable determination of the level of microstrains and characteristic crystallite sizes from the profiles of diffraction peaks.

6. Requested resources, costs and time frames of instrument modernization

The cost of the FSD components to be manufactured or renewed is given in **Table 2** (**Section 4**). Work on the project will be carried out by the employees of the HRFD/FSD group of Sector № 1 (Diffraction), NICM Department, and the personnel of the Spectrometers'Complex Department.

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FSS - Fourier Diffractometer

Leader: G.D. Bokuchava

Main participants: A.A. Kruglov, I.V. Papushkin, V.V. Zhuravlev, V.V. Kruglov

Collaborating organizations: The investigations and methodological developments planned for the FSS diffractometer are of interest to other neutron centers (e.g., ESS), various materials research organizations and a number of industrial enterprises.

1. Abstract

The FSS neutron Fourier diffractometer (Fourier Strain Scanner) successfully operated in 1990-2010 at the FRG-1 steady-state reactor at the GKSS research center (Germany) [1]. The FRG-1 reactor was finally decommissioned in 2010. In view of this, in 2014, the FSS diffractometer was transported to FLNP JINR (Dubna) and placed at the IBR-2 pulsed reactor on beamline 13 [2], which had not previously been used. Over the past few years, a large amount of work has been carried out to develop the beamline infrastructure and adapt FSS to work at a pulsed source [3]. This project outlines plans for further modernization of the FSS Fourier diffractometer.

2. Scientific program, topicality and comparison with the world level

The FSS Fourier diffractometer at beamline 13 of the IBR-2 reactor is intended for investigations of internal stresses in structural materials and industrial products using high-resolution neutron diffraction ($\Delta d/d \approx 5.5\cdot10^{-3}$). In addition to carrying out scientific research, another important area of scientific and methodological activities at FSS is the further development of the neutron correlation RTOF technique for the analysis of elastic neutron scattering by crystals, as well as the development and testing of new detectors, detector electronics and data acquisition electronics. Using FSS, it will be possible to probe new ideas in correlation neutron spectrometry, which can be applied further at the ESS European pulsed neutron source and new neutron source at FLNP JINR.

The FSS is very similar in design to the available IBR-2 diffractometers FSD [4] and HRFD [5]. The FSS, however, has a middle flight path between a Fourier chopper and detector ($L \approx 12.37$ m) and relatively low rotational speed of the chopper (~ 2000 rpm). In the course of the implementation of the project, major attention will be paid to the enhancement of luminosity, increase in the resolving power and solution of the existing technical problems.

3. Scientific and methodological groundwork laid in FLNP JINR

In FLNP JINR over the years of operation of HRFD and FSD diffractometers, considerable experience has been gained in using the neutron correlation Fourier technique at a long-pulse neutron source. During this period, a great number of experiments have been conducted with both diffractometers in the field of structural investigations, physical materials science and engineering sciences.

4. Current status of the instrument and proposals for its modernization

4.1. Current status and main units of FSS

The FSS diffractometer is located at beamline 13 of the IBR-2 reactor at FLNP JINR. In 2014-2019, the major stage of work on the construction of beamline 13, development of its infrastructure, as well as installation and adaptation of the main FSS units and performing a series of test experiments was completed. The main units of the diffractometer are steel conical collimator, mirror neutron guide, Fourier chopper, sample assembly, two 90°-detectors, acquisition and control electronics (Fig. 6).

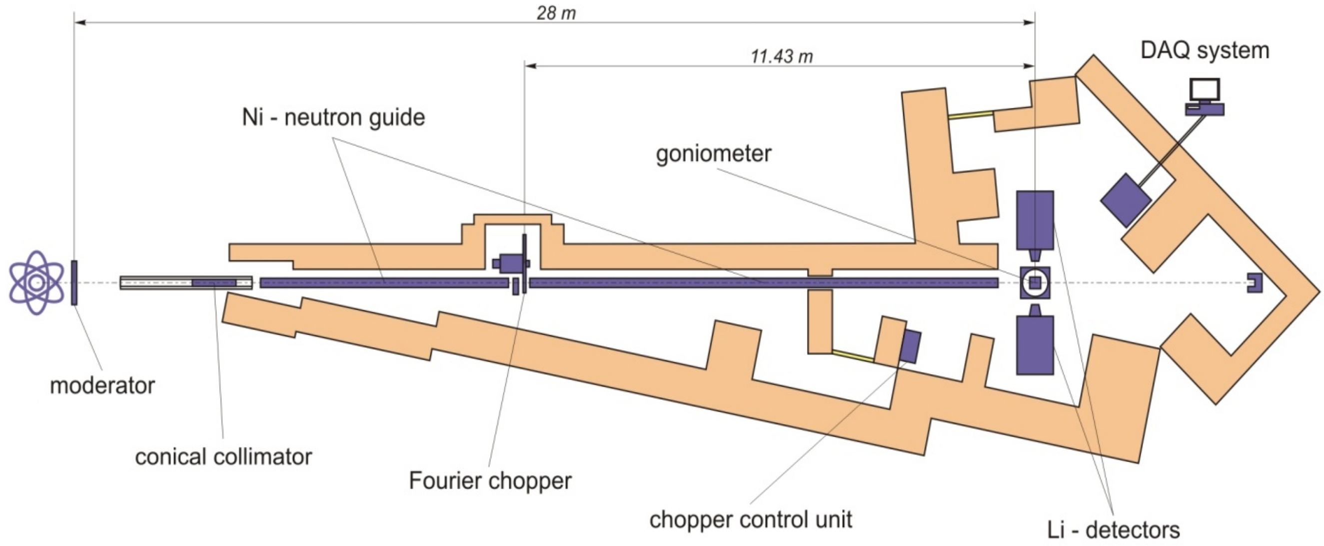


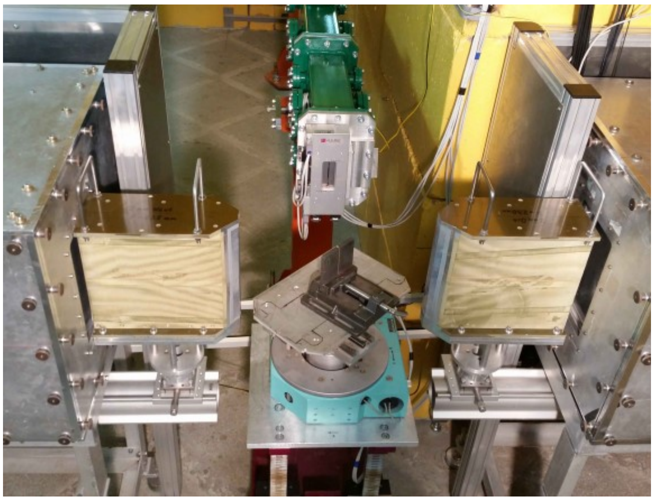
Fig. 6. *Layout of the Fourier diffractometer at beamline 13 of the IBR-2 reactor.*

A **steel collimator** is installed in front of the mirror neutron guide. It is designed to reduce the radiation load on all subsequent elements of the setup and inside has a conical shape both horizontally and vertically. To fit the geometry of the neutron guide, the inlet and outlet openings of the collimator have a rectangular cross section. The angular dimensions of the openings of the conical collimator are chosen to provide the maximum illumination of the neutron guide inlet cross section with respect to the visible surface of the moderator.

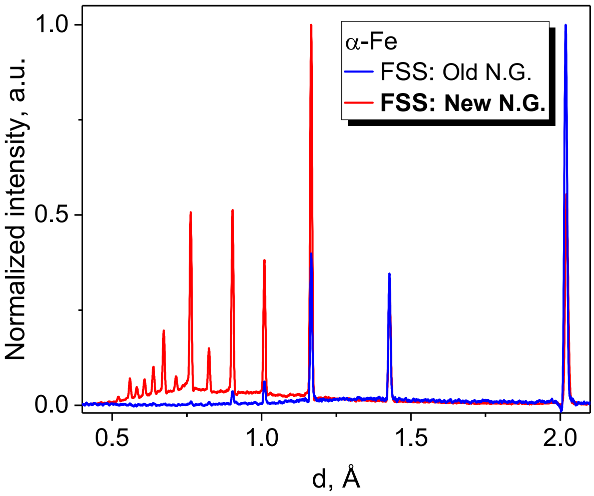
In 2019, to improve the characteristics of the diffractometer, a new **mirror neutron guide** was installed in a steel vacuum housing, which allowed a several-fold increase in the flux of short-wavelength neutrons. The neutron guide is located between the Fourier chopper and the sample place and designed to remove fast neutrons and γ-rays from the beam, as well as reduce losses when transporting thermal neutron flux to the sample position. The new neutron guide is plane-parallel in the horizontal direction (opening width – 10 mm) and linearly converging in the vertical plane (inlet and outlet opening heights are 126 mm and 50 mm, respectively). The sections of the new neutron guide have a super-mirror Ni/Ti coating, m = 2. The radius of curvature of the neutron guide is R = 1900 m, and the characteristic wavelength is $\lambda_c = 0.95$ Å. An automated diaphragm (JJ X-ray, Denmark) made of boron carbide with an adjustable aperture of (0÷30)×(0÷80) mm is installed at the exit of the mirror neutron guide to form an incident beam of the required size.

The FSS **Fourier chopper** is designed for fast modulation of the primary neutron beam and consists of a rotor disk with a diameter of 570 mm fastened to the axis of the engine, and a stator plate fixed to the platform. During the experiment, the disk rotational speed varies from 0 to 2000 rpm according to a certain law (frequency window). The chopper disk has 1024 slits 0.75 mm wide. Metallic gadolinium is used as a neutron absorber. An incremental magnetic encoder is installed on the axis of the electric motor to measure the speed and acceleration of the disk and generate a pickup signal fed to the RTOF analyzer.

The FSS **detector system** consists of two ±90°-detectors Ost and West, assembled from 12 and 15 PEMs, respectively, with NE912 (^{6}Li) scintillation glasses glued on them. The elements of each detector are located in space in accordance with the time-focusing surface. The range of 2θ angles in the scattering plane are 8° for the Ost detector and 10° for the West detector. If necessary, radial collimators with a spatial resolution of 1 or 2 mm can be placed in front of the detectors to define a small gauge volume in the depth of the sample (Fig. 7).



a)



b)

Fig. 7. *a) Sample place at FSS. One can see a HUBER goniometer with a sample, radial collimators in front of ±90-detectors Ost and West, and the end part of the neutron guide with a diaphragm for the incident beam. b) Comparison of diffraction patterns measured before and after the replacement of the neutron guide.*

The FSS equipment includes a **sample table**, consisting of goniometer modules (X, Y, Z, Ω) with a load capacity of 60 kg and additional vertical adjustment.

The FSS **data acquisition system** comprises RTOF analyzers of a new type (list-mode). The list mode suggests the recording of all events. The control system of the diffractometer is based on the Sonix + software package in the Windows (PC) environment.

Main parameters of FSS

Curved neutron guide	mirror, Ni/Ti coating (m = 2)
- length, m	17.32
- radius of curvature, m	1900
Moderator-to-sample distance, m	26.5
Chopper-to-sample distance, m	11.43
Fourier chopper (disk)	high-strength Al alloy
- outer diameter, mm	570
- slit width, mm	0.75
- number of slits	1024
- max. rotational speed, rpm.	2000
- max. beam modulation frequency, kHz	34.1
Thermal neutron pulse width:	
- in low-resolution mode, μs	340
- in high-resolution mode, μs	29.3
Neutron flux at sample position, n/cm²·s⁻¹	$1.2\cdot10^{6}$
Detectors (2θ=±90°)	^{6}Li, with time focusing
Detector resolution $\Delta d/d$ (d = 2 Å)	$5.5\cdot10^{-3}$
d_{hkl}**-range**, Å	0.5 ÷ 3.5

4.2. Proposals for modernization of FSS

The implementation of the FSS project is to be carried out in two stages. In the framework of stage I, the major part of work on the adaptation of the diffractometer at the IBR-2 beamline 13 was completed, and the first test experiments were performed. At this stage, the available units of the FSS diffractometer were mainly used. The plan of activities of stage II (2021-2025) for the modernization of FSS involves work on the enhancement of the diffractometer luminosity, reduction of the background, improvement of the Fourier analysis parameters and equipping the diffractometer with additional sample environment devices.

1) Detector system

To increase the luminosity of the diffractometer, it is necessary to develop and construct a new wide-aperture ZnS(Ag)-scintillator-based detector system with a combined use of electronic and time focusing. The scheme of ASTRA detectors at FSD is planned to be used for the development of 90°-detectors at FSS. A large-solid-angle backscattering ZnS(Ag) detector is to be developed as well.

2) High-resolution scintillation PSD detector in RTOF mode (prototype)

For further development of the correlation Fourier diffractometry and taking into account the prospects of implementation of this method at a new neutron source in FLNP, it is necessary to create a prototype of a high-resolution scintillation position-sensitive detector operating in the RTOF mode. Preliminary estimates show that a detector with a position sensitivity of about 2 mm at a scattering angle of $2\theta = 90°$ can improve the diffractometer resolution by a factor of ~ 2 due to a corresponding decrease in the geometric contribution to the resolution function. In addition to the expected enhancement of the diffractometer luminosity and resolution, detectors of this type can also significantly widen the experimental capabilities of Fourier diffractometers (studies of single crystals, orientation effects in materials, etc.). At present, the development of a concept of the detector prototype and its main parameters is in progress.

3) Fourier chopper

To improve the quality of the correlation analysis, it is planned to replace the Fourier chopper with an advanced variant similar to that developed for the FSD diffractometer (including a vacuum housing, stable pick-up signals, cut-out slits in the rotor and stator, high rotational speed of up to 6000 rpm, flexible control system, high-precision mechanical positioner).

4) Beam-forming system

The proposed detector system requires the installation of wide-aperture multi-slit radial collimators in front of 90° detectors. This system will make it possible to regulate the shape of the incident and scattered neutron beams, and thus, to define a gauge volume with characteristic dimensions of several cubic millimeters inside the sample under study. The collimators will be equipped with mobile platforms with stepper motors, which will allow one to remotely introduce and withdraw them from the working position.

5) Goniometer

For bulky samples and additional equipment, a new goniometer (X, Y, Z, Ω) with a wide range of displacements and a larger load capacity will be installed.

6) Data acquisition system

In view of the plans to install a new Fourier chopper and upgrade the FSS detector system, it is necessary to develop a new version of list-mode correlation analysis electronics (MPD modules) with higher speed, larger number of detector inputs and additional options.

4.3. Operation of the instrument and a cold moderator

The majority of structural materials studied with FSS have a relatively small unit cell parameter, so the greater part of the observed diffraction peaks are in the region $d_{\mathrm{hkl}} \approx 0.6$ - 2.5 Å. In addition, the installation of a cold moderator for IBR-2 beamline 13 is not planned. Thus, experiments at FSS will be carried out using thermal neutrons.

4.4. Expected technical parameters after modernization

After modernization, the FSS diffractometer will have an advanced wide-aperture detector system (0.3 ÷ 0.8 sr) with a high resolving power ($\Delta d/d \approx 2 \div 4{\cdot}10^{-3}$), which will significantly improve the accuracy of determining the structural parameters of various structural materials.

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

For long-pulse neutron sources, the only practical way to achieve high resolution is to use the reverse time-of-flight method in combination with a Fourier chopper (RTOF method), which provides an optimal balance between resolution and luminosity. The experience of upgrading the FSS will be extremely useful for the development of spectrometers on the new neutron source of FLNP.

5. Expected scientific results, comparison with the world level

The gain in luminosity and a high-precision beam-forming system will make it possible to study the distribution of residual stresses in various industrial samples for a reasonable experiment time, as well as accurately determine the level of microstrains and the characteristic sizes of crystallites from the profiles of diffraction peaks. In addition, the improved characteristics of FSS will allow further development of the correlation method and tests of new equipment (detectors, detector electronics and data acquisition electronics).

6. Requested resources, costs and time frames of instrument modernization

The costs of the FSS units to be manufactured and upgraded are given in **Table 3** (**Section 4**).

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RTD - Neutron Diffractometer (Real-Time Diffraction)

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1. Abstract

Powder diffraction is a widely accepted technique for studying kinetics of various processes. However, the vast majority of diffraction experiments deal with systems in equilibrium states when measurements are made in discrete sets of external parameter values (temperature, pressure, magnetic field, etc.). It is assumed that the response of the system under study to external influences is presented correctly. The state-of-the-art development of technology calls for the creation of materials with improved functional (magnetic, electrical, mechanical, etc.) properties, which requires the understanding of microscopic mechanisms and description of the processes leading to the formation of the desired properties. To solve the related problems, the RTD diffractometer was constructed on the basis of the DN-2 diffractometer (beamline 6a). The advantage of RTD is the possibility to follow the kinetics of processes in condensed matter in real time. One of the critical parameters of such kind of experiments is the minimum measurement time interval, in which it is possible to collect the necessary statistics. The experience gained during the operation of RTD allows us to outline the ways for its further development.

2. Scientific program, topicality and comparison with the world level

The RTD diffractometer (Real Time Diffraction) [1, 2] (Fig. 8) was constructed on the basis of the DN-2 diffractometer (beamline 6a). The schematic layout of RTD is shown in Fig. 1. RTD is a conventional time-of-flight diffractometer for detecting elastic neutron scattering. The specialization of RTD is determined by its resolution regarding the interplanar spacing (~ 0.01) and the neutron flux at the sample (~ 5×10^6 n/cm^2/s).

The acquisition of experimental data is performed by:

1) 8-ring backscattering detector (2θ = 156° - 171°) in the range of interplanar spacings d_{hkl} = 0.5 - 6 Å;

2) 9-ring detector at small scattering angles of 2θ ~ 1.0 - 4.5° divided into 16 independent sectors (which allows us to additionally detect azimuthal coordinates of scattered neutrons) in the d_{hkl}-range from 15 Å to 300 Å and greater;

3) three detector banks comprising 8 counters each at $2\theta \sim 30° - 138°$ in the range of $d_{hkl} = 0.5 - 23$ Å;

4) 2D position-sensitive detector (PSD) with a variable angle $2\theta \sim 5° - 140°$, diffraction is observed up to $d_{max} = 80$ Å.

The 2D PSD makes it possible to perform experiments with single crystals. In particular, the combination of the 2D detector and TOF technique for detecting diffraction spectra allows us to study the effects of diffuse scattering in single crystals and analyze local deviations of the structure from the ideal long-range order.

The combination of a medium resolution and a wide interval of interplanar spacings ($d_{hkl} \sim 0.5 - 300$ Å) at the high-luminosity RTD diffractometer makes it possible to refine the crystalline structure of polycrystalline substances of intermediate complexity. The presence of high- and low- temperature devices allows the study of crystalline and magnetic structures, as well as phase transitions in the temperature range from 4 to 1400 K.

The RTD has proven to be a successfully operating instrument. Scientific experiments are carried out in cooperation with scientific organizations and a wide community of users from Russia, Poland, Bulgaria and several other countries.

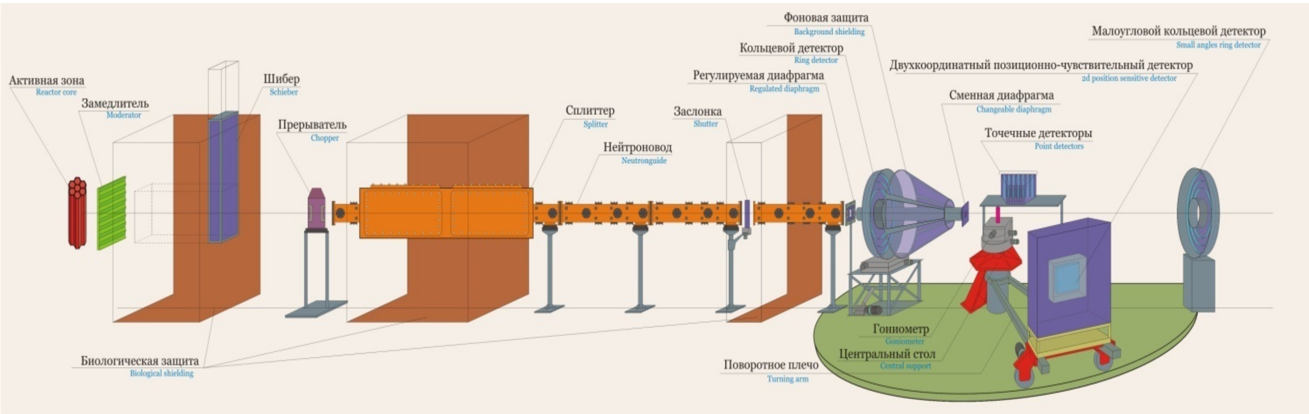

Fig. 8. *Layout of RTD diffractometer.*

3. Scientific and methodological groundwork laid in FLNP JINR

First experiments on real time diffraction at IBR-2 were performed in the mid-1980s after the reactor startup. Interesting results were obtained in the studies of hydration of cement components and kinetics of sorption/desorption of water by lipid membranes [3], solid-phase synthesis of HTSC compounds [4], effects of hydrogen on the structure of HTSC Y-123 [5], kinetics of phase transitions in titanium deuterides [6] and phase transformations of high-pressure metastable ice [7].

In recent years, the medium-resolution time-of-flight RTD diffractometer was successfully used to study nanomaterials [8, 9], crystalline [10] and magnetic structures, chemical reactions and phase transitions (crystallization, solidification, kinetics of hydration-dehydration of lipids and polymers, etc.), diffusion of light elements in ceramic media, domain structure and diffuse scattering in single crystals, low-periodicity and long-period structures (lipid membranes) [3], incommensurate and modulated structures. The main advantage of the RT diffractometer is its high luminosity (on the order of $5x10^6$ n/cm^2/s) and a wide range of available wavelengths (from 1 to 18 Å), which allows one to gain information in the range of interplanar spacings from 0.5 to 300 Å.

Test studies of structural changes in electrode materials were carried out both in specialized electrochemical cells and in commercial lithium-ion batteries [11]. The analysis of the scattering intensity made it possible to follow the ratio of structural phases in the electrodes, as well as the amount of lithium in the cathode. The time changes in the positions of diffraction peaks were followed to obtain information about the change in the size of the unit cell during electrochemical cycling.

4. Current status of the instrument and proposals for its modernization

4.1. Information on the current status of the instrument

The following types of the detector systems are used at the diffractometer:

- Detector system for studying the crystalline and magnetic structures of powders comprising 3 detector banks with 8 SNM-17 counters each (diameter of 18 mm, length of 180 mm, filled with ^{3}He under pressure of 8 atm).
- Ring detector with 8 concentric rings at large scattering angles of 156° - 171° (backscattering).
- 2D position-sensitive detector for studying single crystals and ordered structures with large interplanar spacings (active area of 225 × 225 mm, spatial resolution of ~ 2 mm).
- Ring detector with 9 concentric rings and azimuthal sensitivity at small scattering angles of 1.0-4.5°.

The equipment of RTD includes a three-axis goniometer, a low-temperature module (4 - 320 K) for a closed-cycle refrigerator and high-temperature furnaces (300 - 1000 K).

The characteristics of the diffractometer and its equipment make it possible to study [1-20]:

1) processes in real time such as:

   a) solid-phase chemical reactions,
   b) crystallization,
   c) hydration - dehydration,
   d) phase transitions;

2) crystal structure of powders and single crystals in a wide temperature range from 4 K to 1000 K;

3) magnetic structure;

4) phase transitions;

5) diffuse scattering in imperfect crystals;

6) domain structures;

7) superstructure reflexes of low intensity (~0.1-0.01% of the main peak intensity) in modulated structures;

8) low-dimensional structures with a large unit cell;

9) incommensurate modulated magnetic structures.

Main parameters of RTD

Neutron guide	Ni, mirror
Neutron guide aperture	15 mm × 180 mm
Moderator-to-sample distance	23.85 m
Sample-to-detector distance	0.15 - 2.0 m, variable
Neutron flux at sample position	~ $5*10^6$ n/cm^2/s
Wavelength range	1.0 - 18 Å
Scattering angle range	1 - 170°
Interplanar spacing range	0.6 - 300 Å
Resolution (Δd/d) :	
θ = 80°, d = 2 Å	1 %
θ = 10°, d = 60 Å	10 %

4.2. Detailed description of proposals for modernization of the instrument

The main characteristics that determine the informativeness of the diffraction experiment are luminosity, interplanar spacing range covered in one experimental run and resolution. The modernization of RTD is aimed at increasing the diffractometer luminosity, reducing the background level, developing software and sample environment system (upgrade of equipment for creating and monitoring external conditions on the sample during the experiment). This will increase the number of experiments and significantly expand the capabilities of the diffractometer for conducting experiments in controlled external conditions (temperature, electric and magnetic fields, controlled gas atmosphere and vacuum).

4.2.1. Enhancement of luminosity of the instrument and reduction of background level

It is proposed to significantly increase the luminosity of RTD by implementing a number of measures.

The available detector system at RTD detects diffraction spectra in the range of interplanar spacings from 0.5 to 300 Å with a minimum time resolution down to the duration of a single pulse of the IBR-2 reactor. The maximum and minimum scattering angles on a ring backscattering detector at a sample-to-detector distance of 500 mm are 171 and 156°, respectively, which provides an interplanar spacing resolution of 0.5-1%. In this case, the maximum solid angle is $\Omega_d \approx 0.5$ sr, which is significantly smaller than that at, for example, GEM, ISIS ($\Omega_d \approx 3$ sr):

$$I = \Phi_0 S \left(\frac{\Omega_d}{4\pi}\right) \delta,$$

where Φ_0 is the total neutron flux at the sample in the working wavelength range (Φ_0 is up to 5×10^6 n/cm^2/s), Ω_d is the solid angle of the available detector system (≈ 0.5 sr), S is the sample area (≈ 5 cm^2), δ is the scattering ability of the sample (≈ 0.1). Then the useful count rate (I) reaches ~10^5 n/cm^2/s. Upon increasing the total solid angle to the level of GEM, ISIS ($\Omega_d \approx 3$ sr) or ESS ($\Omega_d \approx 5$ sr), the count rate is expected to be $I \sim 10^6$ n/cm^2/s, which will significantly reduce the time resolution of the real-time mode from a few seconds to milliseconds.

In order to enhance the diffractometer luminosity for research of polycrystals with small and large unit cells, it is proposed to install ZnS(Ag) detector modules symmetrically on both sides of the beam axis at scattering angles of ~150°-120°, thus increasing the solid angle Ω_d up to 2 sr. In the 90° position, we also propose to use ZnS(Ag) scintillation detectors. The design of the detector system should take account of the current trends in the state-of-the-art development of detectors with large solid angles. The ZnS(Ag) detectors developed in FLNP for the FSD and HRFD diffractometers can serve as a basis for the development of the detector system for RTD.

Also, to significantly reduce the background level at the ring backscattering detector, it is proposed to design and install a slit collimation system.

To reduce the background level from the rescattered neutrons generated along a 3-m air path from the sample to the small-angle detector, a cone-shaped tube filled with argon will be installed.

4.2.2. Measures to increase the quality of the diffractometer:

1. To reduce the contribution of the angular divergence and thereby increase the resolution of the diffractometer. For this purpose, movable slit collimators forming the incident beam will be designed and installed. For measurements that do not require high resolution, collimators will be withdrawn from the beam, thereby eliminating the loss in intensity due to collimation.

