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Definition of the optimal suite of instruments

1. Introduction

Research using neutrons covers a wide range of fields of science and technology. The most frequently used group of research methods is neutron scattering, which is designated to directly receive information about the structure and dynamics of the substance at the atomic level. Neutron scattering provides a wide range of possibilities for modern physics, chemistry, biology, and material science. In addition, the neutron is a very convenient object for studying fundamental interactions, because it is involved in all interaction types that are known to date. Historically, research reactors have been used as effective neutron sources. At present, Russia is implementing a project named "Formation of the Instrument Base for the PIK Reactor Complex" (further in the document *National program of PIK*).

2. Description of the approach for instrument's selection

The main challenge in creating a Neutron Center is to identify a set of neutron instruments that would cover the current and future requirements of the scientific community. This task is very ambitious and involves the deployment of enormous intellectual and financial resources, which are certainly limited. This fact should be taken into account when considering the list of instruments and setting priorities. For the instruments of the PIK reactor, an approach was proposed, in which an instrument complex based on a research reactor will be created, containing several high-class instruments. Equipped with high class instruments, PIK at the PNPI has the potential of a large neutron facility with an international impact. It all depends on a timely development of the neutron source (including cold and hot sources) and a balanced instrument suite that meets the needs of the national and international user community.

The National Programme of the PIK reactor includes a large number of instruments specific in different field of neutron sciences. Addition of new bi-spectral source at HEC-2 channel provides new opportunities and fills gaps in the National Programme at reactor PIK. The CREMLINplus project considers the possibility of creating a high-brightness para-hydrogen source with the possibility of bi-spectral beam output. The most suitable devices for such a source could be reflectometers and SANS machines, whose specific feature is the small sample size and increased requirements for the angular divergence of the neutron beam. The bi-spectral source enables measurements in a wide wavelength range, which is an advantage for most modern spectrometers, such as TAS and TOF spectrometers.

During development of National Program instrument park and after consideration of future design of small bi-spectral source on HEC-2 channel, some of the national instruments are planned to move from HEC-3 channel to HEC-2 channel. The design of instruments Harmony, Membrana, IN4, IN3 will be adjusted to the possibilities of the HEC-2 channel developed during the CREMLINplus project, but production of these instruments will be made within the National Programme.

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Bellow we discuss existing National Programme instruments, their science case and what type of instruments should be developed and placed at HEC-2 channel within the CREMLINplus project.

The list of instruments designed for PIK is presented in Table 1. This list leaves apart 7 scientific facilities from the field of nuclear physics, which are also being designed as part of the National Programme.

Table 1. The list of instruments designed on the PIK

Instrument name	Instrument Community	Location	Science discipline	Program
D1	High resolution powder	Reactor hall	Solid state, Magnetism	National Program
D3	High intensity powder	Reactor hall	Solid state, Magnetism	National Program
DC1	Single crystal diffractometer	Reactor hall	Solid state, Magnetism	National Program
IN-1	Thermal TAS	Reactor hall	Solid state, Magnetism	National Program
IN-2	Cold TAS	Neutron guide hall (HEC-3)	Solid state, Magnetism	National Program
SESANS	USANS	Neutron guide hall (HEC-3)	Bio, Chemistry, Magnetism	National Program
SONATA	Vertical reflectometer	Neutron guide hall (HEC-3)	Magnetism, Solid state	National Program
TENZOR	Polarized SANS	Neutron guide hall (HEC-3)	Solid State, Magnetism, Material science	National Program
SANS-2	SANS	Neutron guide hall (HEC-3)	Magnetism, Solid State	-
SEM	NSE	Neutron guide hall (HEC-3)	Bio, Soft matter, Chemistry	National Program
TEX-3	Stress diffractometer	Neutron guide hall (HEC-2)	Materials	National Program
NERO-2	Spectrometer	Neutron guide hall (HEC-2)	Solid state	National Program
TNR	Reflectometer	Neutron guide hall (HEC-2)	Material science	National Program
MEMBRANA	TR-SANS	Neutron guide hall (HEC-2)	Bio, Solid state, Chemistry	National Program
HARMONY	Polarized reflectometer	Neutron guide hall (HEC-2)	Magnetism, Condensed matter	National Program
IN-3	Polarized TAS	Neutron guide hall (HEC-2)	Magnetism, Solid state	National Program
TOF	Time of flight instrument	Neutron guide hall (HEC-2)	Bio, Chemistry, Solid State	National Program