2. To mount the small-angle detector on a rotating platform. This will allow more rapid tests of the detector by measuring spectra in the usual diffraction mode. This measure will reduce the time required to prepare the diffractometer for experiments with the small-angle detector and improve the reliability of the results.

3. To upgrade the available mirror neutron guide for increasing the luminosity of RTD. At present, the RT diffractometer is equipped with a mirror neutron guide, which forms the primary neutron beam on the sample. The 18-m-long neutron guide is located between the moderator and the sample place. It consists of two sections – a curved ~16-m-long head section (radius of curvature of 1850 m) and a straight ~2-m-long end section. The neutron guide is an assembly of rectangular glass sections (dimensions 15×180×500 mm) with a reflective nickel coating of the walls (natural Ni, critical reflection angle $\Theta_c \sim 0.0017\lambda$, where λ is the wavelength in Å). The neutron guide is mounted inside a vacuum housing, which minimizes neutron losses. The curved neutron guide leads to an increase in the neutron flux and a significant decrease in the flux of fast neutrons and gamma-rays on the sample. It is planned to replace the available mirror neutron guide with a supermirror guide (Table 1) with the focusing in two planes (nowadays multilayer coatings provide higher reflectivity and lower roughness of the reflective surface). The preliminary estimates show that such a replacement can increase the neutron flux at the sample position by a factor of 1.5-3. A neutron guide with such characteristics can be manufactured by Mirrotron Ltd (Hungary) or SwissNeutronics (Switzerland).

4.2.3. Sample environment equipment

It is planned to widen the range of possible experimental studies by upgrading the equipment and purchasing the following devices:

1) vacuum furnace to produce high (up to 1800 K) temperatures in polycrystalline samples;

2) cryostat with the possibility of creating a magnetic field in the sample.

3) air-tight cells with the possibility of transmitting electric current through the sample (up to 10 A) for a temperature range of 300 - 1200 K;

4) shaft-type refrigerator with a temperature range of 8 - 290 K;

5) Huber three-circle goniometer with a refrigerator (temperature down to 4 K) and a mini-furnace for performing experiments on single crystals and oriented biological objects;

6) goniometric unit for performing experiments with single crystals at room temperature;

7) unit with mobile permanent (niobium) magnets and a small-sized electromagnet to provide a constant magnetic field in the range from 0 to 2 T.

4.2.4. Development of electronics and software for the RTD diffractometer

The latest update of the software for the measuring module at RTD made it possible to significantly simplify the control of the diffraction experiment. However, when operating in the real time mode, large amounts of data are recorded in separate files. The file processing for subsequent calculations, in particular the calibration using the vanadium spectrum, takes a lot of time. Therefore, it is planned to develop and implement in the measuring module of RTD a semi-automatic procedure of preparation of experimental data for calculations.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

Test experiments with a prototype of the cold moderator, performed as early as in 1994 and 1999, showed a gain factor of 5-10 in the ranges of medium and long wavelengths as compared to the grooved moderator. For crystal structures with a unit cell volume of more than 300 Å^3, the main part of the observed diffraction peaks is concentrated in the region $d_{hkl} \approx 2.5$ - 10.0 Å. Thus, the most optimal moderator temperature is ~ 100 K. The operation with a cold moderator will make it possible to detect diffraction peaks at large d_{hkl} with good statistics for reasonable acquisition times. The possibility of RTD to detect diffraction peaks at large d_{hkl}-values is an important aspect in the study of both magnetic and long-period structures. For example, this concerns the studies of the structure and kinetics of transformations in biological membranes with a period of from 20 to 100 Å or organometallic compounds MIL-101 (a ~ 90 Å).

As a rule, the measurement time of one diffraction spectrum in the normal mode is from 2 to 20 hours. It is important that the real-time mode requires good time stability of the neutron beam intensity. Therefore, the work with a cold moderator is possible with its stable operation for at least one day.

4.4. *Expected technical parameters after modernization of the instrument*

- Increase in luminosity due to the installation of a new neutron guide and increase in the angular aperture of the detector system.

- Increase in resolution during the formation of the incident beam by collimators.

- Improvement of the background conditions on the ring backscattering detector after installation of detector collimators.

- Improvement of the background conditions on the ring detector for small angles after installation of a cone tube filled with argon.

- Improvement of experimental possibilities and quality of the diffractometer after installation of new goniometers and sample environment equipment.

Proposed characteristics of the new neutron guide

Total length	18.0 m
Width of neutron guide (constant)	15 mm
Height of neutron guide (entrance)	200 mm
Height of neutron guide (exit)	100 mm
Supermirror coating	m = 1.75
Reflectivity (at θ_c)	(96 - 98)%
Radius of curvature	1850 m
Characteristic wavelength	1.25 Å
Length of mirror section	0.75 - 0.8 m
Waviness of mirror section	$\leq 1.5 \cdot 10^{-4}$
Glass thickness	~15 mm
Vacuum level	$\leq$ 0.1 MmHg

4.5. *Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR*

The analysis of the possibilities of RTD shows that there is a clear tendency towards the broadening of the range of scientific problems, for which the characteristics of the instrument find effective applications. The medium resolution of RTD, in comparison with high-resolution diffractometers, is compensated by its high intensity, as well as a wide range of its practical applications (studies of magnetic and long-period structures and even structural features of biological objects such as lipid membranes). The possibility of measuring systems both in the equilibrium state and in the real-time mode, is combined with the unique advantage of IBR-2, which is a relatively low pulse frequency compared to spallation sources. The latter is a serious advantage from the point of view of experiments in real time. This makes it clear that a diffractometer of this type should be included in the project for the development of the suite of spectrometers around the new neutron source of FLNP, especially taking into account the extensive experience gained during the operation of RTD.

5. Expected scientific results, comparison with the world level

The upgrade of the sample environment system of RTD and equipping it with the above-listed sample environment devices (shaft-type refrigerator and low-temperature chamber, vacuum furnace, electrochemical cell, Huber three-circle goniometer with a refrigerator) will ***significantly extend the range of possible experiments on the diffractometer***.

The implementation of all proposals on the modernization of RTD (replacement of the neutron guide, increase in the solid angle of the detector, use of ZnS(Ag) scintillators in 90° detectors, installation of collimators, etc.) ***will significantly improve the characteristics of the diffractometer and reduce the time per one experiment***.

6. Requested resources, costs and time frames of instrument modernization

The main units to be upgraded are the mirror neutron guide, backscattering detector, system of detectors located at scattering angles of 30°-138°. The list of the required sample environment equipment and approximate costs are given in **Table 4** (**Section 4**). The project will be realized by the staff of the RTD group of the Diffraction Sector with the participation of employees of the Spectrometers' Complex Department.

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DN-6 - Neutron Diffractometer for Ultrahigh-Pressure Research

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1. Abstract

The high-pressure neutron diffraction technique was first realized at the DN-12 diffractometer for investigations of microsamples [1] developed in cooperation with the NRC "Kurchatov Institute" at the pulsed IBR-2 reactor in FLNP JINR. The diffractometer makes it possible to carry out investigations in a pressure range of up to 7 GPa. During the period of its operation a wealth of experience has been gained in designing, development and modernization of the instrument as well as in the development of the high-pressure neutron diffraction technique. The development and construction of the new DN-6 diffractometer [2] at IBR-2 beamline 6B are a logical extension of the work on the DN-12 diffractometer, which is aimed at significantly increasing the resolving power of the instrument and the pressure range covered in experiments.

2. Scientific program, topicality and comparison with the world level

At present, neutron scattering experiments with high-pressure cells are carried out only in a few most advanced neutron centers in the world. This is due to the fact that this kind of experiments can be done only at high-flux neutron sources on instruments equipped with advanced detector systems that provide good experimental statistics for appropriate data analysis. Until recently, the application of neutron methods, as a rule, has been restricted to the pressure range of 1-2 GPa, because of the use of relatively large samples in cells of the cylinder-piston type. The development of the method of neutron investigations at high pressures employing the technique of sapphire/diamond anvils in combination with low-background neutron diffraction has allowed us to extend the pressure range in experiments to several tens of GPa. Further development of the high-pressure technique, which is aimed at extending the accessible pressure range up to 30-50 GPa, requires an increase in the neutron flux at the sample position and the solid angle of the detector system.

The optimum combination of the intense neutron beam of beamline 6B, mirror neutron guide and a unique multidetector system of the DN-6 diffractometer makes it possible to perform experiments at a pressure of up to 13 GPa using new high-pressure sapphire anvil cells. The use of high-pressure diamond anvil cells will allow experiments with very small sample volumes (0.001 - 0.1 mm^3) and pressures of up to 50 GPa. It should be noted that experimental neutron studies with high pressures are performed only on a few instruments in the world's advanced neutron scattering research centers, including the DISK diffractometer [3] at the IR-8 research reactor of NRC 'Kurchatov Institute' (Moscow, Russia); PERL diffractometer [4] at ISIS RAL (UK); G6.1 diffractometer at LLB (Saclay, France); high-pressure setup [5] for the HRPT diffractometer at the SINQ neutron spallation source (Paul Scherrer Institute, Villigen, Switzerland); high-pressure setup [6] at D20 in ILL (Grenoble, France); HiPPO diffractometer [7] at the Los Alamos Neutron Science Center (USA); PLANET diffractometer [8] at J-PARC (Ibaraki, Japan) and the SNAP diffractometer [9] at the SNS spallation neutron source (ORNL, Oak Ridge, USA).

3. Scientific and methodological groundwork laid in FLNP JINR

The development and construction of the new DN-6 diffractometer [2] at IBR-2 beamline 6B are a logical extension of the work on the DN-12 diffractometer, which is aimed at significantly increasing the resolving power of the instrument and the pressure range covered in experiments. At present, the DN-12 diffractometer [1] is mainly used to carry out investigations of atomic and magnetic structures of condensed matter in experiments with small sample volumes. Further development of the neutron diffraction technique for experiments with ultra-small sample volumes (down to thousandths of a cubic millimeter) requires an enhancement of the neutron flux at the sample position and an increase in the solid angle of the detector system. The intensity of the neutron beam of beamline 6B exceeds the intensity of the neutron beam of beamline 12 by a factor of ~5. The use of a cold neutron moderator at this beamline will significantly widen the possibilities for studying magnetic structures in crystals at high pressures. The optimum combination of the intense neutron beam at beamline 6B, use of a mirror neutron guide and the unique multi-detector system at DN-6 makes it possible to perform diffraction experiments with sample volumes of down to 0.0001 mm^3.

The DN-6 high-intensity diffractometer combines a high neutron flux at the sample position and a highly efficient wide-aperture detector system. Upon reducing the sample volume (required for obtaining experimental data of high quality) down to ~0.002 mm^3, it became possible to carry out unique neutron experiments in the temperature range of 4-300 K due to the improvement in the technical parameters of the neutron diffractometer. At present, such a unique experimental base for performing world-class experiments allows us to obtain new cutting-edge research results.

4. Current status of the instrument and proposals for its modernization

4.1. Information on the current status of the instrument

Main characteristic parameters of DN-6 diffractometer

Thermal neutron flux at sample position	~3.5×10^7 n/cm^2/s
Experimental d_{hkl}-range	
at scattering angle $2\theta = 90°$:	5.7 Å
at scattering angle $2\theta = 42°$:	11.2 Å
Resolution	
$\Delta d/d$ at d = 2 Å:	
at scattering angle $2\theta = 90°$:	0.025
at scattering angle $2\theta = 42°$:	0.030
Characteristic measurement time for one diffraction spectrum:	
typical sample volume $V \sim 50$ mm^3	0.1 h
small sample volume $V \sim 1$ mm^3	2-4 h
ultra-small sample volume $V \sim 0.01$ mm^3	20-40 h
Temperature range	5-320 K

The main units of the new DN-6 diffractometer are shown in Fig. 9.

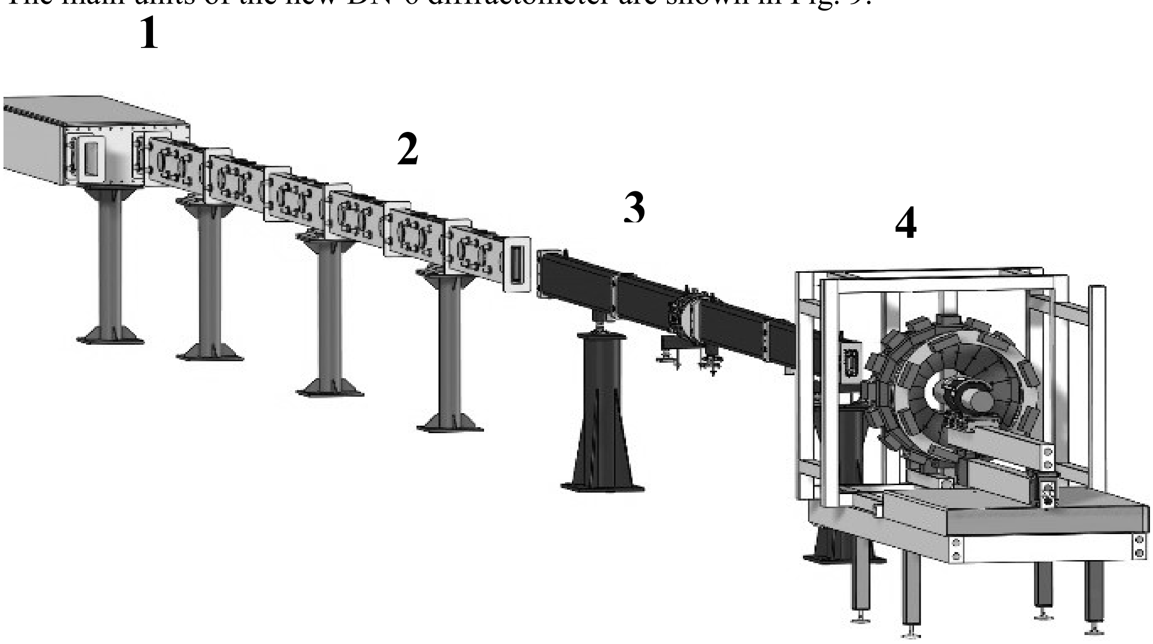

Fig. 9. *General layout of the DN-6 diffractometer at beamline 6B of the IBR-2 reactor. 1 – neutron beam splitter; 2 – curved section of the neutron guide in vacuum housing; 3 – parabolic focusing section of the neutron guide in vacuum housing; 4 – detector system and sample environment system.*

The optimum combination of the intense neutron beam at beamline 6B, use of a mirror neutron guide and the unique multi-detector system at DN-6 makes it possible to perform diffraction experiments with sample volumes of down to 0.0001 mm^3.

The neutron beam is formed by a three-section neutron guide. The first section is a neutron-optical splitter device that divides the incident neutron beam into two beams for the DN-6 diffractometer and the adjacent RTD diffractometer at beamline 6a, respectively. Then follows a 20-m curved section (coating m = 1, total radius of curvature of 1860 m). The dimensions of the neutron beam at the exit of this section are 165 × 15 mm^2. The third (end) section of the neutron guide is a parabolic system with the vertical focusing and coating m = 3 produced by SwissNeutronics (Switzerland). The beam focus (dimensions of 10 × 10 mm) is at a distance of 870 mm from the exit of the neutron guide. The new focusing section of the neutron guide enhanced the total neutron flux at the sample position by a factor of ~6. The total length of the entire neutron guide from the surface of the neutron moderator to the sample position is 30.5 m.

A helium refrigerator ($T \geq 4$ K) and high-pressure cells of different designs (including those with diamond anvils) are used to modify the sample environment. To extend the accessible pressure range, new pressure cells with sapphire and diamond anvils are being designed and manufactured.

A special frame provides fastening of the collimation system, detector system in a protective casing and helium refrigerator on one platform (Fig. 9). Low sample temperatures are achieved using a specially designed cryostat based on a closed-cycle helium refrigerator providing minimum temperatures of T ~ 5 K.

4.2. Detailed description of proposals for modernization of the instrument

1. DN-6 operates in the time-of-flight mode. It has two ring detectors for different scattering angles (see photo of one ring detector in Fig. 10).

Fig. 10. *Photo of one section of 90°-detector at DN-6 diffractometer. The detectors are placed in boron-polyethylene casings for suppressing background and consist of sixteen sectoral collimation modules and detector banks. Red boxes are electronic modules of preamplifiers of neutron counters.*

The first ring detector (Fig. 10) consists of 96 individual ^{3}He-counters arranged in the form of six rings of 16 detectors each with a radius of 350 mm. The detector system provides neutron detection in the range of scattering angles 2θ of 87-93°. Neutron diffraction spectra are obtained by summing the spectra from each detector element with the appropriate correction for the scattering angle.

In the frame of the development of the DN-6 diffractometer, it is planned to put into operation a second ring detector consisting of 96 detector elements, which requires the purchase of standard equipment, including neutron counters, preamplifier boards and electronics modules. The second ring detector has a different technical design intended to detect scattered neutrons in the range of angles 2θ of 35-43°. The electronics of the new detector ring will be based on the MPD32 module, which can provide data acquisition from 240 independent detector elements.

2. To expand the pressure range at the sample position, it is necessary to purchase high-pressure cells and a set of special equipment to support their operation.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

The new DN-6 diffractometer is located at beamline 6B, where a cold moderator is to be installed, which will make it possible to increase the intensity of the incident cold neutron beam in the wavelength range of 4 - 13 Å by a factor of ~7 to 10, which will significantly improve the quality of measured diffraction data in the interplanar spacing range d_{hkl}> 4 Å.

4.4. Expected technical parameters after modernization of the instrument

After modernization of the neutron guide system and installation of the second ring detector, the thermal neutron flux is expected to double. In addition, due to the commissioning of the ring detector for small-angle scattering, the d_{hkl} -range covered in experiments will be extended.

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

A neutron diffractometer for high-pressure research is planned to be built at the new neutron source of FLNP. Thus, the methodological and scientific development of neutron diffraction studies with high pressures is one of the promising and relevant areas for the future FLNP scientific program.

5. Expected scientific results, comparison with the world level

In recent years, pressure-induced modifications of the crystal structure and magnetic order in various materials were studied. A structural antiferroelectric-paraelectric phase transition was observed in double perovskite Pb_2MgWO_6 at high pressures above 0.9 GPa [10]. The structural and magnetic properties of siderite ($FeCO_3$) were studied at high pressures up to 7.5 GPa and complemented by *ab initio* calculations [11]. An unexpectedly large pressure coefficient of the Néel temperature and a decrease in the ordered magnetic moments of iron were revealed. The crystal and magnetic structures of nanostructured manganites [12] were studied at high pressures. At ambient pressure, the ferromagnetic (FM) phase coexists with an A-type antiferromagnetic (AFM) phase. Under high pressure, the volume fraction of the AFM phase increases, while the FM phase is gradually suppressed. The structural and magnetic properties of eskolaite (Cr_2O_3) were studied at high pressures up to 35 GPa [13]. The ground state of the AFM phase, which is magnetoelectrically active in external magnetic fields, was found to be stable in the entire pressure range under study, not confirming a magnetic phase transition that had previously been assumed from optical second-order harmonic generation experiments.

The advantage of the DN-6 diffractometer is that it can be used to study a wide range of systems with intermediate neutron scattering lengths and magnetic moments. For example, the values of the ordered magnetic moment of Cr^{3+} ions in Cr_2O_3 at low temperatures are only about 3 μB [13], which is typical for many transition metal oxides containing Cr, Mn, Fe ions, but significantly less than for most of the corresponding rare-earth elements.

To conclude, the DN-6 diffractometer provides possibilities for routine investigations of wide classes of materials with intermediate neutron scattering lengths and magnetic moments in a significantly extended range of high pressures (at present, in experiments it is possible to achieve a pressure of up to 35 GPa; the potentially possible values are of up to 50 GPa) and low temperatures. The appropriate configuration of the neutron guide system and the multi-element detector system in combination with a set of high-pressure cells with diamond and sapphire anvils makes the parameters of the DN-6 diffractometer comparable or superior to the parameters of the most advanced dedicated instruments in the other leading neutron scattering research centers.

6. Requested resources, costs and time frames of instrument modernization

The costs of the new ring detector and equipment for performing experiments with high pressures are given in **Table 5 (Section 4)**.

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DN-12 - Neutron Diffractometer for Investigations of Microsamples at High Pressures

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1. Abstract

A specialized diffractometer DN-12 for investigations of microsamples has been developed and constructed at the IBR-2 reactor in cooperation with the NRC "Kurchatov Institute" on the basis of the neutron diffraction technique for condensed matter studies at high pressures. The diffractometer makes it possible to carry out investigations in a pressure range of up to 8 GPa.

2. Scientific program, topicality and comparison with the world level

Neutron diffraction is the most direct and informative method for studying the crystal structure and magnetic order in materials. Because of comparatively low intensities of neutron sources, which are many orders of magnitude lower than those of synchrotron sources, the neutron diffraction studies in a fairly wide pressure range (up to 5-7 GPa and higher) have been restricted by the requirement of rather large sample volumes (at least several mm^3). A certain progress has occurred only in the last two decades. The corresponding neutron technique is developed only in a few most advanced neutron research centers in the world, among which is FLNP JINR. The DN-12 diffractometer provides possibilities for performing a complete analysis of both crystal and magnetic structures (from the same set of experimental data) of complex materials under pressure using high-pressure cells with sapphire anvils. At present, neutron scattering experiments with high-pressure cells are carried out only in a few most advanced neutron centers in the world. This is due to the fact that this kind of experiments can be done only at high-flux neutron sources on instruments equipped with advanced detector systems that provide good experimental statistics for appropriate data analysis. Until recently, the application of neutron methods, as a rule, has been restricted to the pressure range of 1-2 GPa, because of the use of relatively large samples in cells of the cylinder-piston type. The development of the method of neutron investigations at high pressures employing the technique of sapphire/diamond anvils in combination with low-background neutron diffraction has allowed us to extend the pressure range in experiments to several tens of GPa. Further development of the high-pressure technique, which is aimed at extending the accessible pressure range up to 30-50 GPa, requires an increase in the neutron flux at the sample position and the solid angle of the detector system.

The optimum combination of the intense neutron beam of beamline 12, mirror neutron guide and a unique multidetector system of the DN-12 diffractometer makes it possible to perform experiments with very small sample volumes down to 1 mm^3 at pressures of up to 8 GPa. The use of a cooled beryllium filter makes it possible to perform inelastic neutron scattering experiments in a wide pressure range. At present, the DN-12 diffractometer [1] is mainly used to study the atomic and magnetic structures of condensed matter at high pressures, 0 - 8 GPa, and low temperatures, 10 - 300 K. Neutron diffraction experiments on the DN-12 diffractometer provide possibilities to simultaneously determine characteristics of the crystal and magnetic structures of functional materials in a wide range of temperatures and external high pressures. Compared to other experimental techniques, the application of high pressure is a direct way to induce controlled changes in potential energy and atomic interactions in crystals (including magnetic interactions) by varying interatomic spacings and angles.

3. Scientific and methodological groundwork laid in FLNP JINR

During the period of operation of the diffractometer a number of successful studies have been performed, which, in fact, formed the basis for a new scientific direction consisting in systematic simultaneous investigation of the crystal and magnetic structure of the whole classes of functional materials widely used in various technologies: complex manganese oxides $R_{1-x}A_xMnO_3$ [2-4], cobaltites [5], organic ferroelectrics [6] and other compounds. It should be noted that besides the DN-12 diffractometer, neutron research with high pressures are performed in NRC ‘Kurchatov Institute’ (DISK diffractometer at the IR-8 reactor); ILL (France, D20 diffractometer), ISIS RAL (UK, PERL diffractometer), LLB (France, G6.1 diffractometer); ORNL (USA, SNAP diffractometer). However, in most cases, there are a number of limitations that do not allow conducting experiments to a full extent. For example, the DISK and G6.1 diffractometers have insufficiently high resolution to analyze fine features of complex atomic structures. The PEARL diffractometer is limited in the range of low temperatures (down to 80 K), as well as in the range of covered interplanar spacings, which is insufficient for analyzing the magnetic structure. The closest in experimental capabilities is the SNAP diffractometer (ORNL, USA). However, the limited range of covered interplanar spacings at this diffractometer is also insufficient for a full analysis of magnetic structures. Therefore, in other neutron centers the diffraction experiments with high pressures are performed only to analyze separately either the crystalline structure of relatively simple materials or the magnetic structure.

4. Current status of the instrument and proposals for its modernization

4.1. Information on the current status of the instrument

The main units of the new DN-12 diffractometer are shown in Fig. 11.

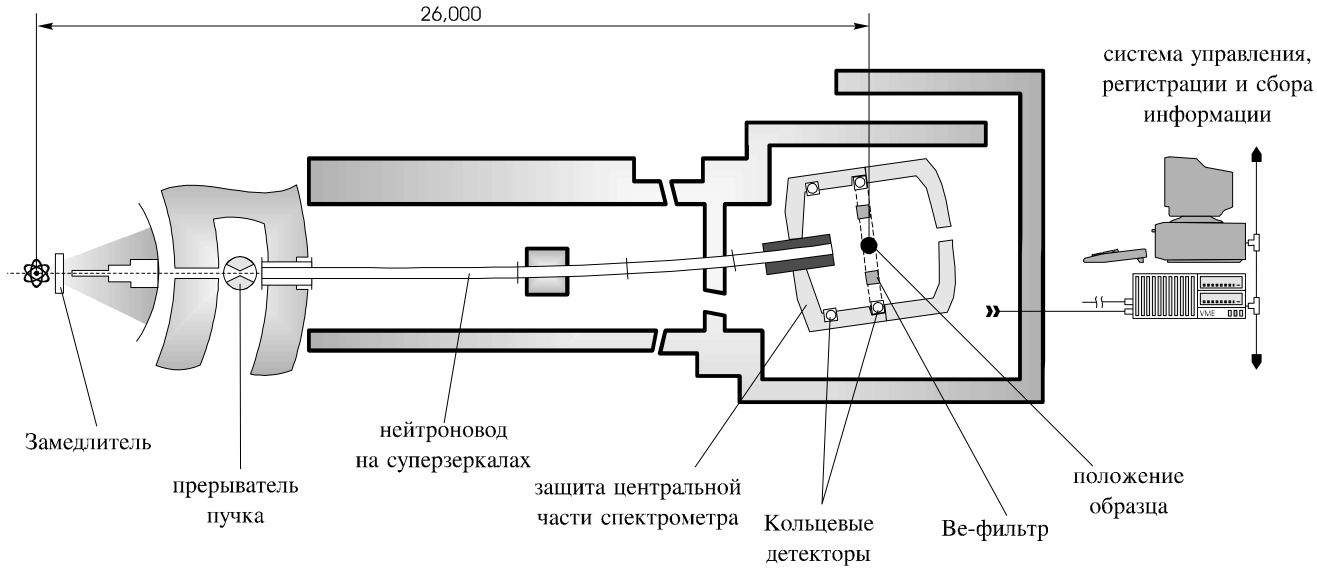

Fig. 11. *Layout of the DN-12 diffractometer.*

Main parameters of DN-12

Thermal neutron flux at sample position (n/cm²/s)		$1.5 \cdot 10^6$
Distances:	**moderator - sample**	26.0 m
	sample - detector	0.4 m
Ranges:	**wavelengths**	0.8÷10 Å
	Scattering angles	45°÷138°
	d_{hkl}	0.6÷10 Å
Resolution (Δd/d, d = 2 Å):	**at 2θ = 90°**	0.022
	at 2θ = 135°	0.012
Solid angle of detector system		0.125 sr
Sample volume, mm³		0.1 - 5
Pressure range		0-10 GPa
Characteristic spectrum measurement time		15-30 h
Temperature range		10-300 K

A closed-cycle helium refrigerator (for cooling down to T = 10 K) and high-pressure cells of different designs are used to modify the sample environment.

4.2. Detailed description of proposals for modernization of the instrument

1. To expand the range of experimental possibilities at the DN-12 diffractometer, it is planned to use a cryogenic system for cooling simultaneously a permanent magnet of up to 5 T and a high-pressure cell (cryocooler system). This device will allow us to conduct diffraction experiments at high pressures in magnetic fields. Therefore, one of the main tasks in the near future will be the commissioning and tests of the magnetic cryocooler. In addition, the design and manufacture of the fixing mechanism for the cryocooler at the DN-12 diffractometer is required. At present, work on the

design and manufacturing of a superconducting permanent magnet, which will expand the experimental possibilities of the diffractometer, is nearing completion.

2. It is planned to upgrade the detector system to increase its solid angle. This will enhance the luminosity of the diffractometer several-fold. To modernize the detector system, it is required to purchase neutron counters, preamplifier boards and electronics modules. The second ring detector has a different technical design intended to detect scattered neutrons in the range of angles 2θ of 35-43°. The electronics of the new ring detector will be based on the MPD32 module, which can provide data acquisition from 240 independent detector elements.

3. For experiments with high pressures, the purchase of sapphire anvils and the development of drawings for a new type of cells with sapphire anvils are required.

4. To expand the pressure range achieved in experiments, it is planned to purchase a large press with a force capacity of up to 100 kN. This will make it possible to conduct experiments with relatively large sample volumes (up to 100 mm^3) at pressures of up to 30 GPa. The unit also provides heating of samples, which will open the possibility of studying P-T diagrams at high temperatures (e.g., for geophysical samples).

5. It is required to purchase a set of special equipment for operating high-pressure cells with sapphire anvils.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

At present, DN-12 is located at beamline 12 of IBR-2, where the installation of the cold moderator is not planned.

4.4. Expected technical parameters after modernization of the instrument

After the modernization of the detector system, it is expected that the instrument luminosity will double. It will also be possible to perform neutron diffraction experiments on studies of P-T-H phase diagrams of materials. The installation and use of the press will expand the range of high pressures up to 30 GPa applied to samples with relatively large volumes (up to 100 mm^3).

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

A neutron diffractometer for high-pressure research is planned to be built at the new neutron source of FLNP. Thus, the methodological and scientific development of neutron diffraction studies with high pressures is one of the promising and relevant areas for the future FLNP scientific program.

5. Expected scientific results, comparison with the world level

The DN-12 diffractometer provides possibilities for routine investigations of wide classes of materials with intermediate neutron scattering lengths and magnetic moments in a significantly extended range of high pressures (at present, in experiments it is possible to achieve a pressure of up to 10 GPa) and at low temperatures. The appropriate configuration of the neutron guide system and the multi-element detector system in combination with a set of high-pressure cells with diamond and sapphire anvils makes the parameters of the DN-12 diffractometer comparable or superior to the parameters of the most advanced dedicated instruments in other leading neutron scattering research centers. The possibility to perform experiments simultaneously at low temperatures, high pressures and magnetic fields are unique and currently not implemented in other neutron centers.

6. Requested resources, costs and time frames of instrument modernization

The costs of the new ring detector and equipment for performing experiments under high pressures are given in **Table 6 (Section 4)**.

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EPSILON-MDS - Strain/Stress Diffractometer

Leader: F.R. Schilling (KIT, Germany)

Main participants: V.V. Sikolenko (KIT/FLNP)

Collaborating organizations: Karlsruhe Institute of Technology (KIT)

Operation of the instrument is supported by the German Federal Ministry of Education and Research

1. Abstract

EPSILON-MDS is a diffractometer for internal stress measurements in geologic and industrial samples. This instrument is a classical high-resolution time-of-flight diffractometer with a long flight path of more than 100 m and fixed scattering angle of 90°, that is best suited for internal stress studies. The instrument is equipped with a pressure device.

2. Scientific program, topicality and comparison with the world level

Current research at EPSILON-MDS focuses on:

- Gaining insight into microstructural processes (strain/stress) occurring before rock failure and earthquake formation.
- Investigation of particular microstructural processes in laboratory experiments under various pressures and temperature conditions.
- Studies of microstructural properties of potential storage rocks for radioactive and chemical wastes in order to assess the risk of waste disposal – in particular, the effect of temperature and fluids.
- Investigation of residual stresses in structural materials.

The high resolution of the EPSILON-MDS instrument makes is possible to investigate materials containing low-symmetrical phases, which is very important for studying rock samples and functional materials, and the large cross section of the beam (50×95 mm^2) allows the investigation of large sample volumes.

3. Scientific and methodological groundwork laid in FLNP JINR

The EPSILON-MDS setup was put into operation in 1993 and since then has been successfully used for implementing the FLNP scientific program. During the modernization of the IBR-2 reactor, it was radically upgraded. A separate beamline was equipped with a 105-m-long mirror neutron guide, and the number of detectors was increased to 81. In recent years, new sample environment equipment has been installed at the instrument, including an axial pressure device, pore pressure stress coupling device for geological applications and an acoustic emission detection system.

4. Current status of the instrument and proposals for its modernization

The EPSILON-MDS diffractometer comprises 9 radial collimator-detector units, each of them containing 9 detectors arranged at scattering angles 2θ ranging from 82 to 98°. The superimposition of diffraction spectra collected by each unit is performed by the time-focusing technique [1].

The diffractometer is equipped with a uniaxial pressure device EXSTRESS for *in-situ* strain experiments with cylindrical samples (external stress is up to 150 MPa). The pressure device allows the rotation of the sample in order to determine textural features. The macroscopic deformation of the sample is measured by means of a laser extensometer. In addition, acoustic emissions can be detected in order to determine the onset and progression of brittle deformation events during sample deformation. The whole diffractometer is placed in a cabin to keep the temperature constant for long-lasting experiments.

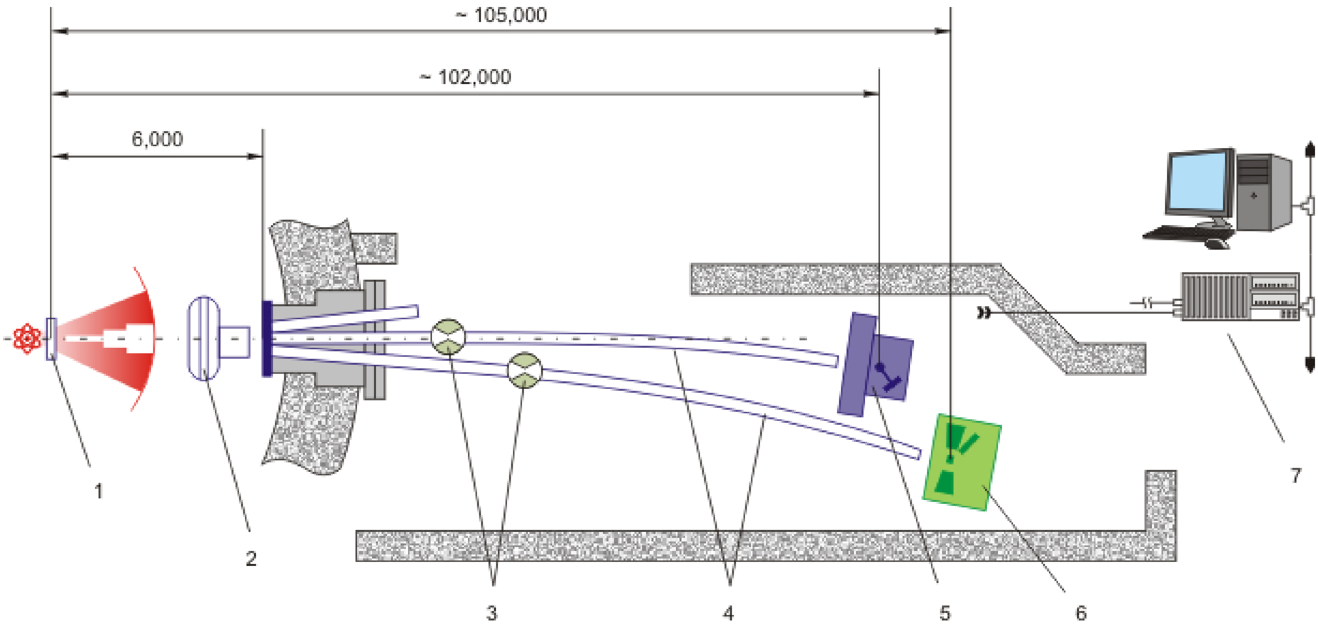

Fig. 12. *General layout at beamline 7A.*

1 – Moderator
2 – Background chopper
3 – λ-choppers
4 – Bent neutron guides (evacuated)
5 – Texture diffractometer SKAT
6 – Strain/stress diffractometer EPSILON-MDS
7 – PC-based experiment control and data acquisition system

The unique feature of beamline 7 of the IBR-2 reactor is that it views both moderators (thermal and cold) simultaneously, therefore the most suitable mode of the moderator complex for Epsilon is the cold mode, when the diffractometer resolves peaks with high d-spacing due to viewing the cold moderator and has a high flux in a short wavelength range due to viewing the thermal moderator.

The strain/stress diffractometer Epsilon is used for the detection of residual and applied strains and operated within the user program. It is planned to upgrade the detector system and the sample environment system by installing a new goniometer. In addition, advanced data analysis methods for determination of spherical strain data are planned to be employed. The neutron guide system is planned to be modernized as well. We are going to close the air gap at the lambda-chopper and insert a focusing part at the neutron guide near the sample position. Also, a possible option is the installation of 2D position-sensitive detectors, which is under consideration.

5. Expected scientific results, comparison with the world level

The new goniometer will also allow us to use this diffractometer for texture measurements, thus expanding its possibilities.

The new detector system will increase the luminosity of the diffractometer and place it among the ranks of the leading world classical instruments for internal stress investigations.

The EPSILON-MDS is a conventional TOF high-resolution diffractometer with a long flight path (105 m). It is a complementary instrument to the existing FSD and FSS. It has a comparable resolution and much lower background due to conventional TOF, but much lower neutron flux due to the longer flight path.

The EPSILON-MDS is perfectly suitable for geological studies. Its unique sample environment system has no analogues among those of other neutron diffractometers throughout the world. The important task is to maintain its competitiveness at the world-class level. A similar instrument should be definitively built at the new future neutron source of FLNP.

6. Requested resources, costs and time frames of instrument modernization

The cost of new equipment is given in **Table 7 (Section 4)**

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SKAT - Texture Diffractometer (project 1)

Leader: Nikolaev D.I.

Main participants: Lychagina T.I., Sikolenko V.V., Sekretarev Z.M., Vasin R.N., employees of NICM Department

Collaborating organizations: FSUE CRICM “Prometey” of NRC “Kurchatov Institute”; Borissiak Paleontological Institute RAS; National Research Nuclear University MEPhI; IMET RAS; Moscow Polytechnic University; Technical University, Prague, Czech Republic; Physical Institute, Prague, Czech Republic; University of Agricultural Sciences and Veterinary Medicine of Iasi, Romania; Danube Delta National Research Institute Tulcea, Romania; Mining and Metallurgical Academy Staszyca, Krakow, Poland

1. Abstract

The SKAT diffractometer successfully operates at beamline 7A-2 of the IBR-2 pulsed reactor. During its operation, a wealth of experience has been gained in respect to the design, development and modernization of the instrument, as well as the development of the technique for measuring spectra to obtain pole figures. Pole figures are necessary to calculate orientation distribution functions, which give a complete quantitative description of the crystallographic texture in polycrystalline samples. Its large beam cross section (50×95 mm^2) makes it possible to install a second ring with detectors (SKAT-2), and provides a natural way to almost double the efficiency of the instrument. A significant improvement in the data quality obtained in the experiments can be achieved by replacing the neutron guide with a more efficient and technologically advanced one.

2. Scientific program, topicality and comparison with the world level

The study of the crystallographic texture of polycrystals is of great interest for the research of metals, alloys, rocks and ceramics, as well as biological objects. Using the SKAT diffractometer, crystallographic textures of all the above types of polycrystals were successfully measured [1–9]. The SKAT diffractometer is one of the best neutron instruments in the world for studying crystallographic textures.

3. Scientific and methodological groundwork laid in FLNP JINR

During the operation of the SKAT diffractometer, a wealth of experience has been gained in respect to the design, development and modernization of the instrument, as well as the development of the technique for measuring spectra to obtain pole figures.

4. Current status of the instrument and proposals for its modernization

4.1. Information on the current status of the instrument

At present, the diffractometer (Fig. 13a) successfully operates within the framework of the user program. However, the intensity of the neutron beam of beamline 7A-2 is insufficient (neutron flux of the order of $\sim 10^5$ n/cm^2/s). With such a neutron flux, 60-80 samples per year are measured with constantly used secondary beam collimators with a divergence of 45 arcmin. If we use the available collimators with a divergence of 18 arcmin, then the number of samples would be 20-40 per year. It should be noted that out of 83 days requested by users for measurements in the first half of 2020, it was possible to allocate only 40.

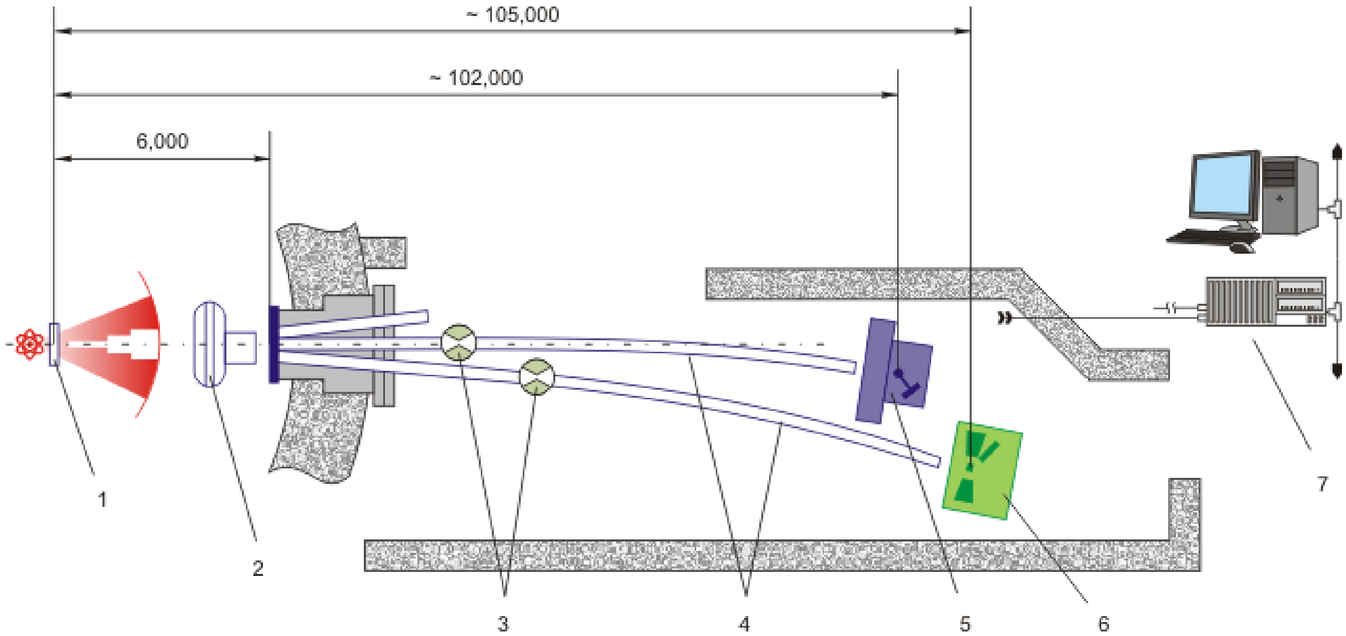

Fig. 13a. *Schematic layout of the SKAT spectrometer: 1 – moderator, 2 – background chopper, 3 – λ-choppers, 4 – curved neutron guides (evacuated), 5 – SKAT texture diffractometer, 6 – EPSILON-MDS diffractometer, 7 – experiment control and data acquisition system.*

Main parameters of the SKAT diffractometer

Flight path	~ 104 m		
Scattering angles 2θ	65° / 90° / 135°		
λ_{max}	7.0 Å / 14.6 Å		
2θ parameters	2θ = 65°	2θ = 90°	2θ =135°
d_{max}			
Maximum resolution Δd/d	$6.2 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$	$3.1 \cdot 10^{-3}$
Flight path of the scattered beam	1.10 m	1.10 m	0.95 m
Neutron guide	Cross-section: 50 mm (width) × 95 mm (height) Radius of curvature: 13400 m Coating: natural Ni (m = 1) Optionally: the chopper blocks each second neutron pulse		
Detectors	Set of 193 detectors based on ^{3}He tubes. P = 4.5 bar Ø = 60 mm		
Collimators	Soller type, Gd coating Angular divergence: 18' / 45' Cross-section: 55 × 55 mm^2		
Sample positioning	3-axis goniometer		
Data treatment	SONIX software PC Windows		

4.2. Detailed description of proposals for modernization of the instrument

- In the case of installation of a second ring with detectors and a goniometer, the available neutron guide cross section will allow measurements with two samples simultaneously. It is proposed to install the second ring for simultaneous measurements with two samples.
- The new neutron guide will make efficient the use of 18'-collimators on the existing ring. In addition to the increased instrument productivity, this will improve the instrument resolution for studying multiphase samples.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

Reflexes in the range of 0.6-5 Å can be effectively studied at the SKAT diffractometer for obtaining pole figures corresponding to the crystallographic indices of planes with interplanar spacing in the specified range. The cold moderator provides the best intensity of diffraction reflexes in the range of 2.8-5 Å, but with worsening intensity in the range of 0.6-2.7 Å. For structural and biological materials, almost all reflexes are in the range of up to 2.5 Å. At the same time, many geomaterials have reflexes in the range of 2.8-5 Å. Thus, the measurement of geomaterial samples is most effective with the cold mode of the moderator. For measurements of samples of structural and biological materials, the operation of the moderator in the thermal mode is more preferable.

4.4. Expected technical parameters after modernization of the instrument

Main expected parameters of the second ring of the SKAT diffractometer (Fig. 13b)

Flight path	~ 105 m
Scattering angles 2θ	90°
λ_{max}	7.0 Å
d_{max}	
Maximum resolution Δd/d	$5.0\cdot10^{-3}$
Flight path of the scattered beam	0.85 m
Neutron guide	Cross-section: 50 mm (width) × 47 mm (height) Radius of curvature: 13400 m Coating: natural Ni (m = 1)
Detectors	Set of 40 detectors based on ^{3}He tubes, P = 4.5 bar Ø = 50 mm.
Collimators	Soller type, Gd coating Angular divergence: 30' Cross-section: 55 × 55 mm^2
Sample positioning	1-axis goniometer
Data treatment	SONIX+ software package for Windows

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

The relevance of the development of the diffractometer is reflected in the fact that in every neutron center in the world there are 1-2 texture instruments. This is due to the need to measure a large number of samples. The measurements are done for only from one-third to one-half of the total number of samples requested in the experimental proposals.

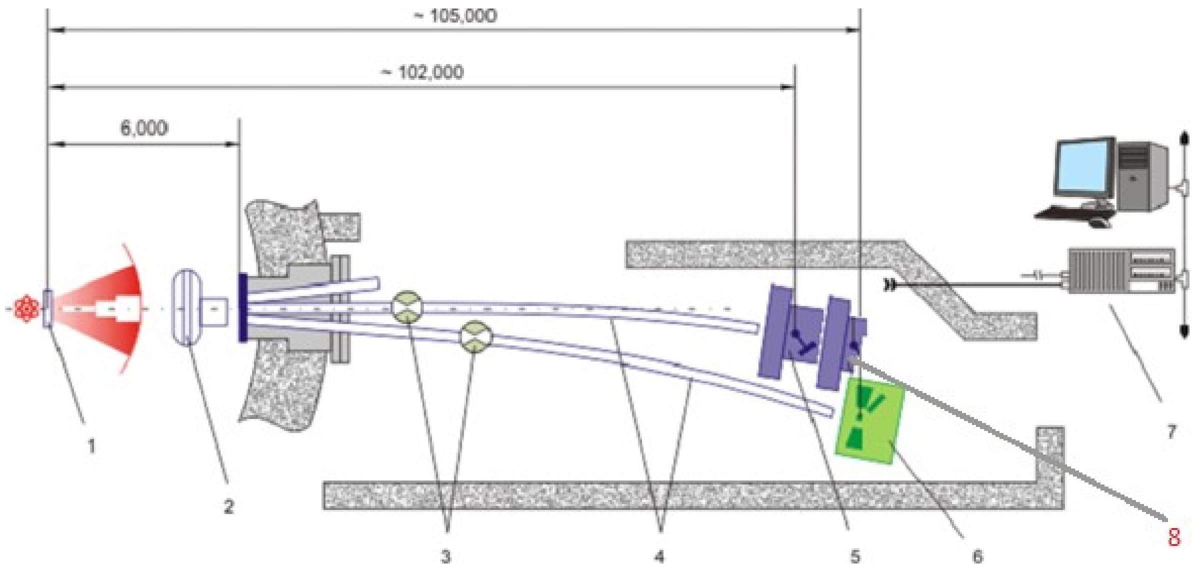

Fig. 13b. Schematic layout of the SKAT - SKAT-2 instrument: 1 – moderator, 2 – background chopper, 3 – λ-choppers, 4 – curved neutron guides (evacuated), 5 – texture diffractometer SKAT, 6 – EPSILON-MDS diffractometer, 7 – experiment control and data acquisition system, 8 – texture diffractometer SKAT-2.

5. Expected scientific results, comparison with the world level

The parameters of the SKAT diffractometer are up to the world-class standards, which allows us to confidently speak about the competitiveness of SKAT as compared to the world analogues. At present, there are about ten instruments (with different degrees of readiness and availability) throughout the world, where it is possible to measure full pole figures for coarse-grained samples. A great demand for these instruments is reflected in the fact that there are 1-2 texture instruments in each neutron center. In this regard, the parameters of the Russian neutron source, the IBR-2 reactor, make it possible to be involved in the overall development of neutron sources and improve the SKAT instrument to maintain its high world-class level from the point of view of the global research infrastructure.

6. Requested resources, costs and time frames of instrument modernization

It is planned to develop and manufacture the second detector ring, which requires the purchase of standard equipment, including neutron counters, collimators, preamplifier boards and electronics modules. To study the crystallographic texture of high-temperature phases in structural materials, it is necessary to purchase heating chambers (up to 1000ºC) and a set of special equipment for their operation.

The costs of the new detector ring and experimental equipment are shown in **Table 8 (Section 4)**.

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SKAT - Texture Diffractometer (project 2)

Leader: Vasin R.N.

Main participants: Employees of SC and NICM Departments

Collaborating organizations:
University of Bonn (Germany)
University of Gottingen (Germany)
Kiel University (Germany)
University of California at Berkeley (USA)
Institute of Geology of the Academy of Sciences of the Czech Republic (Czech Republic)
Institute of Geophysics, Academy of Sciences of the Czech Republic (Czech Republic)
FSUE CRI CM “Prometey” NRC “Kurchatov Institute”
Paleontological Institute RAS (Russia)

1. Abstract

The SKAT diffractometer is operated at beamline 7a2 of the IBR-2 reactor under support of the German Federal Ministry of Education and Research. The main task of the diffractometer is to measure crystallographic textures in rocks and engineering materials. Due t o the high penetrating power of thermal neutrons, it is possible to measure bulk textures and provide the grain statistics necessary for the quantitative texture analysis of coarse-grained materials.

In recent years, the number of beamtime applications at the SKAT diffractometer exceeded the capabilities of the instrument. The proposed development of the detector system and the application of new methods of data analysis will reduce the time of experiments by several times. The use of sample environment systems will expand the range of tasks that can be solved at SKAT.

2. Scientific program, topicality and comparison with the world level

Neutron diffraction texture analysis cannot be attributed to common methods for studying preferred grain orientations. A great number of studies in this area are carried out with laboratory X-ray diffractometers, and in recent decades – at the sources of synchrotron radiation and, in particular, with electron microscopes using electron backscattering (EBSD). However, in comparison with these methods, diffraction of thermal neutrons has a number of unique advantages that make it possible to solve important problems in geophysics and materials science.

Using neutron diffraction, it is possible to study textures in the bulk of materials, in contrast to other methods, which are limited to studying either the surface or extremely small ($<< 1$ cm^3) sample volumes. This is important when studying materials in which sharp local textures or texture gradients are observed. For coarse-grained samples of rocks, alloys and composite materials with grain sizes of the order of several millimeters, the use of neutron diffraction is the only way to provide the grain statistics necessary for quantitative texture analysis. One of the important features of the neutron diffraction texture analysis is that, generally, no special sample preparation is required. This makes it possible to study textures in unique specimens, for example, objects of cultural heritage.

These peculiarities determine the scientific program of SKAT. Investigations of rock textures arecarried out with the aim to analyze deformation processes in minerals and accompanying changes incrystallographic textures [1-3] to gain an insight into the evolutionary processes in the lithosphere. A large amount of research work is aimed at studying the relationship between the preferred grain orientations of various minerals, shape textures, fractures and porosity with elastic rock anisotropy, as well as with the seismic anisotropy of the lithosphere [4-9]. For these studies, it is particularly important to have a possibility of direct comparison of the results of numerical modeling of elastic properties of a material, which is based, among other things, on the information about the textures and mineral composition of the rock obtained in the neutron diffraction experiment, with the results of laboratory ultrasound studies conducted with the same sample. Due to the peculiarities of elastic wave propagation and the models used, the optimum linear size of samples in this case is ~ 5 cm, which ideally matches the capabilities of SKAT.

In the field of materials science, the effect of thermomechanical processing on the preferred orientations of grains in special steels and various alloys is studied [10, 11] in order to optimize production processes. The textures formed during the growth of shells of mollusks of various species are studied [12].

In recent years, we have made several comparisons of the SKAT capabilities with those of other texture instruments, such as neutron time-of-flight instruments (mainly, the HIPPO diffractometer, Los Alamos) and diffractometers at steady-state neutron sources, synchrotron radiation sources, as well as with EBSD [3,4,11]. These comparisons showed that the quality of the results obtained at SKAT is up to the world level. However, the measurement time for one sample at SKAT is usually several times (and sometimes an order of magnitude) longer than that other time-of-flight diffractometers offer. Regarding this parameter, SKAT is inferior to the instruments operating at powerful steady-state reactors, where texture measurements are carried out using the standard technique with sequential measurements of several pole figures.

To summarize, it can be concluded that the scientific program at SKAT is highly relevant. The obtained results are up to the world level. The unique features of the instrument are high angular resolution in pole figures and possibility to perform experiments with large (~100 cm^3) samples. However, the measurement time for one sample is extremely long and unsatisfactory from the viewpoint of the world standards. This is an obstacle for studying extended series of samples. The proposed development of SKAT will eliminate this problem and expand the range of scientific tasks to be solved.

3. Scientific and methodological groundwork laid in FLNP JINR

In FLNP, vast experience has been gained both in operating time-of-flight neutron texture diffractometers and in processing the obtained data. The FLNP employees themselves have developed or participated in the development of software for processing and analysis of texture data, for example, the Beartex software package [13]. The methodological work is conducted to optimize methods for measuring textures, processing and analyzing data [14-17]. The experience in the development and construction of detector systems gained at FLNP makes the proposed development of SKAT easy to implement.

4. Current status of the instrument and proposals for its modernization

4.1. Information on the current status of the instrument

SKAT (Fig. 14) was put into operation in 1998 [18] and shared the beamline with its predecessor, the NSVR texture diffractometer; then, at the same beamline, the construction of the Epsilon diffractometer started. During the modernization of the IBR-2 reactor in 2007-2011, the NSVR diffractometer was dismantled, and SKAT and Epsilon were provided with individual beamlines with separate neutron guides coming from the splitter (Fig. 15). The new curved neutron guide (nickel coating, m = 1) at beamline 7A2 (SKAT) has a cross section of 95 × 50 mm^2 and a radius of curvature of 13400 m [19].

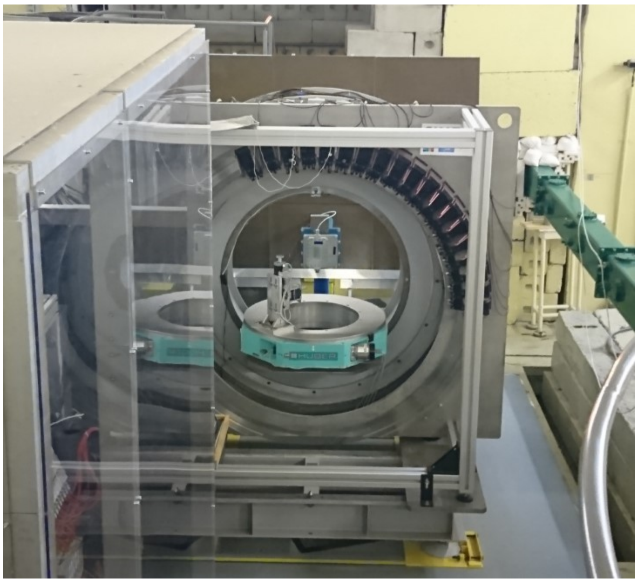

Fig. 14. *SKAT diffractometer in the experimental hall. Right: neutron guide of the NERA spectrometer. Left: "glass" room of the Epsilon diffractometer.*

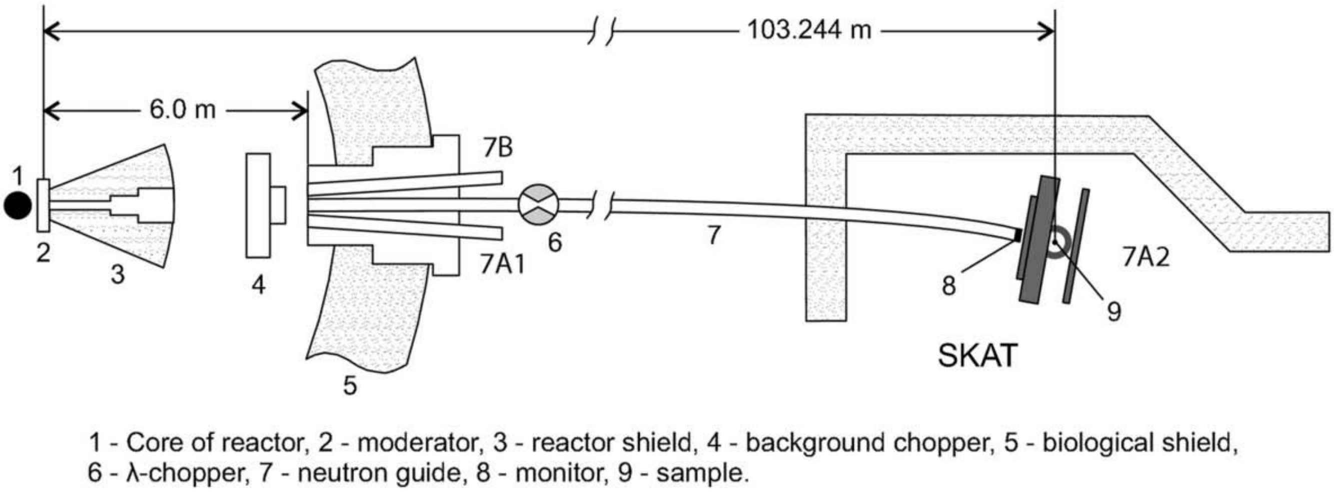

Fig. 15. *Schematic layout of beamline 7A2 [19].*

In the current configuration of SKAT, the detector system consists of nineteen ^{3}He counters mounted on a ring support with a radius of 1 m; 45′ Soller collimators with a cross section of 55 × 55 mm [18,19] are placed at each detector. The total solid angle covered by the detector system is ≈ 0.013 sr. Therefore, in order to provide the coverage of pole figures sufficient to reconstruct the grain orientation distribution functions, the sample is rotated in the goniometer around the axis inclined at an angle of 45° to the incident neutron beam. To obtain complete pole figures in a 5° × 5° grid, measurements are made in 72 sample orientations, i.e. 19 × 72 = 1368 diffraction spectra are collected. The angular resolution in pole figures is ≈ 3° [4].

A large beam cross section allows one to study samples with a volume of up to ≈ 100 cm^3, which is extremely important in research of polymineral coarse-grained rocks. A long time-of-flight path (moderator-to-sample distance is ≈ 103.3 m) in the current SKAT configuration provides the lattice spacings resolution Δd/d of up to ≈ 0.8% at d ≈ 2 Å. There is also a set of 18′ collimators for detectors; their use improves the resolution by ≈ 25%, but significantly reduces the intensity of the recorded spectra and, accordingly, increases the required measurement time. The available wavelength range is ≈ 1-7.3 Å; there is a possibility of using a λ-chopper to "skip" every second reactor pulse and expand the range ~~up~~ to λ ≈ 14.7 Å.

The large distance to the moderator also results in a low neutron flux at the sample. On average, it is 10^6 n cm^2/s and has a strongly asymmetric distribution over the neutron guide cross section (Fig. 16).

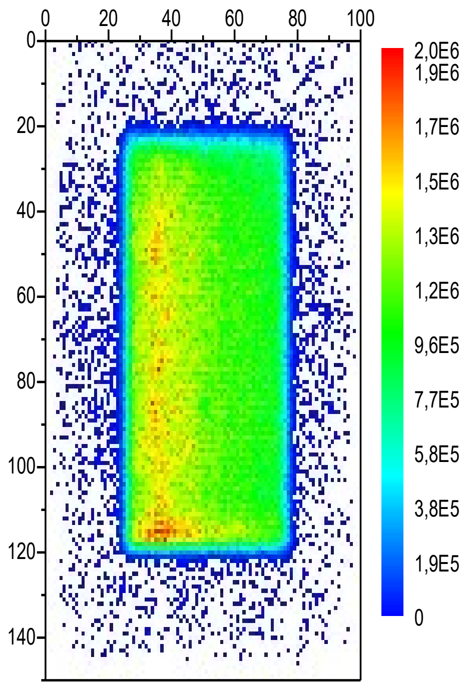

Fig. 16. *Distribution of the neutron flux density in the cross section of the SKAT neutron guide, at a distance of 6 cm from the exit of the neutron guide (measurements and figure by A.V. Churakov).*

It should be noted that the new neutron guide did not lead to an increase in the neutron flux density at SKAT for the thermal mode of the moderator; the gain is observed only for the combined (thermal + cold) mode of the moderator, the use of which increases the neutron flux in the range of wavelengths > 2 Å [20]. Even for the combined mode of the moderator, it takes more than one hour to accumulate diffraction spectra from a large (> 10 cm^3) sample of polymineral rock, i.e. the total measurement time for complete pole figures with a sample rotation step of 5° is more than 3 days, and more than 1 day with a sample rotation step of 15°. If the rock is composed mainly of weakly scattering low-symmetric minerals (for example, feldspars), this time increases.

Therefore, the use of large-volume samples is not only a distinctive feature of SKAT, but also an urgent necessity for providing a reasonable measurement time.

4.2. Detailed description of proposals for modernization (construction) of the instrument

The main problem of SKAT is a very long measurement time per one sample, which will increase with a decrease in the power of the IBR-2 reactor. To reduce the measurement time for each sample orientation, it is necessary to increase the neutron flux. However, the design and modernization of a 100-m-long neutron guide require considerable time and financial investment. Therefore, it is proposed to perform the neutron flux simulation in the case of dismantling the splitter of channel 7 (after consideration and approval by the Epsilon and NERA groups). The maintenance of high vacuum in the splitter faces difficulties, which is one of the main sources of neutron flux loss. The dismantling of the splitter can provide a gain in the neutron flux for all three instruments at beamline 7 (SKAT, Epsilon,NERA).

The reduction in the measurement time at SKAT can also be achieved by reducing the number of sample orientations in the measurement. The operating instruments such as HIPPO (LANSCE), GEM (ISIS), iMateria (J-PARC MLF), as well as the time-of-flight diffractometers under construction as POWTEX (FRM II), BEER (ESS), that are used for measuring crystallographic textures, are equipped with either numerous arrays of detectors installed at different scattering angles, or large-area position sensitive detectors. They provide simultaneous measurements along a large number of directions of scattering vectors and, as a result, a high speed of measurement of sample textures (down to several minutes for steel samples at the iMateria diffractometer, no sample rotation is required [21]). For data analysis, a modified Rietveld method, the so-called RITA (Rietveld Texture Analysis), is used [22].

The installation of additional detectors at SKAT will make it possible to measure a sample over a fewer number of orientations and thus reduce the measurement time. SKAT is already equipped with mounting places for detectors at scattering angles of $2\theta = 65°$ and $2\theta = 135°$ in addition to the main 90°-detector ring (Fig. 17). By placing there ^{3}He counters with Soller collimators, we will achieve good c overage of pole figures to reconstruct orientation distribution functions with high resolution. The installation and tests of the new detectors can be carriedout without suspending physicsexperiments, since the 90°-detector ring remains unchanged. The adaptation of the data analysis software upon completion of the proposed development of the SKAT diffractometer using RITA can be done very quickly using the experience with the previous implementation of the software for the current SKAT configuration [3].

The shortening of the measurement time for one sample after the installation of additional detectors at SKAT will lead to a relatively frequent sample change (≈ 3-4 samples per day). Normally, the regular procedure of closing the beam shutter of channel 7, placing a new sample and opening the shutter again takes about 12 min; also, during this period the experiments at the Epsilon diffractometer and the NERA spectrometer are suspended. In order to save “beam time”, it is proposed to develop and install an automatic sample changer with a capacity of 6-8 samples. As a rule, the weight of rock samplesmeasured at SKAT does not exceed 0.2 kg; large steel samples can weigh more than 0.5 kg. Therefore,the sample changer must provide a change of non-standard samples weighing up to 1 kg.

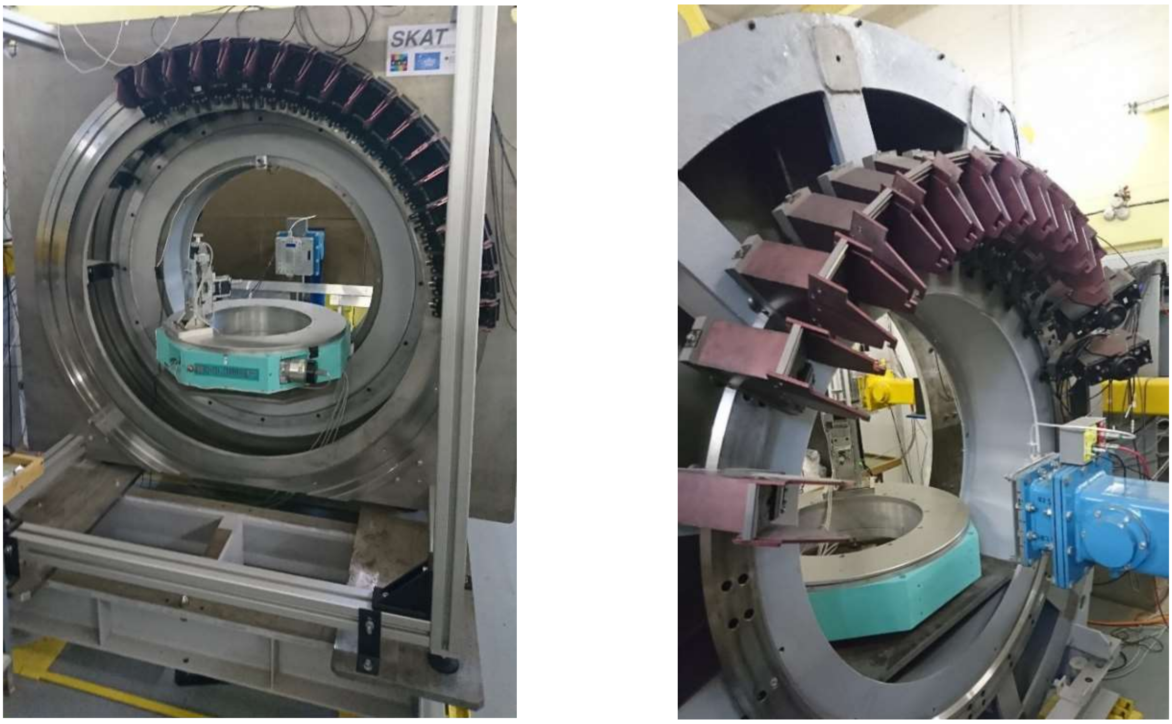

Fig. 17. *Currently available mounting places for detectors at scattering angles 2θ = 65° (left) and 2θ = 135° (right) at the SKAT diffractometer.*

In order to further develop the experimental technique and improve the SKAT characteristics, it is planned to order, manufacture and install a small PSD detector (50 × 50 cm) with good spatial resolution (<0.5 cm). This will increase the solid angle of the detector system, assist in testing and polishing the technique for measuring textures using 2D detectors, and improve the quality of measurements.

In addition, currently SKAT is one of the few instruments that is not equipped with sample environment systems. To expand the range of scientific tasks, which can be solved at the instrument, it is planned topurchase a compact furnace for sample heating of up to ~ 1000 °C.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

The use of a combined (thermal + cold) mode of the moderator at channel 7 increases the neutron flux in the range of wavelengths > 2 Å. This is of great importance for texture analysis of rocks, which are mainly composed of minerals with large lattice parameters (~ 10 Å). The comparative analysis of identical samples has shown that the use of the combined mode of the moderator leads to an increase in neutron statistics in the most interesting wavelength range by a factor of ≈ 4 on the average, which is especially important for accurate determination of strong textures and volume fractions of accessory (~ 1 vol.%) minerals (Fig. 18) [20]. At the same time, for weakly textured, well-scattering materials, especially for cubic and hexagonal metals and alloys, in which almost all diffraction peaks are in the range of lattice spacings of < 3 Å, the gain factor when using the combined mode of the moderator is negligible, and they can be measured at the thermal mode of the moderator. Since at SKAT polymineral rocks are measured most of the time, it is optimal to schedule at least 7 out of 9 reactor cycles per year with the combined mode of the moderator.

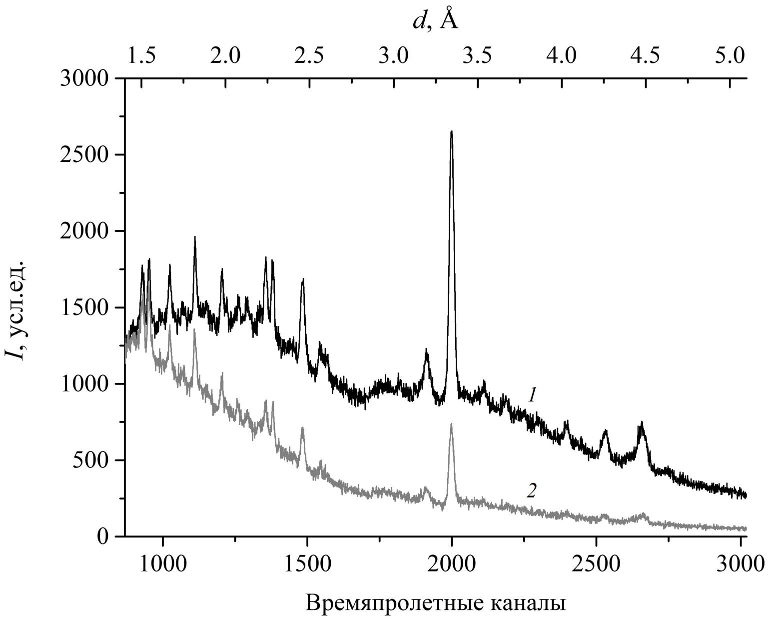

Fig. 18. *Diffraction spectra of a sample of metamorphosed slate measured with the SKAT diffractometer at the combined (1) and thermal (2) modes of the moderator. The measurement time is 2 hours, the scattering vector lies in the plane of rock foliation [20].*

4.4. Expected technical parameters after modernization of the instrument

The estimates made for the SKAT diffractometer [19] showed that ~ 350 spectra are sufficient for qualitative determination of the orientation distribution function, even for polymineral rocks in which a strong overlap of diffraction peaks is observed. For simple single-phase materials, ~ 150 spectra are sufficient; the relatively non-uniform coverage of the pole figure in this case does not lead to texture distortions. This is confirmed by the conclusions made when analyzing data from the iMateria time-of-flight neutron diffractometer [21]: ≈ 132 spectra are sufficient to determine the orientation distribution function for a non-uniform coverage of the pole figure with a good angular resolution.

Thus, at SKAT equipped with three detector sets at scattering angles of $2\theta = 65$, 90, and 135°, the measurements at 4–8 sample orientations will be sufficient, compared to the currently commonly used36–72 sample orientations, reducing the required measurement time several-fold. The optimal measurement grids with 6 sample orientations are shown in Fig. 19. Spectra from detectors at $2\theta =$ 65° will have better intensity and the covered range of lattice spacings will be extended up to ≈ 6.8 Å. Spectra from detectors at $2\theta = 135°$ will have ~1.5-fold higher resolution, allowing better separation of peaks frommultiphase samples in the middle range of lattice spacings (Fig. 20).

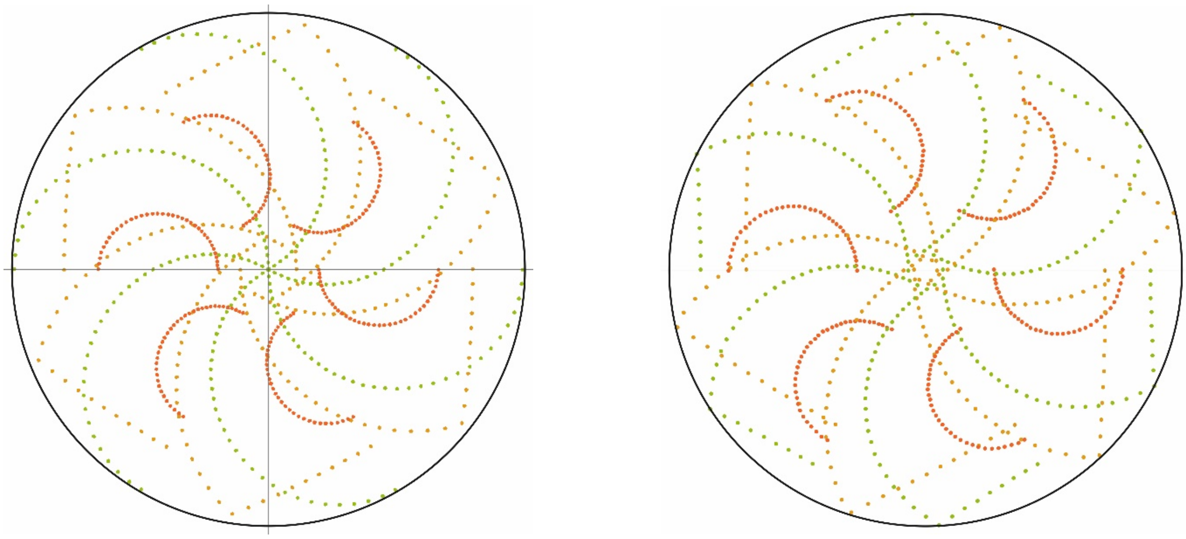

Fig. 19. *Coverage of pole figures when the sample rotation axis is inclined at 45° (left) and 52.5° (right) to the incident beam with the detectors at scattering angles 2θ = 65° (yellow), 90° (green) and 135° (red). The sample rotation axis is in the center of the stereographic projection, 6 orientations of the sample.*

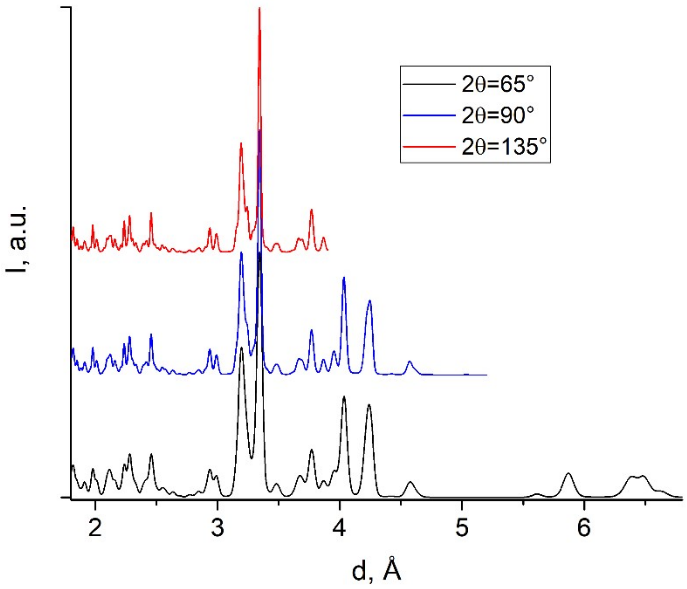

Fig. 20. *Normalized neutron time-of-flight spectra of rock (granite) consisting of common minerals: quartz, two feldspars and mica (biotite), from standard 90°-detectors of SKAT with 45' collimators and expected (simulated) spectra for 65°- and 135°-detectors.*

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

As noted above, an advanced time-of-flight neutron texture diffractometer should have a multi-detector system that covers the largest possible solid angle to minimize the number of sample rotations and the experiment time, which potentially opens up possibilities for *in situ* measurements of textures during deformation processes, phase transformations, etc. Therefore, the proposed development of SKAT is undoubtedly important for the development of the concept of a suite of instruments at the future next-generation neutron source of FLNP.

5. Expected scientific results, comparison with the world level

As noted above, the scientific program at SKAT is up to the world level, and the main problem is the long sample exposition time, which does not allow measuring extended series of samples. The proposed development of SKAT should eliminate this drawback.

The use of 2D PSD detectors will make it possible to measure materials with very sharp textures or small grain misorientations.

The new compact furnace will allow measuring crystallographic textures at various temperatures, in particular, for studying changes in crystallographic textures during phase transitions. This topic is of unfailing interest from the point of view of geophysics/mineralogy, and, mainly, in materials science, for example, in the study of alloys undergoing thermoelastic martensitic transformations.

6. Requested resources, costs and time frames of instrument modernization

The time frames and costs of SKAT units to be manufactured and upgraded are given in **Table 9 (Section 4)**.

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YuMO - Small-Angle Neutron Scattering Instrument

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Collaborating organizations: MSU, MIPT, A.N.Belozersky Institute of Physico-Chemical Biology of MSU, PNPI

1. Abstract

The project aims at creating and developing the small-angle neutron scattering instrument operating at IBR-2 beamline 4. The implementation of the project will allow us to improve the quality of obtained data (by changing the detector type), expand the range of available scattering vectors, increase the experimental data acquisition rate, and improve the resolution and background conditions. The development and construction of new position-sensitive detectors, including a direct-beam detector, will make it possible to conduct experiments with anisotropic samples and expand the possibilities of the sample environment system (magnetic field, fluid rotation, etc.). As a result of the modernization, the already existing wide community of users of the instrument will be significantly enlarged.

2. Scientific program, topicality and comparison with the world level

Small-angle neutron scattering is widely applied for investigations of the nanoscale structure of matter, being an effective method for studying fundamental problems and for solving important technological problems. Using the YuMO instrument (Fig. 21), studies are conducted in the field of condensed matter physics, physical chemistry of dispersed systems, aggregates of surfactants, biophysics and biology, polymeric substances, metallurgy, materials science, etc. [17-45]. The most important feature of small-angle scattering is the possibility to analyze the structure of disordered systems. This method, for example, is often the only way to obtain structural information about systems with chaotic and partially ordered distributions of density inhomogeneities with sizes of 10-10000 Å. It makes it possible to study the dispersed structure of alloys, powders, glasses (phase separation mechanisms, size and degree of polydispersity of particles), structural features of polymers in various states of aggregation, weight and geometric characteristics of biological macromolecules and their complexes, biological nanoscale structures, such as biological membranes and viruses. The significant difference in coherent neutron scattering lengths of hydrogen and deuterium together with the possibility of specific deuteration of macromolecules and nanoscale structures make the small-angle neutron scattering technique an indispensable tool for studying biological, colloidal objects, as well as polymers and liquid crystals.

3. Scientific and methodological groundwork laid in FLNP JINR

One of the first neutron small-angle instruments that appeared in the world was a setup in ILL. At time-of-flight sources, the first small-angle instrument was constructed at JINR, at IBR-30 in 1975. Over the past almost half a century, numerous methods and designs have been proposed and developed, including: two-detector data acquisition system, direct axial geometry, long total flight and collimation paths, use of vanadium calibration standard during the experiment, specific geometry of detectors, including direct-beam detector. In the framework of methodological activities, programs of raw data treatment and fitting of scattering curves were successfully developed in collaboration with LIT JINR. Experiments are under discussion to verify the results obtained in the course of the theoretical work on small-angle scattering on deterministic fractals.

The YuMO small-angle scattering diffractometer is the most in-demand instrument at the IBR-2 reactor. During its operation, several hundred journal papers based on the experiments performed with YuMO were published. The range of research areas at the YuMO instrument is continuously expanding.

4. Current status of the instrument and proposals for its modernization

4.1. Information on the current status of the instrument

At present, the YuMO instrument has a number of specific features, including: two-detector data acquisition system, direct axial geometry, long total flight and collimation paths, use of vanadium calibration standard during the experiment, specific geometry of detectors, including direct beam detector, wide wavelength range, chopper, as well as full experiment automation, including primary data processing and additional sample environment options (temperature, pressure, and magnetic field) [1-16].

The instrument (viewing the grooved moderator) has a high flux at the sample position, and due to its two-detector system, – a wide dynamic range. The modernization of the instrument carried out earlier opened up new possibilities.

4.2. Detailed description of proposals for modernization of the instrument

The parameters of the instrument to be improved after the implementation of the project are: range of available scattering vectors Q_{min} - Q_{max}, experimental data acquisition rate, type of neutron detectors, resolution, and background conditions.

1) The extension of the Q-range will be achieved by replacing the detectors, eliminating the air gaps along the neutron flight path, and improving the collimation of the neutron beam. Two position-sensitive detectors (PSD) and one direct-beam detector are to be installed. The first PSD will be located in the nearest position (2–8 meters from the sample), in the case of the second PSD, there will be a possibility of changing positions and placing it at a distance from 5 to 13 meters from the sample. The introduction of a two-detector system will require, in turn, changes in the collimation system, electronic equipment (data acquisition system) and qualitative changes in the software. In addition, a combined analysis of experimental data from different detectors will require methodological improvements in the existing approach. These changes will be based on

methodological [7–11] and scientific [12] achievements, as well as on already partially developed software [11], which will significantly reduce the project costs.

2) The enhancement of resolution (first of all of spatial resolution of PSD) will require improving spatial alignment of the detectors, which in turn will call for development, construction and installation of alignment mechanisms for large detectors and vanadium standards.
3) An increase in the data acquisition rate will be achieved by means of simultaneous detection of scattered neutrons by several detectors positioned so as to cover the entire required (available) range of scattering vectors, by increasing the efficiency and active areas of the detectors, as well as by improving the background conditions.
4) Since at YuMO, the width of the resolution function for the momentum transfer is mainly determined by the angular contribution (the contribution from the pulse width is small), its decrease will be achieved by improving the spatial resolution of the detector and of the corresponding collimator.
5) The possibility to measure samples with small scattering cross sections will be provided by significantly reducing the background with the help of a new chopper and a new collimation system, as well as by using advanced detectors and detector electronics.
6) The range of sample environment equipment will be expanded to enable investigations with additional conditions at the sample. This, in the first place, concerns the possibility of conducting rheological studies, investigations under high pressure and magnetic field, experiments with the rotation of the sample and over an extended temperature range.
7) The modernization of the instrument will be accompanied by corresponding changes in the software.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

Almost all present-day small-angle scattering instruments operate at cold neutron sources. This is primarily due to the need to perform experiments in the widest possible range of momentum transfer, Q, and to achieve the minimum possible Q. The installation of a cold moderator at a steady-state reactor results not only in an increase in the wavelength (and consequently in a decrease in the value of the scattering vector modulus and the appearance of the possibility of studying larger objects), but also in the gain in the neutron flux by more than one order of magnitude. Therefore, there developed a world-wide paradigm of the necessity to use cold moderators. The situation at the IBR-2 pulsed reactor is quite different. The low average reactor power (2 MW) is compensated by the wide range of wavelengths used. As a result, the YuMO instrument with a direct view of the grooved moderator at room temperature makes it possible (in the absence of a neutron guide) to provide a high neutron flux at the sample position [9]. The use of a cold moderator gives only a small gain in the range of small angles with a non-optimal detector position. The flux in the used wavelength range decreases by a factor of 3-5 in the cold moderator mode. It is known that the background component of the reactor is determined only by the reactor power. Therefore, the signal-to-noise ratio also decreases by a factor of 3-5. This makes it impossible to conduct experiments with low forward scattering intensity, which nowadays make up the majority of experiments with biological and polymeric materials.

We propose alternative ways of increasing the neutron flux from the grooved moderator by a factor of 1.4-1.5 over the entire range of wavelengths used. Such solutions exist not only in calculations, but have also been implemented in practice.

4.4. Expected technical parameters after modernization of the instrument

Main parameters of the existing and modernized YuMO instruments at IBR-2 beamline 4

Parameters	Before modernization	After modernization
Flux at the sample	10^7 - $4{\cdot}10^7$ n/(s cm^2)	10^7 – $4{\cdot}10^7$ n/(s cm^2)
Wavelength range	from 0.5 Å to 8 Å	from 0.5 Å to 10 Å
Q-range	$8{\cdot}10^{-3}$ - 0.5 Å^{-1}	$4{\cdot}10^{-3}$ - 1 Å^{-1}
Size range of objects under study	10 - 500 Å	8 - 1500 Å
Measured scattering cross section	0.01 cm^{-1}	0.005 cm^{-1}
Calibration method	V standard during experiment	V, H_2O, graphite
Collimation type	Axial	Axial
Detector system	2 detectors of scattered neutrons, direct-beam detector	2 PSD of scattered neutrons, direct-beam PSD, monitor
Automatic sample changer	14 samples in thermostatted box	25 samples in thermostatted box
Temperature range	from –20°C to +130°C	from –20°C to +200°C
Q-resolution	5 - 20%	2 - 8%
Controlled parameters	Starts, temperature, V-standard, sample position	Starts, temperature, V-standard, sample position, detector position, monitor, chopper, reactor power

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

The key parameter for a small-angle neutron diffractometer is the flux at the sample. At the new neutron source of FLNP, the flux is projected to be increased by a factor of 10. This can significantly improve the parameters of the instrument, reduce the measurement time per experiment, and improve the resolution of the diffractometer. Using a start frequency of 5 Hz or even 10 Hz without an additional satellite peak is a preferred option for the YuMO instrument. The important aspect of the project is its implementation without the discontinuation of the user program.

5. Expected scientific results

The small-angle neutron scattering technique is one of the main methods for studying the structure of condensed matter. This is evidenced by three international conferences held in Dubna. Every year, up to 100 experiments, both methodological and scientific, are carried out with the instrument. The YuMO setup is the most in-demand instrument within the user policy at IBR-2. It is expected that in the coming years the demand for measurements by this method will continue. First of all, this is due to a wide variety of tasks solved with YuMO, ranging from biology to materials science. At the same time, the instrument already allows performing kinetic measurements with 1-min exposition time. At the new source, with an increase in the flux up to a factor of 10, it will be possible to carry out measurements with the time resolution of tens of seconds, which will significantly expand the range of tasks to be solved. The replacement of the ring detectors with PSD (including the direct-beam detector) will not only broaden the spectrum of tasks (with a magnetic field, rheological devices, etc.), but also improve the resolution and qualitatively change the data acquisition system. Judging by the publications, some of which are listed below, many publications are already at the highest world level (Scientific Reports, 2019.9 (1): p. 15852.– journal from the Nature Publishing Group, Macromolecules, 2017. 50 (1): p. 339-348, BBA, etc.). Taking into account the upcoming changes in the quality of the instrument, it is expected that the level of publications will continue to grow in both quantity and quality. Thus, the modernization will make it possible to qualitatively change the instrument by 2025, provided the project is properly financed.

6. Requested resources, costs and time frames of instrument modernization

The work on the project will mainly be carried out by the employees of two FLNP Departments, LIT and the YuMO group.

The cost and terms of production (purchase) of some YuMO units within the project are given in **Table 10 (Section 4)**.

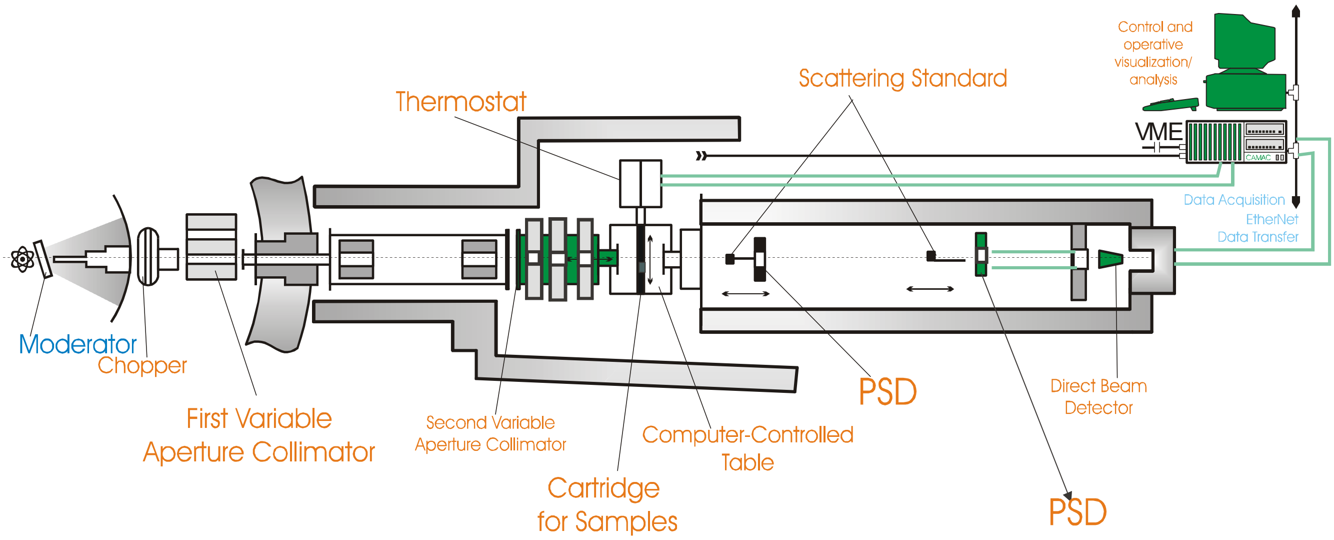

Fig. 21. *Schematic layout of the modernized YuMO instrument.*

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GRAINS - Neutron Reflectometer with Horizontal Sample Plane

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1. Abstract

The GRAINS (GRAzing Incidence Neutron Scattering) time-of-flight neutron reflectometer with a horizontal sample plane is located at beamline 10-B of the IBR-2 reactor. The instrument is designed to study nanostructured interfaces in the solid and liquid states by measuring the specular reflection coefficient and the intensity of diffuse scattering of a beam of thermal/cold neutrons. The modernization is aimed at improving the quality of neutron reflectometry experiments, including the reduction in the measurement time per reflectivity curve, increasing the range of momentum transfer, reducing the background, and widening of the capabilities of the sample environment system for conducting *in situ* experiments under various conditions.

2. Scientific program, topicality and comparison with the world level

The GRAINS (GRAzing Incidence Neutron Scattering) time-of-flight neutron reflectometer with a horizontal sample plane is located at beamline 10-B of the IBR-2 reactor [1,2]. The instrument is designed to study nanostructured interfaces in the solid and liquid states by measuring the specular reflection coefficient and the intensity of diffuse scattering of a beam of thermal/cold neutrons. The classical analysis of specular reflection in neutron reflectometry (NR) allows reconstructing the profile of the scattering length density in the studied object along the direction perpendicular to the interface between the media over a depth of up to several hundred nanometers with a resolution of 1 nm. The analysis of off-specular (diffuse) neutron scattering provides the characterization of lateral correlations on surfaces and interlayer boundaries. The use of specialized liquid cells in neutron reflectometry allows one to vary the contrast in the reflectometry experiment at interfaces with liquid media and to obtain more detailed information on the structure of surface inhomogeneities at a level of 1-100 nm. The cold mode of operation of the neutron moderator available for beamline 10 allows measurements in a wider dynamic range of momentum transfer.

The scientific program includes the following areas related to the physics of soft matter:

- Adsorption of nanoparticles (including magnetic nanoparticles) on solid surfaces;

- Electrochemical interfaces;
- Thin films, including polymer and composite films;
- Biological macromolecules and lipid layers on the surface;
- Liquid crystal films.

The GRAINS project includes a wide configuration of modern capabilities of neutron reflectometry in horizontal geometry. First of all, it involves the creation of conditions for complex studies of interfaces containing liquid components with the help of unpolarized and polarized neutrons and the testing of methods for obtaining and analyzing specular reflection and off-specular (diffuse) scattering. At present, these conditions have been implemented at the instrument, which allowed the GRAINS reflectometer to be included in the user program at the IBR-2 reactor (since 2015) and made it available for interdisciplinary research [3-11].

3. Scientific and methodological groundwork laid in FLNP JINR

When designing GRAINS, we used the experience of development of two other successfully operating reflectometers at the IBR-2 reactor (REMUR, REFLEX) [12] with a vertical sample plane. The GRAINS reflectometer implements geometry with a horizontal sample plane (vertical scattering plane), which opens up possibilities for studying interfaces with liquid media. So far, two neutron reflectometers of this type have been created at the neutron sources of the Russian Federation: REVERANCE (steady-state reactor VVR-M, PNPI NRC KI, Gatchina) [13, 14] and HORIZON (pulsed spallation source IN-06, INR RAS, Moscow) [15, 16]. However, the operation of both instruments is currently carried out in a limited mode due to the peculiarities of operation of the neutron sources, which creates a need for the development of more available instruments to support the experimental activities of numerous users of neutron reflectometry. The GRAINS reflectometer, as noted above, successfully operates in the framework of the IBR-2 user program.

4. Current status of the instrument and proposals for its modernization

4.1. Information about the current status of the instrument

The GRAINS reflectometer (its schematic layout is shown in Fig. 22) is located at the IBR-2 reactor, beamline 10-B. The main elements of the reflectometer are the moderator, neutron guide, chopper, beam-forming system, sample table and detector system. The characteristics of the units of the GRAINS reflectometer are given in Table 1. The beam is formed using a set of collimating devices and a long (up to 1 m) deflecting mirror – a principal element that separates the thermal neutron beam from fast background neutrons and directs it to the horizontally placed interface at a certain angle. Then, the reflected or scattered beam enters the detector system. The axis of the channel is directed to the moderator, which can operate in two modes: cold (22 K) and thermal (300 K). The experimental samples are fixed in special holders in a horizontal plane on a five-axis goniometric table (HUBER), which is mounted on an anti-vibration platform (JRS Scientific Instruments). The sample holder is provided with thermostating (Julabo F25-MA thermostat) in the temperature range from –15 to + 180 °C.

Neutrons behind the sample are detected by a detector system consisting of the main large-area gas two-dimensional position-sensitive detector (2D PSD) and an additional standard gas point detector. PSD is a multiwire proportional chamber with delay-line readout with universal data acquisition and storage system (developed in SC Department of DCMRD, FLNP JINR [17, 18]). The detectors are mounted on a movable platform placed behind the sample at a certain distance (Fig. 22); the plane of PSD and the axis of the counter are always perpendicular to the beam axis. The experiment is fully automated, control is provided (including remote access control) using the universal SONIX+ software package for the IBR-2 spectrometers (developed in SC Department of DCMRD, FLNP JINR [19–21]).

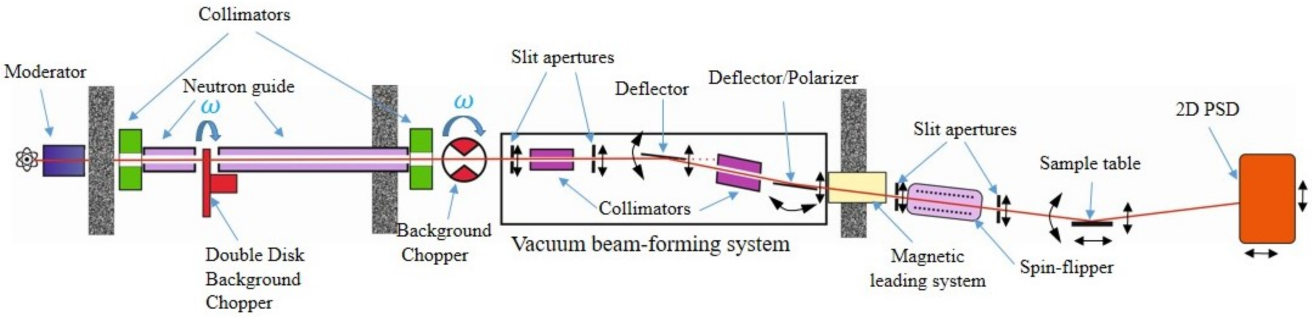

Fig. 22. *Schematic layout of the GRAINS reflectometer, current configuration.*

During five years after the GRAINS reflectometer was put into operation and included in the suite of instruments for users, it has proved effective in *in situ* studies of solid/liquid interfaces. This is due to a comparatively small characteristic measurement time per reflectivity curve: 1 hour in the dynamic range $q_z = 0.05$-1.2 nm^{-1}. Measurements in the maximum possible range using several grazing angles are limited only by strongly scattering systems due to a relatively high background: the minimum reflectivity is 10^{-5}.

4.2. Detailed description of proposals for modernization of the instrument

The modernization is aimed at improving the quality of NR experiments. To this end, measures are proposed to (1) improve the quality of reflectivity curves obtained in the experiment; (2) expand the possibilities of the sample environment system for conducting *in situ* NR experiments under various conditions. They include:

1) Installation of additional drum-type background choppers

At present, there is one drum chopper at the instrument: horizontal slit, rotation frequency of 5 Hz, fixed transmission function, released in 2010 (SiNaTech Ltd., Gatchina). This chopper ensures the performance of the reflectometer. There is a disk-type chopper installed in the beamline (under adjustment): two disks with opposite rotation, rotation frequencies of 5 and 10 Hz, variable transmission function, released in 2019 (MIRROTRON Ltd., Budapest). To expand the possibilities of fine-tuning of the transmission function, it is proposed to install two new (instead of one old) drum choppers with opposite rotation. This will make it possible to "cut off" the background component of the disk chopper at the fronts of the transmission function, as well as expand the range of accessible wavelengths in the cold region of the spectrum. In addition, these choppers can be used to scan the spectrum of background neutrons in the intervals between reactor power pulses, which is an important task in the development of the instrument with respect to the background reduction.

2) ***Modernization of the detector system***

The modernization of the detector system basically implies the installation and adaptation of a vacuum tube after the sample holder for alignment with the elements used in polarization analysis: a spin flipper and a wide-angle polarization analyzer. The goal is to reduce the contribution to the background component from re-scattering in the air after reflection. Also, an additional set of monitor neutron detectors is required to reduce the load on the main detectors when performing simultaneous measurements of spectra of incident and reflected beams, and the background.

3) ***Modernization of the polarizer assembly***

At present, the polarizer uses two polarizing mirrors (each 50 cm long) mounted on a metal support. This design did not justify itself, since over time, due to the fatigue of the material, a kink appeared between the mirrors, which led to the splitting of the beam. This makes it impossible to use the polarizer at the moment. The polarizer should be replaced with a principal change in its design. A similar problem occurred with the non-polarizing mirror beam deflector. It was successfully eliminated in 2017. The new assembly was manufactured by MIRROTRON Ltd., Budapest, using a polymer support for the mirror.

4) ***Magnetic system***

In 2019, for reflectometry measurements in external magnetic fields with controlled field strength, an electromagnet from GMW Associates, USA, was purchased (H-shape, dipole electromagnet, current of up to 70 A, gap of up to 96 mm, maximum field strength of 1.5 T, weight – 700 kg). The installation and adaptation of this magnet require the creation of a special sample unit with the development, manufacture and installation of a magnet cooling and power supply system.

5) ***Sample environment system***

The development of the sample environment system is associated with the creation and production of specialized reflectometry cells for *in situ* studies at interfaces of different types (liquid/solid, liquid/air) under various conditions (temperature, external electric field, external magnetic field, humidity, pressure, etc.), as well as the use of parallel measurements with complementary methods (impedance spectroscopy, ellipsometry, viscometry). Costs in this area are determined by high technological requirements for the processing of elements of cell parts from metals and plastics, as well as by the use of special materials and the creation of special planar structures (depending on the purpose of the experiment) on the surface of crystal blocks (substrates).

4.3. Current technical parameters for the thermal and cold modes of the moderator

Neutron wavelength range, nm	0.05 - 1.0 (cold) 0.05 - 0.7 (thermal)
Grazing angle, mrad	0 - 25
q_z-interval covered, nm^{-1}	0.05 - 2
Angle resolution, %	2 - 10
Neutron flux at sample position, cm^{-2}·s^{-1}	1 (cold) - 2 (thermal) × 10^6
Sample dimensions, cm	(2 × 2) - (7 × 15)
Deflecting mirror	Supermirror NiTi, $m = 2$, $L = 1$ m
Detectors	2D PSD, ^{3}He, 20 × 20 cm, spatial resolution 2×2 mm 1D cylindrical counter, ^{3}He, ∅ 18 mm, $L = 190$ mm

4.4. Expected technical parameters after modernization of the instrument

Neutron wavelength range, nm	0.05 - 1.5 (cold) 0.05 - 0.7 (thermal)
Grazing angle, mrad	0–25
q_z-interval covered, nm^{-1}	0.05–2
Angle resolution, %	2–10
Neutron flux at sample position, cm^{-2}·s^{-1}	1 (cold) - 2 (thermal) × 10^6
Sample dimensions, cm	(2 × 2) - (7 × 15)
Deflecting mirror	Supermirror NiTi, $m = 2$, $L = 1$ m
Detectors	2D PSD, ^{3}He, 20 × 20 cm, spatial resolution 2×2 mm 1D cylindrical counter, ^{3}He, ∅ 18 mm, $L = 190$ mm
Polarizer	Supermirror, $m = 2$, $L = 1$ m
Analyzer	Fan-type, $m = 2$
Sample environment system	External magnetic field, 1.5 T Thermostat, –50 ÷ +150°C

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

The development of reflectometry at IBR-2 in the direction of studying interfaces in soft matter is fully consistent with modern world trends. At almost all neutron sources of both pulsed and steady-state types, neutron reflectometers with a horizontal sample plane have been actively developed and put into operation over the past ten years with an emphasis on the use for soft matter research. It should be noted that the time-of-flight technique is mainly implemented at steady-state sources.

5. Expected scientific results

As a result of the modernization, the background component in reflectivity curves is expected to decrease down to 10^{-6}, which will allow measurements in the maximum accessible q_z-range. A significant expansion of experimental capabilities with respect to the classes of experimental systems is also expected due to the modernization of the sample environment system.

A promising area of research is the study of the structure of oriented phospholipid bilayers, representing real models of cell membranes. The investigation of ion transport channels and protein adsorption in these systems can be essential for the development of new drug delivery systems, as well as for the study of the transport mechanism itself. An important research objective is the determination of the size, distribution, physical and chemical behavior of oriented lipid membranes. This information can be obtained from experiments on oriented lipids or synthesized membranes under various conditions. A study of their transverse and lateral structure, as well as composition and fluctuations, can be carried out in *real time*.

The interest in systems containing magnetic nanoparticles is primarily connected with the possibility to control the properties of these systems by means of an external magnetic field. These systems include magnetic fluids, magnetic polymer films, Langmuir-Blodgett films with magnetic nanoinclusions, magnetic gels, including elastomers, and other magnetic composite materials. Particular prospects are associated with the use of magnetic nanoparticles in biomedical applications, such as targeted drug delivery to tumors; tumor diagnostics (magnetic resonance imaging), tumor therapy (magnetic hyperthermia).

Using neutron reflectometry, details of the internal structure of copolymer films with various structures on surfaces and interfaces are actively studied. *In-situ* time-of-flight experiments will provide information on structural changes in the process of self-organization that occurs during hybridization. Among systems, which can be efficiently studied by neutron reflectometry, are polymer glasses, liquid crystal films, and nanocomposites based on them.

A classic problem well studied for bulk systems is the study of phase separation in mixed liquid systems. The semi-empirical theory of this phenomenon created so far allows a fairly complete classification of the types of separation depending on the interaction potentials in the components of solutions. At present, an extremely interesting problem is the study of the behavior of mixed solutions at interfaces. Modern structural methods, such as neutron reflectometry in the horizontal geometry of the sample, will make it possible to advance in solving this problem.

6. Requested resources, costs and time frames of instrument modernization

The modernization period is 3 years. The cost of the main units of GRAINS is given in **Table 11 (Section 4)**.

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REFLEX - Reflectometer with Polarized Neutrons

Leaders: V.I. Bodnarchuk, A.V. Nagornyi

Main participants: V.V. Sadilov, S.P. Yaradaykin, A.S. Doroshkevich, A.M. Tkachenko

Collaborating organizations: PNPI NRC KI, JCNS@FRMII Garching (Germany), «DonIPE» (Donetsk)

1. Abstract

The REFLEX reflectometer with polarized neutrons is used for time-of-flight studies of thin-film magnetic and non-magnetic nanostructured objects at room temperature. Its long flight path allows measurements with high time and angular resolutions.

In addition to scientific research, the REFLEX reflectometer is used to perform methodological studies on diagnostics of the quality of neutron-optical structures, as well as to study and develop new polarized neutron techniques.

2. Scientific program, topicality and comparison with the world level

The REFLEX reflectometer (Fig. 23a) is located at beamline 9 of the IBR-2 reactor. The feature of the beamline is that it is a tangential channel with respect to the moderator, i.e. the radiating surface is the flat end part of the thermal water moderator. As a result, the neutron flux density of beamline 9 is lower than that available at the beamlines of other two reflectometers of the IBR-2 reactor (REMUR and GRAINS), whose beam axes originate from the flat part of the cold moderator. In addition, the head part of the REFLEX reflectometer, which is located in the ring corridor of the reactor, is not optimal because of the limitations imposed by the technological equipment of the reactor and the system of cold moderators. This limits the possibilities for effective background suppression at the beamline and narrows the possibilities of reflectometry measurements at the instrument. Nevertheless, the availability of a polarized beam and good angular resolution of the instrument make it possible to solve a certain range of problems related to the investigation of magnetism of layered nanosystems, interlayer diffusion processes, surface roughness, etc.

To increase the efficiency of using beamline 9, the REFLEX reflectometer is mainly used in methodological research. It is actively employed for testing new neutron-optical systems, polarization control devices, detector systems, etc. One of the promising areas of methodological development is the creation of a neutron spin-echo instrument with a time-of-flight mode. The spin-echo method is quite well developed for steady-state neutron sources [1-4]. It is based on the use of either coils with a constant magnetic field or radio-frequency spin flippers as precession arms. In both cases, the working spectral region is limited to a value of the order of $\Delta\lambda/\lambda \sim$ 15-20%, which in most cases is substantially less than the total spectral range of the pulsed source. In this regard, the use of the spin-echo technique on pulsed sources is limited, although some attempts have been made to adapt the existing techniques to the time-of-flight mode [5]. For pulsed neutron sources, two methods of using spin-echo techniques have been proposed. The first one consists in using adiabatic RF spin-flippers in the precession arms [6, 7]. This method has been brought to practical implementation at the OFF-SPEC reflectometer of the ISIS pulsed source [8]; this mode is currently undergoing debugging and tuning for the instrument. The second method was proposed in [9] and is based on the use of spin-rotators in the precession arms, in which magnetic fields increase linearly with time. In practice, the magnetic fields in this method are modulated in time (sawtooth-shaped magnetic pulses). This approach in the version of the elastic spin echo for small-angle neutron scattering is being developed at the REFLEX instrument. The wide spectral range that can be used within the framework of this method will cover the area of the studied objects on a scale from 100 Å to 15000 Å, which will significantly supplement the capabilities of existing small-angle scattering instruments at the IBR-2 reactor. In addition, the neutron spin-echo method does not require strong beam collimation, and polarization analysis is carried out for the entire scattered beam without scanning over a certain range of solid angles. This feature compensates a comparatively low flux at REFLEX, thus making the method most appropriate for the further effective development of the instrument.

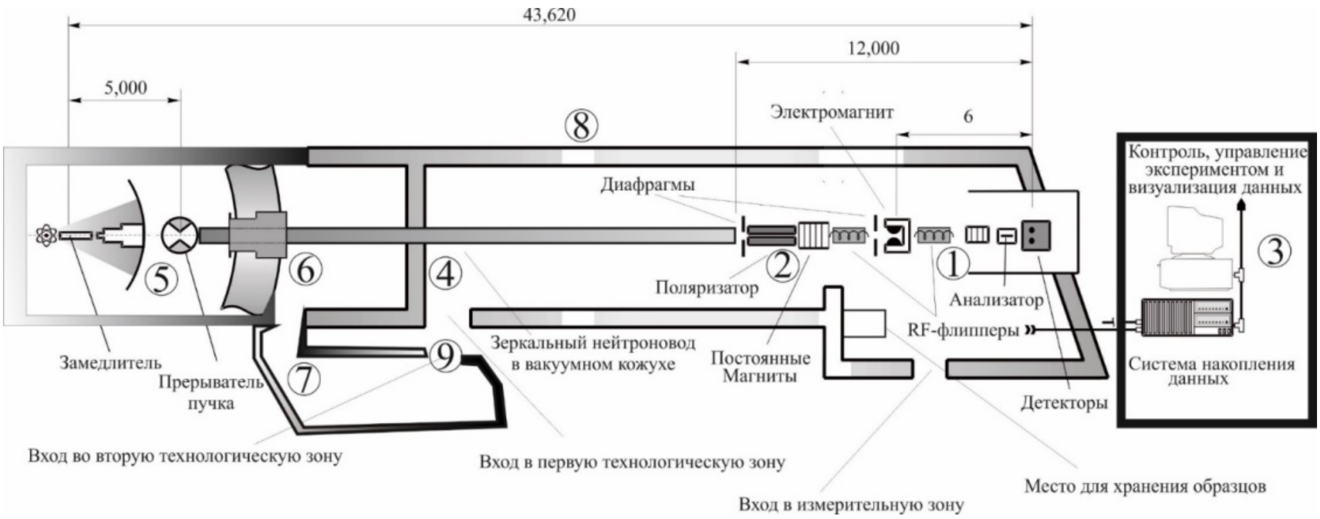

Fig. 23a. *Layout of the REFLEX instrument.*

3. Scientific and methodological groundwork laid in FLNP JINR

The REFLEX reflectometer team has extensive experience in creating and developing instruments at the IBR-2 reactor and other sources [10-12]. In the frames of the modernization of the REFLEX reflectometer, numerous units, instrument elements were successfully designed and implemented in the currently operating instrument.

In the framework of the joint project on the design of a small-angle spin-echo instrument in Julich Research Center (Germany), all elements of the spin-echo setup, including electronic power supply units of spin-rotators, were developed and tested at IBR-2. Along with this work, the possibility for implementing such a technique at the IBR-2 reactor was demonstrated.

A virtual model of the future prototype of a spin-echo small-angle scattering setup as an option at REFLEX was designed using the VITESS software package for Monte-Carlo simulation of neutron instruments [13]. The main parameters of the setup were optimized.

At present, the necessary power sources, a cooling system for power electronics and spin-rotator coils have been developed and manufactured.

4. Current status of the instrument and proposals for its modernization

At present, the REFLEX instrument is included in the user policy program, within which the scheduled reflectometry experiments with solid samples are carried out. Most of submitted experimental proposals concern the analysis of specular reflection from various layered nanostructures and are aimed at establishing the structural characteristics of thin films: layer thicknesses, roughness of interlayer boundaries and free surfaces, scattering density characteristics of matter in the layers. For analysis of the structures containing layers of magnetic materials, the REFLEX reflectometer offers a polarized neutron beam option with a possibility of full polarization analysis of the beam scattered (specularly reflected) from the sample.

4.1. Information about the current status of the instrument

The equipment upgrade carried out in recent years has significantly improved the REFLEX parameters and simplified the measuring process. However, there are a number of factors that limit the capabilities of the reflectometer. For example, the head part of the REFLEX reflectometer, which is located in the ring corridor of the reactor, is not optimal because of the constraints imposed by the technological equipment of the reactor and the system of cold moderators. This limits the possibilities for effective background suppression at the beamline. A relatively high background imposes limitations on the dynamic range of the measured reflectivity curves. The background chopper installed in the ring corridor was designed to be placed on a flight path twice as long as its actual position, and therefore, the time window of the chopper does not sufficiently suppress the background of thermal neutrons. The first section of the neutron guide is installed at a distance of more than 5 m from the shutter. As a result, the neutron guide collects the flux from an area much larger than the shutter opening, which also worsens the background conditions for reflectometry measurements.

At present, active work is underway to improve the background conditions at REFLEX in order to maximize its potential.

Main parameters of the REFLEX reflectometer

Beam-forming system	supermirror (m=1.2) neutron guide 27 m long, 10×80 mm^2
Wavelength range	1.4 - 10 Å
Q-range	0.001- 0.13 Å^{-1}
Neutron flux at sample position	10^5 s^{-1}cm^{-2}
Q-resolution	3 - 10 %
Sample-to-detector distance	2 - 6 m
Minimum sample dimensions	20×20 mm^2
Magnetic field at sample position	<0.4 T
Spin-flippers	2 radio-frequency adiabatic spin-flippers
Polarizer	Transmission type, V-shape, Fe/Si, m=5
Analyzer	Transmission type, Fe/Si, m=3.6 (also FeCo/TiZr supermirror, m=2, is available)
Detectors	2D PSD 200×200 mm^2, ^{3}He; ^{3}He proportional counter

4.2. Detailed description of proposals for modernization of the instrument

The long-term development of the REFLEX instrument is planned to focus on the following areas:

4.2.1. Sample Environment Equipment

- Modernization of the magnetic system at the sample location. The magnet should produce a magnetic field at the sample position of at least 1 T.
- Development and installation of a cryogenic system to ensure low temperatures of down to 2 K at the sample.

The modernization of the sample environment system will allow studies of magnetic thin-film structures with a low Curie temperature, superconducting films near the superconducting transition temperature. At present, these studies cannot be performed at the instrument.

4.2.2. Modernization of automation system

- Installation of automated collimation systems: a) at the exit of the neutron guide, b) in front of the sample, c) behind the sample.
- Development and installation of a new table in place of the sample with a system for adjusting the sample position.
- Development of automated control over the position of the detector system (for moving perpendicular to the beam axis when setting up a convenient measurement mode).

4.2.3. Modernization of background chopper

The reflectometry method is extremely sensitive both to the quality of the shape of neutron pulses produced by a mechanical chopper as well as to background conditions. The available mechanical drum chopper for the REFLEX instrument has a large neutron transmission window (40 ms). During the development of the chopper, there was a lack of clarity regarding the possibility of its installation in the ring corridor of the reactor, so the window was designed taking into account the possible location at a large distance from the moderator. The long-term use of the chopper in the ring corridor has almost exhausted the resource of reliable operation. It is necessary to develop a more reliable design of the chopper with the provided options for regulating the delays and the window width of the neutron pulse. Therefore, the design and installation of a new mechanical chopper at beamline 9 of the IBR-2 reactor is a first-priority task for the development of the REFLEX instrument for its operation both in the reflectometry mode and in the spin-echo mode currently being developed.

4.2.4. Background suppression

The creation of enhanced background shielding around the neutron guide is also an important task for the development of the REFLEX instrument. The section in the beginning of the neutron guide in the ring corridor of the IBR-2 reactor is of particular importance, since at the moment it does not have protection from radiation coming from neighboring beamlines. In the framework of the REFLEX instrument development, it is planned to develop and construct shielding walls and housings made of neutron-absorbing materials (including borated polyethylene) in the IBR-2 reactor ring corridor.

It is also necessary to develop and install background shielding of the detector system, as well as to provide an option for installation of a vacuum tube between the sample and the detector system.

4.2.5. Creation of a measuring mode of spin-echo small-angle scattering

The spin-echo technique for elastic neutron scattering has been developing at the REFLEX instrument for a long time. Over the next 5 years, it is planned to create a separate module with a spin-echo small-angle scattering setup, which will allow us to perform experiments at users' requests. The new option will significantly expand the experimental capabilities of the instrument.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

The implementation of the project of the new cold moderator, taking into account the channel geometry, could expand the dynamic range in reflectometry measurements provided the background of thermal neutrons is low.

4.4. Expected technical parameters after modernization of the instrument

The main project, under which the further methodical development of the REFLEX instrument will be carried out, is the creation of a spin-echo small-angle diffractometer (Fig. 23b). Preliminary calculations and simulation of the future setup, taking into account the real parameters of the neutron beam at beamline 9 made it possible to evaluate the parameters of the future instrument.

1	Guide field
2	RF-flipper
3	Coupling coil 1
4	Coupling coil 2
5	Metal zero-field shielding
6	Mu-metal zero-field shielding
7	Spin-rotator A
8	Spin-rotator B
9	Spin-rotator C
10	Spin-rotator D
11	Sample position
12	Water cooling system
13	Spin-rotators power supply
14	Analyzer
15	PSD detector
16	Coupling coils power supply

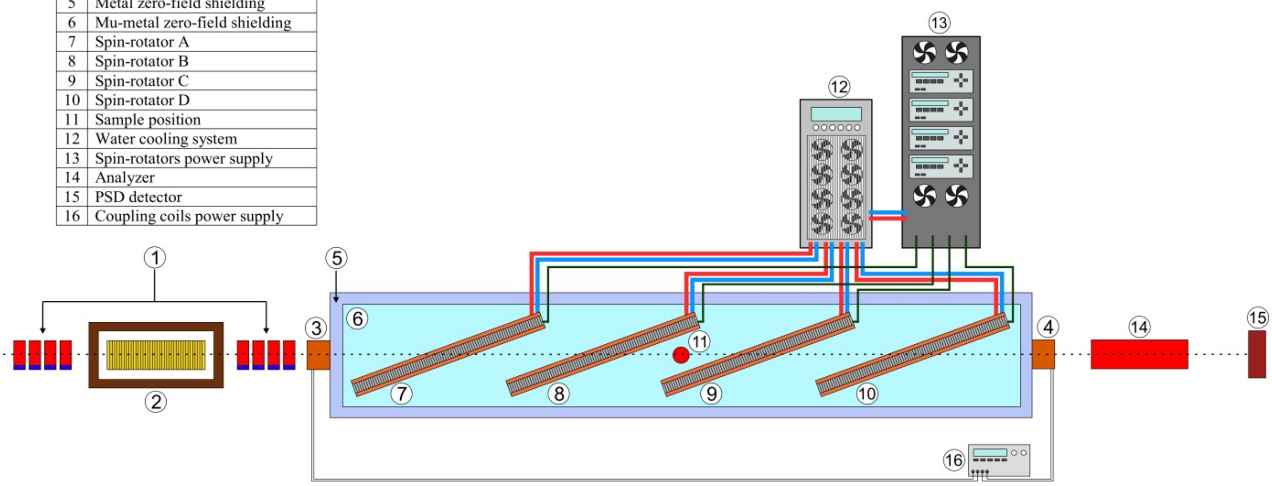

Fig. 23b. *Schematic diagram of the spin-echo small-angle diffractometer at beamline 9 of the IBR-2 reactor. The spin-echo scheme is implemented on the basis of spin rotators (7-10) with a magnetic field inside, linearly increasing along their axes with a time gradient* $\dot{B}$. *The axes of spin rotators are tilted to the beamline axis to increase sensitivity to the neutron scattering angle.*

Wavelength range, Å	1.2 - 6
Spin-echo length range, Å	100 - 15000
Magnetic field gradient, G/s	$3.75 * 10^5$
Pulse frequency, Hz	200
Tilt angle of coils, degrees/deg./°	10 - 15
Dimensions of spin rotator coil, mm × mm × mm	350 × 80 × 40
Distance between spin-rotators, m	1

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

The REFLEX instrument is a convenient setup for testing new methods of neutron scattering, which can be implemented at the future neutron source at JINR in the coming years. In this regard, the development of the REFLEX instrument will certainly contribute to the methodological and scientific support of the instrument development regarding the concept of the new source.

5. Expected scientific results

The spin-echo small-angle diffractometer operating in the time-of-flight mode will be the first instrument of this kind in Russia. The evaluation of the parameters of the future setup allows us to state that it can significantly expand the capabilities of the existing and future conventional small-angle instruments at the IBR-2 pulsed reactor.

The experience gained in the development of this technique can be applied both to the existing and future pulsed neutron sources.

6. Requested resources, costs and time frames of instrument modernization

The terms and cost of modernization of the REFLEX reflectometer are listed in **Table 12 (Section 4)**.

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REMUR - Reflectometer with Polarized Neutrons

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IPM RAS (Nizhny Novgorod)
INR (Debrecen, Hungary)

1. Abstract

The development of the REMUR reflectometer involves a further extension of the range of the instrument possibilities and is aimed at improving the detector system, enhancing the luminosity and suppressing the background from fast neutrons and gamma-radiation.

2. Scientific program, topicality and comparison with the world level

The interaction of various types of order parameters gives rise to unusual phenomena that underlie the development of nano- and microelectronics. In this regard, the studies of this interaction are important from both fundamental and applied points of view. A number of such phenomena are the result of the interaction between superconducting pairs and magnetization, which occurs in ferromagnetic-superconducting structures. In bilayers, trilayers, and periodic structures, the unusual phenomena have been predicted including the triplet superconductivity, cryptoferromagnetism, inverse proximity effect, spontaneous Meissner effect, paramagnetism of the Meissner state and others. So far, we have observed some varieties of cryptoferromagnetism, the spontaneous Meissner effect and Meissner paramagnetism. It should be noted that the theoretical predictions are not fully realized in practice due to irregularities in heterostructures under study. This requires both experimental and theoretical efforts. The heterostructures with magnetic layers having a more complex, namely, helicoidal magnetic structure, are of current interest. In this case, superconductivity in magnetic layers can occur at higher temperatures.

Experiments with polarized neutrons are rare, however, they allow us to reveal phenomena by studying structures at nanoscale. Recent advances in neutron reflectometry relating to the detection of secondary radiation, make it possible to study elemental distributions in magnetic structures. This will allow us to study, for example, the nature of the Meissner paramagnetism, as well as to determine the degree of polarization of superconducting pairs induced by ferromagnets.

3. Scientific and methodological groundwork laid in FLNP JINR

In two last decades, the investigations performed by the REMUR group were focused mostly on two topics. The first topic concerned the condensed matter research, in particular the discovery and studies of phenomena in ferromagnetic-superconducting structures [1-14]. We investigated 18 structures that differ in the composition of layers and elements. The main results on the effect of superconductivity on magnetic structures characterized by a linear scale from fractions of nanometers to hundreds of angstroms are as follows:

- Suppression of magnetization by superconductivity due to the isotropic distribution of the directions of domain moments (cryptoferromagnetism in the domain structure) and the anticollinear ordering of the moments of the cluster system (cryptoferromagnetism in the cluster system).
- Temperature reversibility of the inhomogeneous magnetic state.
- Correlation in the behavior of magnetic structures at different spatial scales, in particular, the interaction of a cluster system with a domain structure.
- Two-stage transformation of the domain structure.
- Reorientation of magnetic moments in the system during a zero-field superconducting transition to a spontaneous Meissner phase.
- Diamagnetism of a periodic ferromagnetic-superconducting structure, coherent superconducting length in gadolinium (4 nm).
- Meissner paramagnetism of F-S structures.

The second research topic is related to the development of neutron reflectometry methods. Scattering methods, in particular, GIND and GISANS, were developed. Reflectometry with the detection of secondary radiation (charged particles, gamma-rays and neutrons experiencing a spin-flip) was realized [15–16].

4. Current status of the instrument and proposals for its modernization

The last modernization of the reflectometer was carried out in 2003. Since then, a part of the equipment has aged, and its performance has deteriorated. So, for example, the long-wavelength dependence of the polarization efficiency of the polarizer has worsened. It is necessary to manufacture a new super-mirror polarizer (m = 2).

The available disk chopper has a low transmission, which reduces the luminosity. In this regard, it is necessary to replace the disk chopper with a drum one.

The use of the gamma-radiation detection channel with the available cryostat is now problematic because of the large diameter of the cryostat, which does not allow placing a gamma-detector close to the structure under study. A new cryostat should increase the detector aperture by a factor of about 20-30. For the new cryostat, it will be necessary to manufacture an electromagnet with the poles of a special shape, which will create a magnetic field directed in the plane of the structure under study. This development is relevant for the concept of a suite of instruments for the project of a new neutron source of FLNP.

Specular reflection of neutrons in experiments on layered structures is accompanied by the scattering from roughnesses, clusters, and crystalline structures. For example, in studies of ferromagnetic-superconducting structures, a superconductivity-induced correlation was observed in the behavior of structures of different scales. In this regard, it is necessary to develop, manufacture and install two detectors: one for detecting clusters with a linear size of 1-20 nm and the other for detecting interplanar spacings of the crystal lattice in the range of 0.2-1 nm.

Main parameters of REMUR before and after modernization

Parameters	Before modernization	After modernization
Total flux at sample position	$2 \cdot 10^5$ n/(s·cm^2)	$4 \cdot 10^5$ n/(s·cm^2)
Wavelength range	1 - 10 Å	1 - 15 Å
Q-range	$2 \cdot 10^{-3}$ - 1 Å^{-1}	$1 \cdot 10^{-3}$ - 1 Å^{-1}
Size range of objects under study	1 nm - 100 μm	1 Å - 100 μm
Flux at 10 Å		An increase by a factor of 20 due to a new chopper
Polarization efficiency	0.8 at 2 Å	An increase up to 0.95 at 2 Å
Background count by gamma-ray detector		A decrease by a factor of 5
Detector system for neutrons	Direct-beam PSD	Direct-beam PSD, backscattering PSD
Distance between gamma-ray detector and structure under study in cryostat	18 cm	3 cm
Temperature range	1.5 - 300 K	1.5 - 300 K
Q-resolution	$2 \cdot 10^{-3}$ at 10 Å	$1.3 \cdot 10^{-3}$ at 15 Å
Magnetic field range	20 Oe - 3 T	20 Oe - 3 T

5. Expected scientific results, comparison with the world level

The future investigations are expected to yield valuable data on new phenomena resulting from the interaction of various kinds of order parameters, in particular, magnetization and density of superconducting pairs. The behavior of helicoidal structures in layered structures with rare-earth elements depending on temperature and magnetic field is planned to be studied.

6. Requested resources, costs and time frames of instrument modernization

The time frames and cost of upgrading the REMUR reflectometer are given in **Table 13 (Section 4)**.

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NRT - Neutron Radiography and Tomography Station

Leader: D.P. Kozlenko

Main participants: B.N. Savenko, S.E. Kichanov, E.V. Lukin, A.V. Rutkauskas, I.Yu. Zel’, G.M. Aidanov, K. Nazarov, M. Kenesarin

Collaborating organizations: NRC "Kurchatov Institute", Moscow, Russia; Petersburg Nuclear Physics Institute, NRC KI, Gatchina, Russia; Institute of Archeology, RAS, Moscow, Russia; Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH), Bucharest, Romania

1. Abstract

Neutron radiography is an imaging technique based on various degrees of attenuation of the neutron beam passing through components of the sample under study with different chemical composition, density, and thickness. It is used to obtain information on the internal structure of the studied materials with a micrometer-scale spatial resolution. The functional elaboration of neutron radiography is neutron tomography. In this method, three-dimensional reconstruction of the internal structure of the object under study is performed from a set of individual single-plane radiographic projections obtained for different angular positions of the sample relative to the direction of the neutron beam. At the IBR-2 high-flux pulsed reactor, the NRT experimental station was built to conduct research using the neutron radiography and tomography method.

2. Scientific program, topicality and comparison with the world level

Neutron radiography is a method of obtaining neutron images of objects under study. Different intensity losses in the neutron beam passing through components of the sample under study with different chemical composition, density, and thickness provide information on the internal structure of the studied materials with a micrometer-scale spatial resolution [1, 2]. This method of nondestructive testing is characterized by a deeper penetration into materials compared to the complementary method of X-ray radiography and has a number of advantages in the investigation of objects containing both light (e.g., hydrogen or lithium) and heavy elements.

All modern and newly developed neutron sources are equipped with neutron radiography and tomography stations [1, 2]. At present, neutron radiography is widely used in research of materials and products for nuclear technologies, paleontological and geophysical objects [3-5], and objects of cultural heritage [6-10]. It should be noted that much attention is now being paid to unique studies of physical and chemical processes in fuel cells and batteries, processes connected with the penetration of hydrogen or water into the mass of various materials. The functional elaboration of neutron radiography is neutron tomography. In this method, three-dimensional reconstruction of the internal structure of the object under study is performed from a set of individual single-plane radiographic projections obtained for different angular positions of the sample relative to the direction of the neutron beam.

The availability of advanced CCD-camera-based detectors for neutron imaging and the development of high-flux neutron sources have given a new impetus to the development of methods of neutron radiography and tomography and the construction of specialized experimental stations at neutron centers throughout the world. One of the basic facilities of the Joint Institute for Nuclear Research is the modernized high-flux IBR-2 reactor, which is one of the most intense pulsed neutron sources in the world. It should be noted that the pulsed character of the operation of the IBR-2 reactor opens up wide prospects for the implementation of energy-selective neutron imaging using the time-of-flight technique [4], in which the contrast of the object elements consisting of various materials can be enhanced by choosing the optimal energy range of incident neutrons.

3. Scientific and methodological groundwork laid in FLNP JINR

In recent years, a neutron radiography and tomography station [1-4] has been created at beamline 14 of the IBR-2 reactor. Its methodological possibilities allow the successful implementation of scientific and applied experiments to analyze the internal structure of various objects both in fundamental and applied research [4-10].

The parameters of the station and its experimental capabilities make it possible to carry out neutron experiments at a high world level with paleontological [1], astrophysical [5] and engineering [1, 2] objects. Significant scientific groundwork has been laid for nondestructive research of cultural heritage objects using neutron radiography and tomography [6-10] including unique studies of coins of Ancient Greece [6] and Bulgaria [7], objects of ancient Russia's cultural heritage [8-10].

4. Current status of the instrument and proposals for its modernization

4.1. Information about the current status of the instrument

A schematic drawing of the main units of the experimental setup for neutron radiography and tomography is shown in Fig. 24.

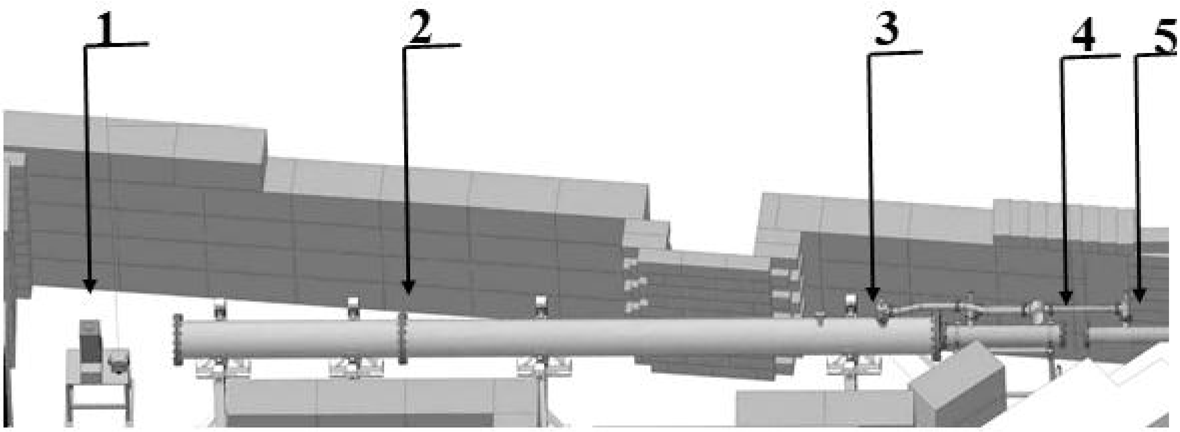

Fig. 24. *Schematic drawing of main units of the neutron radiography and tomography station at beamline 14 of the IBR-2 reactor: 1 – detection system and system of rotating and inclined goniometers for positioning samples in the neutron beam; 2 – vacuum housing of the system of collimators forming the neutron beam; 3 – vacuum post for pumping air from the housing of the collimation system; 4 – position of single-crystal bismuth filter for neutron beam; 5 – embedded tube for collimators forming the beam from the reactor moderator.*

The neutron beam is formed using a system of collimators consisting of four annular cylindrical inserts made of borated polyethylene alternating with additional steel rings for structural rigidity. The inner diameters of the annular collimators increase from 5 cm at the inlet to 23.7 cm at the exit of the neutron beam from the collimation system. It is known that the spatial resolution of radiography stations, and therefore the quality of obtained neutron images, depends on the characteristic parameter L/D, which is determined by the ratio of the distance, L, between the inlet aperture of the collimation system and the sample position to the diameter of the inlet aperture of the collimators, D. The higher the value of the parameter L/D, the better the spatial resolution of neutron images. The length L for the new neutron radiography and tomography station is 10 m, and the diameter of the inlet of the collimator, D, is 5 cm, which corresponds to L/D = 200. The design of the collimation system makes it possible to reduce the diameter of the inlet aperture down to 0.5 cm, thus achieving L/D = 2000. These values of the characteristic parameter L/D are similar to the parameters of leading neutron radiography stations at world neutron centers. The collimation system is placed in a vacuum housing to reduce losses in the intensity due to the neutron scattering in the air.

The total flux of thermal neutrons at the sample position is $\Phi \sim 5.5(2) \times 10^6$ n/cm^2/s. The spectral wavelength distribution for thermal neutrons in the incident neutron beam was also measured using a point ^{3}He gas counter (Fig. 25). It has a pronounced maximum at $\lambda \sim 1.8$ Å.

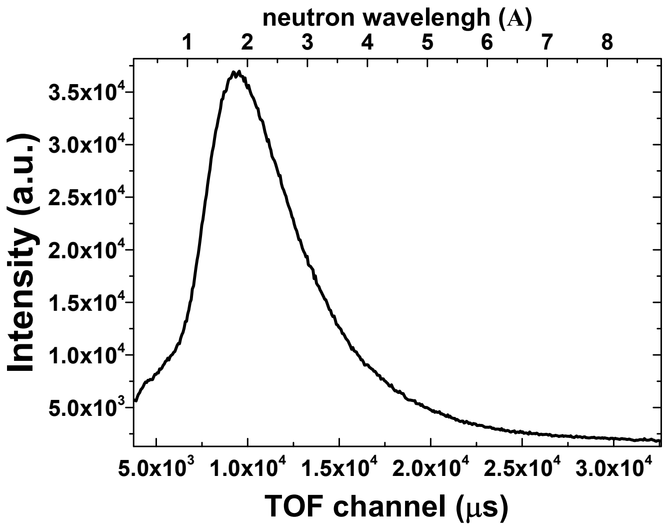

Fig. 25. *Neutron spectrum at the sample position obtained at the neutron radiography and tomography station at beamline 14 of the IBR-2 reactor.*

A detector system based on a CCD video camera is used in the experimental station for neutron radiography and tomography. The conversion of neutrons into photons recorded by the CCD video camera is performed using a 0.2-mm thick ^{6}LiF/ZnS scintillator plate manufactured by RC TRITEC Ltd. (Switzerland). To protect the video camera from radiation, the light from the scintillator is reflected by a rotating mirror tilted at an angle of 45° with respect to the axis of the incident neutron beam, and hits the optical system of the video camera. All optical systems of the detector are in a light-protective housing. The technical parameters of a high-sensitivity high-resolution video camera and its optical system are presented in Table 1. The size of one pixel of a neutron radiographic image is 51x51 μm, and the spatial resolution of images recorded for a neutron beam size of 20×20 cm is 154 μm.

Main technical parameters of the experimental station for neutron radiography and tomography

Characteristic collimation parameter:	200-2000
Diameter of inlet aperture of collimation system, D	5 - 50 mm
Distance between system aperture and sample position, *L*	10 m
Size of neutron beam (field-of-view, *FOV* of station)	20 × 20 cm^2
Characteristic parameters of detecting video camera	
Type of high-sensitivity video camera	VIDEOSCAN-11002-2001
Size of CCD sensor (pixels)	4008 × 2672
Size of CCD sensor (mm)	36 × 24
Size of one pixel in sensor (μm)	9 × 9
Cooling	Based on Peltier element, down to –25ºC
Parameters of optical system of video camera	Based on Nikon lens with a focal length of 50 mm and an aperture width of 1:1.4D

Tomography experiments are performed using the system of HUBER goniometers with a minimum rotation angle of down to 0.02° and a remote control system. The high neutron flux at the sample makes it possible to reduce the exposure time down to 10 s per one image.

The obtained neutron images are corrected for the background noise of the detector system and normalized to the incident neutron beam using the ImageJ software package. The tomographic reconstruction of the studied object from a set of angular projections is performed using the H-PITRE software. The VGStudio MAX 2.2 software package from Volume Graphics (Heidelberg, Germany) is used for visualization and analysis of obtained 3D data.

4.2. Detailed description of proposals for modernization of the instrument

4.2.1. From the point of view of further development of the technique, it should be noted that the pulsed character of the IBR-2 operation opens up wide prospects for the implementation of energy-selective neutron imaging: the total neutron scattering cross section in crystalline materials has sharp discontinuities at certain wavelengths (the so-called Bragg edges), therefore, by choosing the optimal neutron energy range in the experiment, it is possible to enhance the contrast of the components of the studied object made of a certain material for more detailed analysis. The selection of the neutron energy range is planned to be realized using the time-of-flight technique, which will significantly expand the possibilities of research at the experimental station for neutron radiography and tomography. It is planned to develop, manufacture and purchase special neutron detectors with large active areas and fast electronics to implement the time-of-flight technique for recording neutron radiographic images.

4.2.2. To expand the capabilities of the NRT station for neutron experiments in real time, it is necessary to develop and manufacture a detector system based on a high-speed camera with an sCMOS sensor. The new detector system requires the purchase of optical, mechanical and protective components: video cameras, mirrors, fasteners, borated polyethylene plates, software.

4.2.3. To improve the background conditions at the sample and detector system, it is necessary to design, manufacture and install a neutron filter system based on a sapphire single crystal.

4.2.4. To improve the optical parameters of the detector system, it is necessary to purchase optical components: lenses, CCD cameras, guard rings, new types of scintillators, etc.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

The NRT experimental station is currently located at beamline 14 of IBR-2, where no cold moderator is planned to be installed.

4.4. Expected technical parameters after modernization

It is expected that the parameters of the detector module for conventional neutron radiography and tomography will be improved. The development and manufacturing of a module based on a high-speed camera will allow us to study fast processes: penetration of liquids into materials, melting or phase transformations in materials, processes in cements and cement pastes. The production and installation of a sapphire filter will improve the characteristics of the neutron beam by suppressing the background parasitic gamma-rays and fast neutrons.

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

At the new neutron source of FLNP, it is planned to construct several stations for neutron radiography and tomography investigations, including a station for energy-selective neutron imaging. Thus, the methodological and scientific development of the research direction of neutron radiography and tomography is one of the promising and relevant research areas for the future FLNP scientific program.

5. Expected scientific results

The development of the detector system and background conditions for the neutron beam at beamline 14 of the IBR-2 pulsed high-flux reactor already allows us to successfully implement the scientific program for research of a wide range of scientific and technical objects using the method of neutron radiography and tomography. World-class results were obtained in studies of engineering devices and components, objects of cultural heritage, paleontology, astrophysics, structural materials, etc. The commissioning of a high-speed recording camera will expand the experimental capabilities of the station and will make it possible to study fast processes, for example, in cement materials or cooling heat pipes.

It should be noted that the pulsed character of the IBR-2 operation opens up wide prospects for the implementation of energy-selective neutron imaging using the time-of-flight technique, in which the contrast of the object elements consisting of various materials can be enhanced by choosing the optimal energy range of incident neutrons. For this purpose, it is planned to purchase special detector systems based on sCMOS sensors and Medipix chips.

6. Requested resources, costs and time frames of instrument modernization

The costs of the stages of modernization of the experimental station are presented in **Table 14 (Section 4)**.

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PROJECTS OF NEW INSTRUMENTS

New Inverse-Geometry Inelastic Neutron Scattering Spectrometer

Leader: D.Chudoba

Main participants: Ye.A. Goremychkin, A.V. Belushkin, A.A. Kruglov, V.I. Bodnarchuk, A.V. Churakov, A.N. Chernikov, P. Bilsky, V.I. Sukhanov

Collaborating organizations:

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PNPI NRC KI, St. Petersburg
Saint-Petersburg State University, St. Petersburg
INR RAS, Moscow

Poland:
INP PAS, Kraków
AMU, Poznań
FRAKO-TERM, Toruń
JU, Kraków

1. Abstract

At present, two inelastic neutron scattering (INS) spectrometers operate in FLNP, including the DIN-2PI spectrometer with direct geometry and the NERA spectrometer with inverse geometry.

The parameters of the NERA spectrometer, which has been upgraded in recent years, make it possible to carry out INS experiments at a good level, comparable to that provided by instruments of the same type operating in advanced neutron research centers. Nevertheless, all possible options for upgrading NERA have essentially been exhausted, and since it was put into operation in the late 1990s, many of its units have become obsolete. So, the development of a new inverse-geometry spectrometer based on advanced technologies will make it possible to create an instrument significantly superior to similar setups in other neutron centers.

The state and parameters of the DIN-2PI spectrometer do not meet present-day requirements for resolution and luminosity, and its modernization to improve these characteristics is practically impossible due to the current location of the instrument (too close to the active core).

Thus, although the two INS spectrometers provide certain possibilities for studying the condensed matter dynamics, they are not up to the world-class level of instruments of this type and do not fully satisfy the needs of the user community. In order to make FLNP competitive in this area of research, it is necessary to build new INS spectrometers using advanced neutron optics and new optimum design to provide high resolution, low background and wide range of energy transfer. Nowadays, the high technologies employed in neutron guides and optical devices make it possible to use the maximum brightness of IBR-2, which, in combination with the optimal design, will help to achieve record parameters at the new INS instruments. The first phase of the project for the development of new INS

instruments involves the construction of a new spectrometer with inverse geometry at beamline 2 of the IBR-2 reactor.

2. Scientific program, topicality and comparison with the world level

There are several experimental methods for spectroscopic studies of condensed matter dynamics aimed at obtaining information about the structure, chemical bonds, and molecular interactions in materials under study. Infrared (IR) absorption spectroscopy and Raman spectroscopy are probably the best-known examples and the most popular methods used for this purpose. Inelastic neutron scattering (INS) is also a spectroscopic method for studying atomic and molecular dynamics, which, in combination with advanced quantum-chemical calculations and complementary experimental methods, provides unique information about certain vibrational properties of materials. There is an ever-growing demand for inelastic neutron scattering instruments, which is determined by the advantages of INS as compared to the optical vibrational spectroscopy:

1. No selection rules,
2. Isotopic sensitivity (isotopic substitution to hide or highlight selected molecular fragments),
3. High penetrating power of neutrons,
4. Minimum energy release in the sample,
5. Possibility to study chemical processes in situ,
6. Possibility to study magnetic excitations using polarized neutrons,
7. Experimental information as a function of both energy transfer and momentum transfer,
8. Relatively simple theoretical description and modeling.

The possibility of neutron spectroscopy to see overtones and their combinations is unique, and, in this respect, INS is clearly superior to IR and Raman spectroscopy (in optical methods such vibrations contribute about 1% of the spectral intensity, whereas in INS spectra they can be up to 75% of the intensity).

The planned research program of the new INS spectrometer with inverse geometry encompasses studies of the dynamics of:

1. methyl groups in molecular crystals;
2. molecular crystals and glass-forming agents at low temperatures in combination with the studies by complementary techniques and *ab initio* quantum-chemical calculations;
3. pharmaceutical substances in bulk (native) state and in the form of “micronized” or amorphized powders;
4. materials in spatial confinement: “hard” nanomatrices (for example, membranes) and “soft” confinement (for example, microfibre);
5. materials for energy storage, for example, solid polymer electrolytes with plasticizers for lithium batteries;
6. catalysts;
7. photonic materials for industrial applications.

Every advanced neutron research center in the world operates one (e.g. ISIS, ORNL) or even more (e.g. ILL) highly efficient optimized INS spectrometers. The development of a high-quality INS spectrometer optimized for low wave numbers has good prospects for realization at the IBR-2 pulsed reactor.

3. Scientific and methodological groundwork laid in FLNP JINR

Considerable experience has been accumulated in FLNP JINR in using neutron spectroscopy on the basis of operation of KDSOG, NERA and DIN-2RI spectrometers, at which numerous experiments on the dynamics of condensed matter were carried out.

4. Proposals for design of the instrument

4.1. Information on the current status of the project

At present, a concept of the spectrometer has been developed, and the simulation of its main units has been done.

4.2. Detailed description of proposals for design of the instrument

4.2.1. Layout and main units of the instrument

The new inelastic neutron scattering spectrometer with inverse geometry will be installed at beamline 2 of the IBR-2 reactor (building 117/1). The main units of the spectrometer include mirror neutron guide, cascade of choppers, sample assembly, analyzer made of highly-oriented pyrolytic graphite and a beryllium filter, and detectors. The proposed layout of the new spectrometer is shown in Fig. 26.

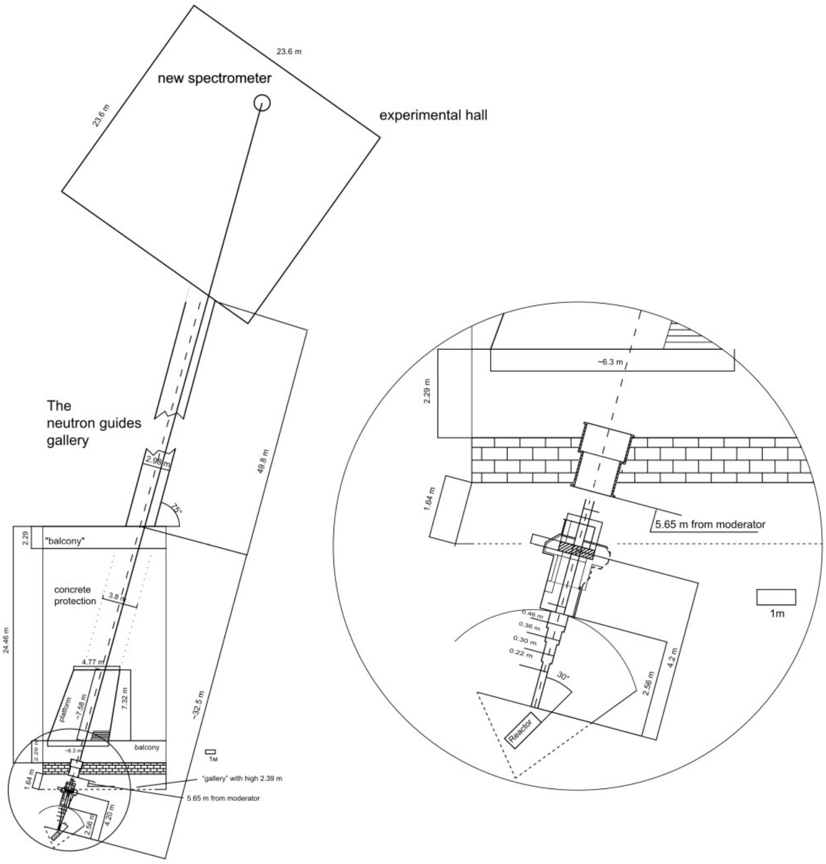


Fig. 26. *Layout of the new INS spectrometer at beamline 2 of the IBR-2 reactor.*

Since the spectrometer will be placed in the existing building 117/1, the optimal distance from the moderator surface to the sample was chosen to be 105 m, which gives the optimal time resolution over the entire range of energy transfer.

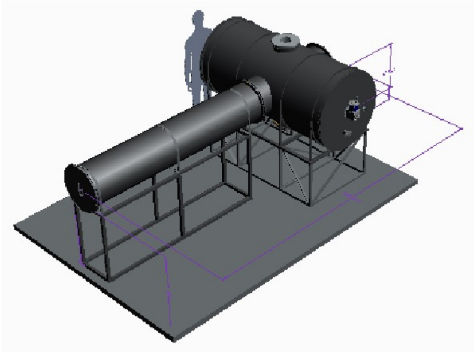
Neutron-optical elements of the mirror neutron guide will be optimized for a wavelength range of 0.5 - 1 Å (energy transfer range of 80 - 330 meV). The end part of the neutron guide (length ~25 m) will be convergent. In addition, two possible beam sizes on the sample (3 ×3 cm^2 and 1 × 1 cm^2) will be available. The distance between the exit of the neutron guide and the sample place will be 0.35 m.

In accordance with the strategic development plan, a place will be reserved for a second direct-geometry spectrometer at beamline 2.

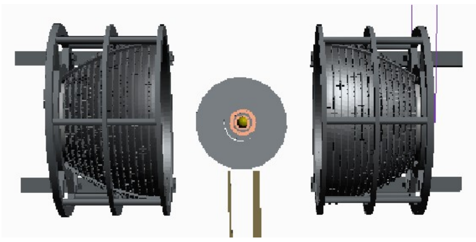
The inverse-geometry spectrometer at beamline 2 will operate with the existing thermal grooved moderator. For a direct-geometry spectrometer, a wide spectrum of incident neutrons (thermal and cold) is preferable, therefore, in the future, it is planned to install a bi-spectral moderator (the cold part is a mesitylene-based moderator mounted above the grooved moderator).

4.2.2. Geometry of the instrument

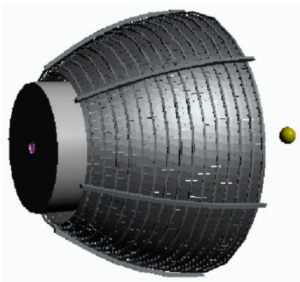
The schematic drawing of the new INS spectrometer with inverse geometry is shown in Fig. 27.



a)



b)



c)

Fig. 27. *The geometry of the new INS spectrometer with inverse geometry: a) general layout; b) two symmetric parts of the spectrometer with pyrolytic graphite analyzers; c) one part of the spectrometer with beryllium filter and detector.*

The new inverse-geometry spectrometer will consist of two symmetrical parts. Each of them is shaped as a paraboloid of revolution and lined with plates of highly-oriented pyrolytic graphite. It is proposed to install approximately 700 plates (dimensions 15 × 30 mm) on each part. At the moment, the necessary engineering and design work to optimize the spectrometer is underway.

The scattering scheme by the sample is shown in Fig. 28.

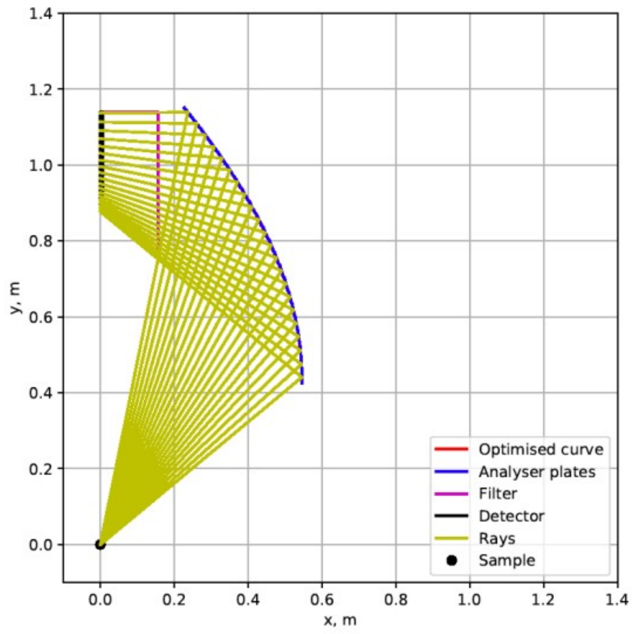


Fig. 28. *Scattering scheme and detection of neutrons at the new spectrometer with inverse geometry.*

4.3.3. Detector system

It is planned to install one detector in each arm of the spectrometer. Each detector comprises one or several cylindrical counters inscribed in a circle with a diameter of 50 mm. The counters will have a thin metal wall (0.2-0.3 mm) and will be filled with ^{3}He.

4.4. Expected technical parameters

<u>Features of the new INS spectrometer:</u>

- large solid angle, more than five times greater than at NERA;

- advanced neutron optics (manufactured by SwissNeutronics) together with neutron beam focusing will give a significant gain in the neutron flux density at the sample place.

The total gain in luminosity compared to NERA can exceed a factor of 50, which will allow one to perform experiments with a sample mass of several hundred milligrams.

5. Requested resources, costs and time frames of instrument construction

The time frames and costs of the stages of the spectrometer construction are given in **Table 15 (Section 4)**.

SANSARA - Small-Angle Neutron Scattering Instrument

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1. Abstract

The SANSARA (Small-Angle Neutron Scattering And RAdiography) instrument is a small-angle neutron scattering (SANS) diffractometer combined with a neutron radiography (NRG) station located at beamline 10a with cold neutrons. The construction of a new advanced small-angle neutron scattering instrument at IBR-2 with the most efficient realization of the capabilities of neutron scattering, is an important part in the development of structural methods for studying nanosystems at the reactor. Following the current trends in the development of neutron centers, the instrument is a general-purpose small-angle diffractometer aimed at providing a wide range of possibilities for conducting SANS experiments. The optimization of the setup follows the conventional configuration of a SANS instrument at a cold neutron source. To enhance the efficiency of using cold neutrons, it is proposed to combine a SANS diffractometer with a neutron radiography station.

2. Scientific program, topicality and comparison with the world level

The SANSARA (Small-Angle Neutron Scattering And RAdiography) setup is a small-angle neutron scattering (SANS) diffractometer combined with a neutron radiography (NRG) station located at beamline 10a with cold neutrons.

Small-angle neutron scattering is one of the widely used methods of structural studies of nano-objects – systems whose properties are determined by structural features at a level of 1-100 nm. The scientific program of small-angle instruments includes a variety of research areas:

- Complex fluids, including magnetic fluids, surfactant solutions, anisotropic fluids, liquid crystals, etc.
- Magnetic nanocomposites
- Polymers, including magnetic polymers
- Biological macromolecules, membranes, vesicles
- Liposomes, including magnetosomes
- Dispersions of carbon materials
- Inhomogeneities in structural materials

Today, every advanced neutron center runs at least one such instrument. Moreover, there is a tendency to create several small-angle instruments in one center, optimized for different types of tasks. This concept provides the most effective use of this method. The small-angle scattering instrument is a 'fast-payback' project in the scientific sense, since the average time per one experiment is only a few hours. The latter factor determines the possibility of conducting a complete study using neutrons in a relatively short time. The small-angle scattering instruments operating today at IBR-2 cannot satisfy the growing demand for research using this method. Thus, analyzing the statistics of the use of neutron instruments at the IBR-2 reactor within the user policy over the past 10 years, one can conclude that there is a stable excess of experimental proposals over the capacity of the YuMO setup, operating at the level of world standards. In view of the current boom in nanosciences, one can only expect an increase in demand for SANS experiments in the nearest future. The use of neutron scattering in the study of nanosystems is determined by two factors: (1) wide possibilities of contrast variation based on the isotopic substitution of atoms in the systems under study; (2) magnetic neutron scattering, which allows obtaining information on magnetic correlations in magnetic systems. Thus, the construction of a new advanced small-angle neutron scattering instrument at IBR-2 with the most efficient realization of the capabilities of neutron scattering, is an important part in the development of structural methods for studying nanosystems at the reactor.

3. Scientific and methodological groundwork laid in FLNP JINR

The YuMO time-of-flight small-angle neutron scattering instrument [1], which is oriented to work with the thermal moderator (T = 300 K) and uses collimation with the direct view of the moderator [2], is successfully operating at the IBR-2 pulsed reactor. To obtain a scattering curve in the range $q = 0.05 - 5\ \mathrm{nm}^{-1}$, a special procedure is used with a continuous calibration to the vanadium standard placed in front of the detector. The time spent on the calibration is compensated by a high peak intensity when using the thermal moderator, which reduces the characteristic measurement time per one curve to an interval of 10 - 90 min (depending on the cross section of the sample).

The main advantage of YuMO is a two-detector system with large-area ring detectors for detecting isotropic scattering and central openings in the detectors allowing the direct beam to pass. This feature makes it possible to realize a record (~100) dynamic q-range (scanning range in one measurement run). Thus, the setup can be effectively used to study changes in the nanoscale range (10-100 nm) in real time (time resolution down to 1 min).

This feature, however, imposes some limitations. Since the instrument is optimized for the thermal moderator, there is a limitation in resolution at the minimum q-value, which narrows the sensitivity in the size range (submicron region). Also, because of the direct view of the source, the background level is comparatively high. The detector openings complicate the use of conventional designs of position-sensitive detectors (PSD), as well as the use of direct measurement of the transmission and corresponding calibration.

The design of the new SANS instrument is aimed at eliminating the above limitations, which is possible due to the availability of a cold moderator. The natural compensation will be a decrease in the average beam intensity at the sample. The availability of a large-area 2D PSD with the conventional procedure for obtaining and calibrating scattering curves at two detector positions (short and long flight paths) will allow experiments for a large number of equilibrium systems, including systems with scattering anisotropy (oriented systems, magnetized magnetic systems). In turn, this will make it possible to focus the YuMO scientific program on the study of kinetic phenomena.

4. Proposals for design of the instrument

4.1. Information about the current status of the project

The concept, simulation and selection of the optimal configuration and moderator temperature, as well as estimates of the instrument parameters were published in [3].

The schematic layout of the proposed instrument is presented in Fig. 29. For the implementation of the project, it is proposed to use channel 10 of the IBR-2 reactor, which is currently split into two beamlines: 10a and 10b. At present, the GRAINS reflectometer (reflectometer with a horizontal sample plane) is operating at beamline 10b [4]. Beamline 10a is equipped with a head part with a neutron guide (supermirror m = 2) and a background chopper in the ring corridor. Also, the head part is followed by the previously installed multi-slit optical beam deflector (bender), a supermirror m = 2, bending angle of 8 ° at a length of 2 m.

4.2. Detailed description of proposals for design of the instrument

The main factors determining the parameters of SANSARA are: (1) minimization of fast neutron background; (2) measurement in a wider (with respect to small q-values) range of momentum transfer.

The implementation of (1) is provided by the tangential nature of beamline 10 relative to the reactor core and the use of a neutron bender with the beam axis diverted from the direct view of the neutron moderator.

The implementation of (2) is provided by the availability of a cold moderator at beamline 10.

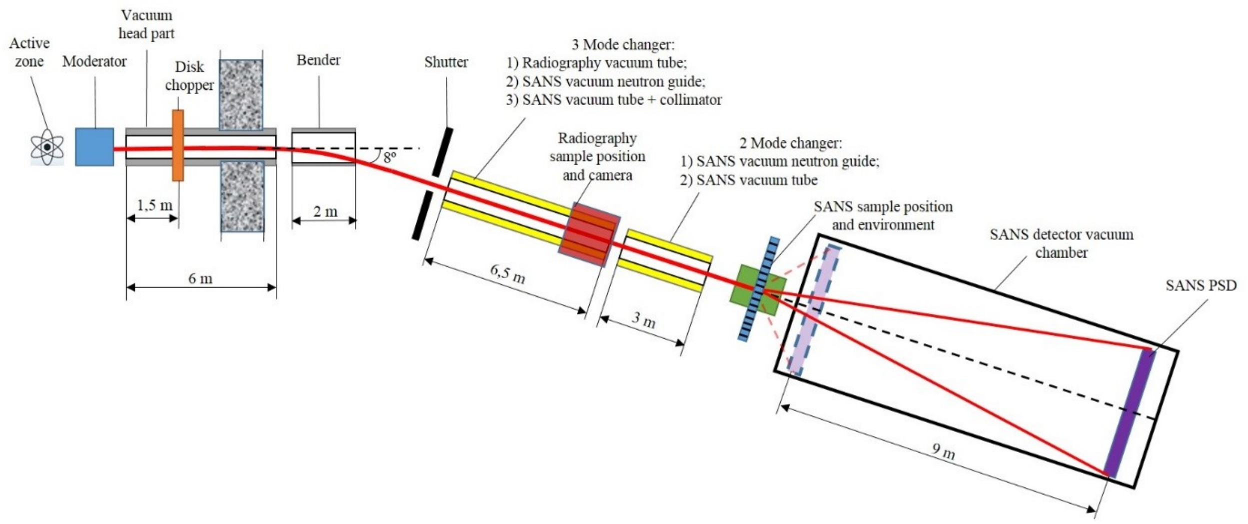

Fig. 29. *Schematic layout of SANSARA.*

A replaceable beam-forming system together with an additional shutter are installed behind the bender (Fig. 30). The system provides the following options: NRG (radiography) and SANS (small-angle neutron scattering). Switching between the options is provided by three separate beam-forming units in the vertical direction (one unit for NRG and two units for SANS) via remote control.

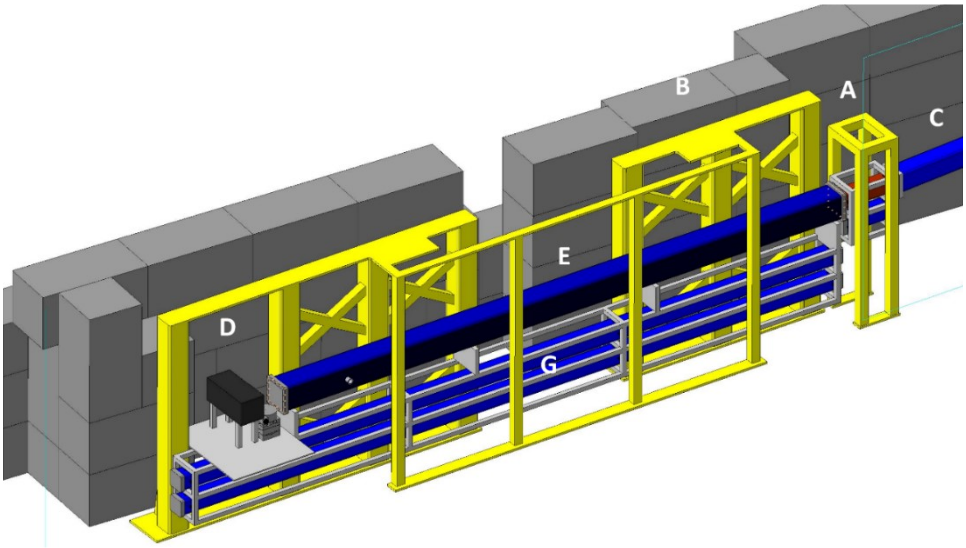

Fig. 30. *Conceptual view of the beam-forming system of the SANSARA instrument in the experimental hall of IBR-2. Main units: (A) movable shutter with a vacuum tube; (B) mechanical part for changing the vertical position of neutron guides to form a beam; (C) bender; (D) NRG platform; (E) NRG vacuum tube; (G) two SANS beam-forming units (neutron guide and vacuum tube).*

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

For the most efficient use of neutron scattering in terms of sensitivity to the size range, the SANS instrument with the conventional configuration requires a cold moderator with a temperature of 30 K. The availability of cold neutrons additionally allows the use of neutron-optical devices to separate fast and cold neutrons and significantly reduce the background level at the sample. Also, to enhance the efficiency of using cold neutrons, this research technique can be relatively easily combined with other methods, such as neutron radiography and tomography. As a result of the use of a bender (beam deflector) optimized for a temperature of 30 K, the instrument is intended only for operation in the cold mode of the moderator.

4.4. Expected technical parameters

Beam size	50×50 mm^2
Neutron wavelength range:	0.5 - 15 Å
q-range	0.001 - 1 Å^{-1}
Angular resolution	5 - 20 %
Sample dimensions	5×5×1 - 20×50×50 mm
Neutron flux at sample position	1.0×10^6 cm^{-2} s^{-1}
Detector	2D PSD, efficiency > 50% (0.2 nm) 64×64 - 80×80 cm^2, resolution 5×5 - 10×10 mm^2 count rate 10^5 - 10^6 s^{-1}

4.5. Relevance of the instrument development for the concept of a suite of spectrometers within the project of a new neutron source at JINR

The construction of the instrument is fully consistent with the current trends in methodological development. Over the past five years, general-purpose small-angle diffractometers have been designed and are successfully operating at almost all neutron sources, both pulsed and steady-state. Their main task is to meet a huge demand for this technique. Among the examples are GP-SANS - General Purposes SANS (SNS), Sans2d (ISIS), KWS-2 (FRM-II), Bilby (ANSTO).

5. Expected scientific results

The SANS technique, which is used in solving a wide range of fundamental and applied problems within a broad research scope related to the nanoscale structure of matter, remains one of the most popular methods among neutron scattering techniques. Such kind of problems are very important and of great current interest in various sciences, including condensed matter physics, physics and chemistry of complex liquids and dispersed systems, including solutions of surface-active agents and polymers, biophysics and molecular biology, materials science. The most important area of application of small-angle scattering is the analysis of the structure of disordered systems using non-destructive testing with an emphasis on obtaining direct structural information about systems with chaotic and partially ordered arrangement of density inhomogeneities with sizes of the order of 1 - 100 nm. This includes dispersed structures of alloys, powders, and glasses (phase separation mechanisms, particle size and degree of polydispersity), structural features of polymers in various states of aggregation, weight and geometric characteristics of biological macromolecules and their complexes, biological supramolecular structures, such as biological membranes and viruses.

6. Requested resources, costs and time frames of instrument construction

The construction period is 3 years. The requested resources are listed in **Table 16 (Section 4)**.

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Neutron Radiography and Tomography Station with Cold Neutrons

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1. Abstract

Neutron radiography is an imaging technique based on various degrees of attenuation of the neutron beam passing through components of the sample under study with different chemical composition, density, and thickness. It is used to obtain information on the internal structure of the studied materials with a micrometer-scale spatial resolution. To radically improve the neutron radiographic contrast in neutron radiography experiments, cold neutrons are required. In addition, a low-background neutron source is preferred for realization of the energy-selective neutron imaging method. Therefore, it is planned to develop and implement a neutron radiography mode at beamline 10a of the IBR-2 reactor, where the source of cold neutrons is a curved multi-module neutron guide – a neutron 'bender'.

2. Scientific program, topicality and comparison with the world level

Neutron radiography is a method of obtaining neutron images of objects under study. Different intensity losses in the neutron beam passing through components of the sample under study with different chemical composition, density, and thickness provide information on the internal structure of the studied materials with a micrometer-scale spatial resolution [1, 2]. This method of nondestructive testing is characterized by a deeper penetration into materials compared to the complementary method of X-ray radiography and has a number of advantages in the investigation of objects containing both light (e.g., hydrogen or lithium) and heavy elements. All modern and newly developed neutron sources are equipped with neutron radiography and tomography stations [1, 2]. At present, neutron radiography is widely used in research of materials and products for nuclear technologies, paleontological and geophysical objects [3-5], and unique objects of cultural heritage [6-10].

The availability of advanced CCD-camera-based detectors for neutron imaging and the development of high-flux neutron sources have given a new impetus to the development of methods of neutron radiography and tomography and the construction of specialized experimental stations at neutron centers throughout the world. One of the basic facilities of the Joint Institute for Nuclear Research is the modernized high-flux IBR-2 reactor, which is one of the most intense pulsed neutron sources in the world. It should be noted that the pulsed character of the operation of the IBR-2 reactor opens up wide prospects for the implementation of energy-selective neutron imaging using the time-of-flight technique [4], in which the contrast of the object elements consisting of various materials can be enhanced by choosing the optimal energy range of incident neutrons.

At the IBR-2 high-flux pulsed reactor at beamline 14, the NRT experimental station has already been successfully operating for research using the neutron radiography and tomography technique. However, the neutron spectrum at beamline 14 is shifted to the region of fast neutrons with a relatively small fraction of thermal and cold neutrons. Therefore, to improve the contrast in neutron radiographic experiments, a neutron beam is required with a spectral redistribution towards the region of cold neutrons.

3. Scientific and methodological groundwork laid in FLNP JINR

In recent years, a neutron radiography and tomography station [1-4] has been created at beamline 14 of the IBR-2 reactor. Its methodological possibilities allow the successful implementation of scientific and applied experiments to analyze the internal structure of various objects both in fundamental and applied research [4-10]. The parameters of the station and its experimental capabilities make it possible to carry out neutron experiments at a high world level with paleontological [1], astrophysical [5] and engineering [1, 2] objects. Significant scientific groundwork has been laid for nondestructive research of cultural heritage objects using neutron radiography and tomography [6-10] including unique studies of coins of Ancient Greece [6] and Bulgaria [7], objects of ancient Russia’s cultural heritage [8-10].

4. Current status of the project and proposals for the construction of the instrument

4.1. Information about the current status of the project

In the framework of the project of a new neutron radiography station with the “cold” neutron spectrum, it is planned to place the equipment at beamline 10 of the IBR-2 reactor. A special optical device is currently installed at beamline 10a, a neutron bender, at the exit of which a squared neutron beam with dimensions of 60 × 60 mm is formed with a spectral distribution shifted to the region of “cold” neutrons. Along with it, it is planned to construct a new small-angle scattering instrument at the same beamline 10a. To divide experimental time between several techniques, it is proposed to install a multi-module system with a mechanical equipment changer (Fig. 31).

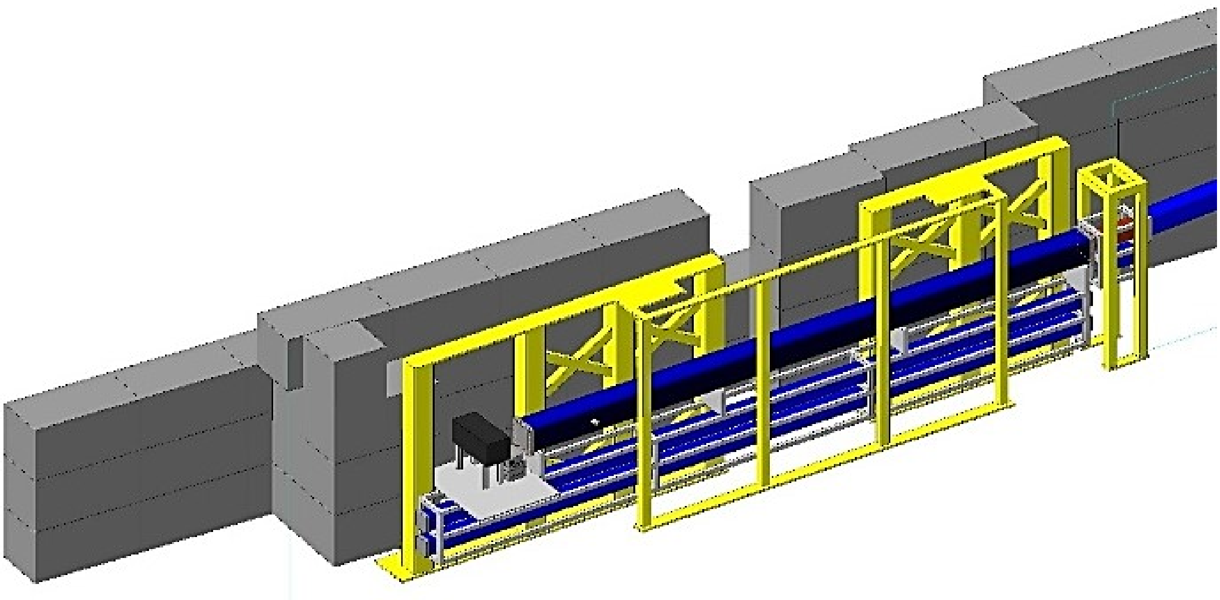

Fig. 31. *Schematic drawing of a multi-module changer for replacing equipment for small-angle neutron scattering and neutron radiography. One of the modules is a system for neutron radiography and tomography at the cold neutron source.*

One of the modules of this system is planned to be used as a basis for a new neutron radiography and tomography station. The first test experiments (Fig. 32) on neutron imaging at beamline 10a have already been conducted.

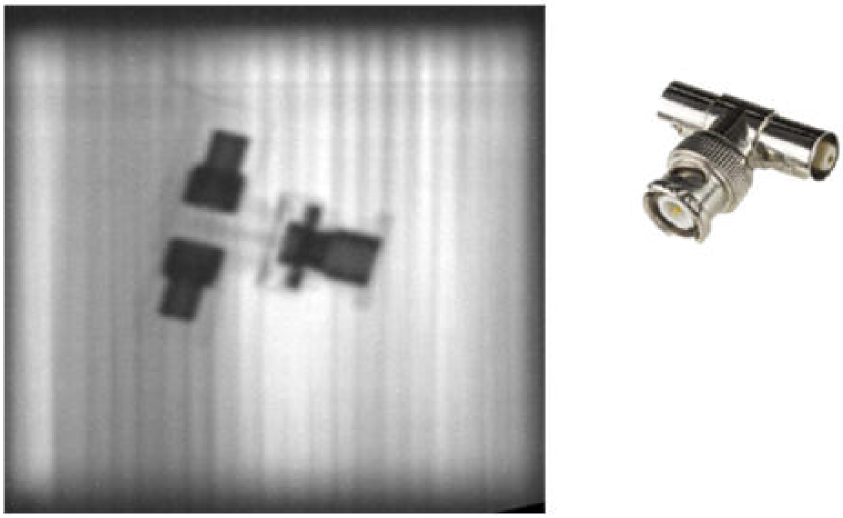

Fig. 32. *Test neutron image of a metal connector obtained at beamline 10a at the exit of the neutron bender. Periodic stripes visible in the neutron image correspond to the absorbing elements between transmission slits of the bender.*

4.2. Detailed description of proposals for the construction of the instrument

The implementation of the project of a new experimental neutron radiography and tomography station at beamline 10a requires design work, purchase of equipment and its installation on a movable module.

It is suggested that the neutron beam is formed by a neutron bender with initial dimensions of 60 × 60 mm, and then, using a 10-m long collimation system consisting of circular cylindrical inserts made of borated polyethylene, it expands up to 120 mm at the exit of the neutron beam from the collimation system. The collimation system will be placed in a vacuum housing to reduce losses in intensity due to neutron scattering in the air.

As a detection system, it is intended to use a detector module with replaceable CCD video cameras of various types. The conversion of neutrons into photons will be performed using scintillator plates of various types (from standard ^{6}LiF/ZnS to gadox Gd_2O_2S). The light from the scintillator is reflected from rotating mirrors tilted at an angle of 45° with respect to the axis of the incident neutron beam, and hits the optical system of the video camera. All optical systems of the detector will be in a light-protective housing. Tomography experiments will be performed using a system of goniometers with a minimum rotation angle of down to 0.01° and a remote control system.

The obtained neutron images will be corrected for the background noise of the detector system and calibrated to the incident neutron beam using the ImageJ software package. The tomographic reconstruction of the studied object from a set of angular projections will be performed using the H-PITRE software. For visualization and analysis of the obtained 3D data, the VGStudio MAX 2.2 software package from Volume Graphics (Heidelberg, Germany) is intended to be used.

4.3. Technical parameters important for operation at thermal and cold modes of the moderator

A new mode for experiments on neutron radiography and tomography will be realized at beamline 10, where a cold moderator operates. This will increase the incident flux of cold neutrons in the wavelength range of 4-13 Å by a factor of ~ 7-10.

4.4. Expected technical parameters

The construction of a neutron radiography station at a cold neutron source will allow conducting standard classical experiments on neutron radiography and tomography with high radiographic contrast. The redistribution of the spectrum towards the region of slower neutrons, as well as improved background conditions for the sensitive optical components of cameras will make it possible to use a wider range of technical solutions in the field of recording neutron images: from simple CCD cameras to highly sensitive cameras based on sCMOS sensors. Experiments with detectors based on Timepix and Medipix chips will also be possible. In this case, the method of energy-selective neutron imaging with low-background conditions will be implemented.

4.5. Relevance of the instrument creation for the concept of a complex of spectrometers in the project on a new neutron source at FLNP

At the new neutron source of FLNP, it is planned to construct several stations for neutron radiography and tomography investigations, including a station for energy-selective neutron imaging. Thus, the methodological and scientific development of the research direction of neutron radiography and tomography is one of the promising and relevant research areas for the future FLNP scientific program.

5. Expected scientific results

The construction of a neutron radiography station at a cold neutron source will allow conducting standard classical experiments on neutron radiography and tomography with high radiographic contrast. The redistribution of the spectrum towards the region of slower neutrons, as well as improved background conditions for the sensitive optical components of cameras will make it possible to use a wider range of technical solutions in the field of recording neutron images: from simple CCD cameras to highly sensitive cameras based on sCMOS sensors. Studies of engineering devices and components, objects of cultural heritage, paleontology, astrophysics, building materials, etc. are planned.

Experiments with detectors based on Timepix and Medipix chips will also be possible. In this case, the method of energy-selective neutron imaging with low-background conditions will be implemented.

6. Requested resources, costs and time frames of instrument construction

The costs of the design and development stages of the construction of the experimental station are presented in **Table 17 (Section 4)**.

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4. REQUESTED FINANCIAL RESOURCES FOR PROJECTS

The tables below summarize the cost (in k$) and desired periods of manufacturing (purchase) of units and equipment necessary for the implementation of the projects presented in Sections 2 - 3.

Table 1. HRFD - High-Resolution Fourier Diffractometer

Description	Cost, k$	Realization period	Notes
Backscattering detector	600	2021-2023	Manufacturing in FLNP
Cryo-furnace	150	2021	Purchase
Magnet with its own cooling and heating system for samples	400	2022-2023	Manufacturing in FLNP
Positioning platform	60	2021	Purchase
Fourier-chopper	350	2023-2025	Purchase
Infrastructure	50	2021-2025	Purchase and installation
TOTAL:	**1610 k$**		

Table 2. FSD - Fourier Stress Diffractometer

Description	Cost, k$	Realization period	Notes
Backscattering scintillation detectors	350	2021-2025	Manufacturing in FLNP
New version of list-mode correlation analysis electronics	30	2020-2022	Manufacturing in FLNP
Development of software for spectrum reconstruction from list-mode data	15	2022-2024	Order
Mirror neutron guide	240	2022-2024	Order
TOTAL:	**635 k$**		

Table 3. FSS - Fourier Diffractometer

Description	Cost, k$	Realization period	Notes
Backscattering scintillation detectors	300	2021-2025	Manufacturing in FLNP
ZnS-based 90°-detectors	100	2021-2025	Manufacturing in FLNP
High-resolution scintillation PSD detector (prototype)	30	2021-2025	Manufacturing in FLNP
Manufacturing of new Fourier chopper	350	2021-2025	Order
Radial collimators	100		Order
Device for moving radial collimators	10		Order
Goniometer	90		Order
New version of list-mode correlation analysis electronics	30	2020-2022	Manufacturing in FLNP
Development of software for spectrum reconstruction from list-mode data	15	2022-2024	Order
TOTAL:	**1025 k$**		

Table 4. **RTD - Neutron Diffractometer (Real-Time Diffraction)**

Description	Cost, k$	Realization period	Notes
Supermirror neutron guide (m ≈ 2) with two-plane focusing	400	until 2024	Purchase
Backscattering detector system ($\Omega_d \approx 2$ sr) with electronic components and slit collimators	350	until 2023	Purchase and order in FLNP
90° ZnS scintillation detector system and electronic components	300	until 2025	Purchase and order in FLNP
Rotating platform for small-angle detector	35	2021	Purchase of units and manufacturing in FLNP
High-temperature furnace (1800°C)	70	2022	Purchase
Electrochemical cell with possibility of transmitting electric current through the sample (up to 10 A) for a temperature range of 20-900°C	20	2022	Order in FLNP
Huber three-circle goniometer with refrigerator down to 4 K	120	2021	Purchase
Compact furnace for Huber three-circle goniometer	30	2022	Purchase
Shaft-type refrigerator (8-290 K).	70	2022	Purchase and manufacturing in FLNP
Cryostat with possibility of producing a magnetic field at the sample	100	2021	Purchase
Unit for producing a magnetic field in the range from 0 to 2 T	30	2021	Purchase and order in FLNP
Modernization of electronics and software	30	2021	Order in FLNP
Radiation shielding screen "TISSA-RP" with Pb glass for channels 5-6	3	2021	Purchase
Infrastructure	30	2021-2023	Purchase and installation
TOTAL:	**1588 k$**		

Table 5. DN-6 - Neutron Diffractometer for Ultrahigh-Pressure Research

Description	Cost, k$	Realization period	Notes
Protective casing of borated polyethylene for ring detector for small-angle scattering	45	2022	
Helium neutron detectors, 100 pcs	50	2022	
Set of high-pressure cells with diamond anvils	40	2023-2024	
Equipment for preparing high-pressure cells with diamond anvils for experiments: machine for drilling gaskets, gas charging machine for cells, sets of diamond anvils, gaskets, supports made of hard-alloy material	70	2022-2025	
Electronic components for ring detector for small-angle scattering	155	2022	
Special microscope to control loading of ultra-small samples in a high-pressure cell with diamond anvils	70	2022, 2025	
TOTAL:	**430 k$**		

Table 6. DN-12 - Neutron Diffractometer for Investigations of Microsamples at High Pressures

Description	Cost, k$	Realization period	Notes
Commissioning of cryogenic system for cooling simultaneously permanent magnet of up to 5 T and high-pressure cell (cryocooler system)	105	2021- 2023	
Purchase of accessories for the cryocooler system: mechanical fasteners, positioner, radiation shielding, vacuum equipment and accessories, vacuum sensors	85	2021 - 2023	
Modernization of the detector system to increase its solid angle. Design and manufacture of fixing mechanism for cryocooler. Purchase of neutron counters and DAQ electronics.	105	2021 - 2023	
Purchase of high-pressure cells and accessories: sapphire anvils, hard-alloy supports, gaskets, toolkits	99	2021-2025	
Protective casing of borated polyethylene for ring detector	55	2022-2023	
Purchase of high-pressure press with necessary infrastructure of compressors and accessories.	550	2022-2025	
Monocular microscope with a large focal length for adjusting anvils in high pressure cells and accessories	40	2022-2023	
TOTAL:	**1039 k$**		

Table 7. **EPSILON-MDS - Strain/Stress Diffractometer**

Description	Cost, k$	Realization period	Notes
Goniometer HUBER	10	2021-2024	
New neutron guide	1200	2021-2024	
Electronics for new detector system	100	2021-2024	
TOTAL:	**1310 k$**		

Table 8. **SKAT - Texture Diffractometer (project 1)**

Description	Cost, k$	Realization period	Notes
New neutron guide	1200	until 2025	
Helium neutron detectors, 40 pcs.	50	until 2021	
Manufacturing of radial collimators	40	until 2023	
HUBER goniometer	10	until 2023	
Bearing ring	70	until 2022	
Electronics and computers	60	until 2021	
Sample environment equipment	45	until 2022	
TOTAL:	**1475 k$**		

Table 9. **SKAT - Texture Diffractometer (project 2)**

Description	Cost, k$	Realization period	Notes
^{3}He counters with a set of collimators and data acquisition electronics	100	2021-22	Order/Manufacturing in FLNP
Compact furnace (up to 1000°C)	40	2021-22	Order
Simulation to optimize the SKAT neutron guide in case of dismantling the splitter on channel 7	5	2022-23	Order
Automatic sample changer	30	2021-23	Order/Manufacturing in FLNP
2D PSD	75	2022-25	Order/Manufacturing in FLNP
TOTAL:	**250 k$**		

Table 10. **YuMO - Small-Angle Neutron Scattering Instrument**

Description	Cost, k$	Realization period	Notes
Development and construction of prototype of 2D solid-state direct-beam detector	30	2021-2023	
Development and construction of 2D large-area detectors	280	2021-2025	
Data acquisition electronics of PSD of new type	75	2021-2024	
Development and installation of changeable collimator	70	2021-2022	
Development and construction of chopper	45	2021-2023	
Optimization of collimation base	90	2022-2025	
Modernization of instrument units and sample environment equipment	155	2021-2025	
TOTAL:	**745 k$**		

Table 11. **GRAINS - Neutron Reflectometer with Horizontal Sample Plane**

Description	Cost, k$	Realization period	Notes
Drum choppers	200	2021-2023	
Polarizer assembly	100	2021-2025	
Detector system	150	2021-2024	
Magnetic system	100	2021-2022	
Sample environment system	150	2021-2023	
TOTAL:	**700 k$**		

Table 12. **REFLEX - Reflectometer with Polarized Neutrons**

Description	Cost, k$	Realization period	Notes
Polarization analyzer m = 5	35	2021	
Background suppression equipment	30	2022	
Mechanical chopper	25	2022	
Automation system	15	2022	
Magnetic sample system	40	2024	
Cryogenic sample system	100	2024	
Fan-type polarization analyzer	120	2024	
Spin-echo diffractometer	300	2025	
TOTAL:	**665 k$**		

Table 13. REMUR - Reflectometer with Polarized Neutrons

Description	Cost, k$	Realization period	Notes
Drum chopper	20	2021	Purchase
Closed-cycle helium cryostat	80	2021	Purchase
Pumping system	45	2022	Purchase
1. Ring PSD for direct scattering 2. Backscattering detector	60 60	2021 2022	Manufacturing in FLNP Manufacturing in FLNP
Neutron polarizer	35	2022	Purchase
TOTAL:	**300 k$**		

Table 14. NRT - Neutron Radiography and Tomography Station

Description	Cost, k$	Realization period	Notes
Medipix detector for energy-selective neutron imaging	150	2021	
Vacuum pump for pumping out the casing of Medipix detector for energy-selective neutron imaging	25	2021	
Protective casing of borated polyethylene for Medipix detector for energy-selective neutron imaging	45	2022	
Module of detector system based on high-speed camera with sCMOS sensor. Production of protective module for camera	55	2022-2023	Development
High-speed camera with sCMOS sensor. Optical components for camera: camera lens, a set of lenses, guard rings, etc.	80	2023-2025	
Protective casing for sapphire filter. Single-crystal sapphire filter	65	2022-2024	Development Purchase
Additional accessories for the available CCD-based detector system	110	2021-2025	Purchase
TOTAL:	**530 k$**		

Table 14. **New Inverse-Geometry Inelastic Neutron Scattering Spectrometer**

Description	Cost, k$	Realization period	Notes
Neutron guide	2000	2021-2024	
Analyzer (graphite plates)	300	2021-2023	
Detectors	10	2022-2023	
Vacuum tank	400	2021-2022	
Sample environment	300	2023-2024	
Repairs of experimental building	100	2021	FLNP infrastructure
TOTAL:	**3110 k$**		

Table 15. **SANSARA - Small-Angle Neutron Scattering Instrument**

Description	Cost, k$	Realization period	Notes
Changeable beam-forming system	450	2021	
Detector system for PSD (SANS mode)	500	2021-2023	
2D PSD (SANS mode)	1500	2021-2023	
Monitor	50	2021	
Sample assembly with thermostating	300	2021-2023	
Electromagnet (SANS mode)	100	2023-2025	
Control system	100	2021-2023	
TOTAL:	**3000 k$**		

Table 16. **Neutron Radiography and Tomography Station with Cold Neutrons**

Description	Cost, k$	Realization period	Notes
Design of individual components and their location on the platform of the module changing mechanism	45	2021-2022	
Purchase of main components of new neutron radiography station: vacuum tubes for collimation system, collimators, vacuum equipment, goniometer and electronic components	90	2021-2023	
Design and manufacture of a detector system for neutron radiography and tomography	180	2021-2023	
Purchase of recording cameras based on CCD and sCMOS sensors, neutron scintillators	140	2021-2022, 2024-2025	
Purchase of Timepix detector for time-of-flight neutron imaging	135	2023-2025	
Purchase of specialized software for analysis of experimental data	70	2021, 2024	
TOTAL:	**660 k$**		

Summary table of requested financing for projects

№	Instrument	Project title	Requested financing, k$
1.	HRFD	HRFD - High-Resolution Fourier Diffractometer	1610
2.	FSD	FSD - Fourier Stress Diffractometer	635
3.	FSS	FSS - Fourier Diffractometer	1025
4.	RTD	RTD - Neutron Diffractometer (Real-Time Diffraction)	1588
5.	DN-6	DN-6 - Neutron Diffractometer for Ultrahigh-Pressure Research	430
6.	DN-12	DN-12 - Neutron Diffractometer for Investigations of Microsamples at High Pressures	1039
7.	EPSILON-MDS	EPSILON-MDS - Strain/Stress Diffractometer	1310
8.	SKAT	SKAT - Texture Diffractometer (project 1)	1475
		SKAT - Texture Diffractometer (project 2)	250
9.	YuMO	YuMO - Small-Angle Neutron Scattering Instrument	745
10.	GRAINS	GRAINS - Neutron Reflectometer with Horizontal Sample Plane	700
11.	REFLEX	REFLEX - Reflectometer with Polarized Neutrons	665
12.	REMUR	REMUR - Reflectometer with Polarized Neutrons	300
13.	NRT	NRT - Neutron Radiography and Tomography Station	530
14.	INS_NEW	New Inverse-Geometry Inelastic Neutron Scattering Spectrometer	3110
15.	SANSARA	SANSARA - Small-Angle Neutron Scattering Instrument	3000
16.	NRT_COLD	Neutron Radiography and Tomography Station with Cold Neutrons	660
		TOTAL:	**19 072 k$**