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Instrument name	Instrument Community	Location	Science discipline	Program
BioDiff	Monochromatic single-crystal diffractometer	Neutron guide hall (HEC-2)	Bio	CREMLINplus
Neutron Spin Echo	High resolution NSE	Neutron guide hall (HEC-2)	Bio, Soft matter, Chemistry	CREMLINplus

3. General layout

Based on the results of the analysis of the instruments to be designed under the National Programme and the CREMLINplus project, the layout of the neutron stations on the HEC-2 and HEC-3 channels was proposed (Fig. 1). Neutron instruments designed as part of the CREMLINplus project are to be placed on the neutron guides of the HEC-2. As noted in Table 1, some of the installations belong simultaneously to the CREMLINplus project and the National Programme (TAS, MEMBRANA, HARMONY, TOF).

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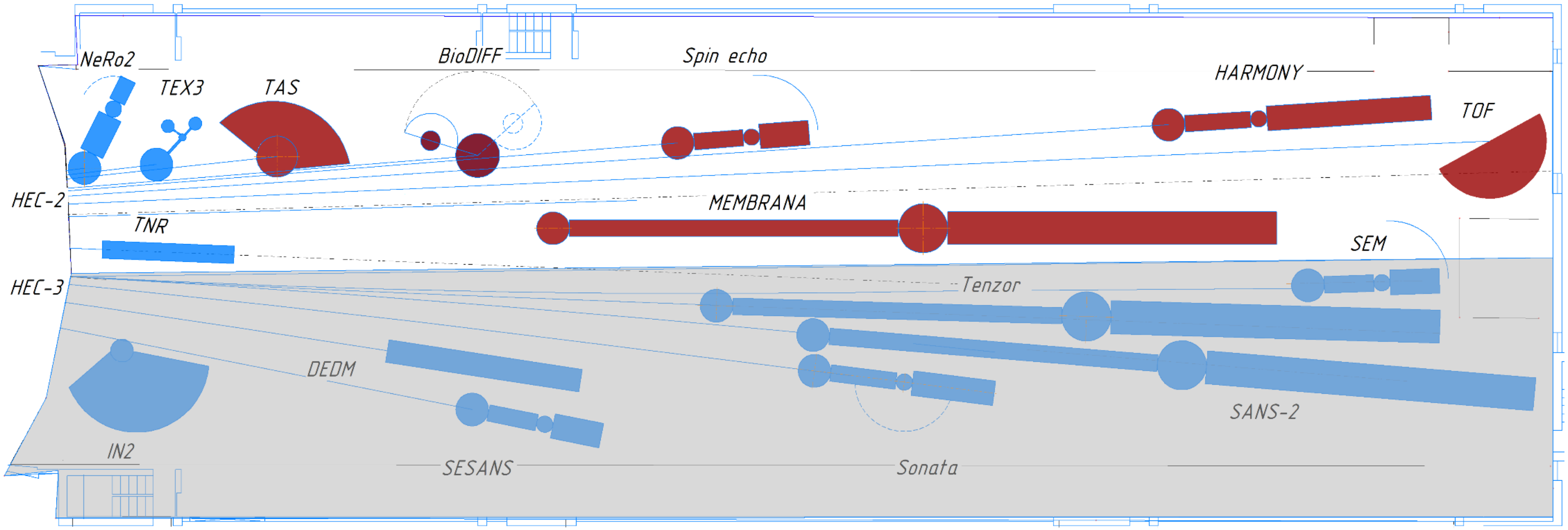

Fig. 1. Layout of the Instrument Suite (red colour – CREMLINplus, blue colour – National Program)

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4. Brief overview of the National Programme

4.1. Diffraction

The diffraction block of the National Programme includes four instruments: D1 (powder, high resolution, thermal), D3 (powder, high flux, thermal), DC1 (4-circle/single crystal, thermal) and TEX2 (4-circle, stress diffractometer).

D1 – High resolution powder

D1 is designed as traditional powder diffractometer for structural studies of crystals and for Rietveld analysis of large structures such as fullerenes, zeolites with adsorbed molecules, etc. [1]. D1 is located close to the reactor (distance from source to monochromator ~ 8 m) and has quite high monochromator take-off angle 112.5-155° (three possible position) (Table 2).

Table 2. Parameters of D1

Instrument	D1
Monochromator type	Ge (533)
Monochromator take-off angle ($2\theta_M$)	112.5°,120°, 155°
Available neutron wavelengths (λ_M), Å	1.2 - 2.8
Angular range of detectors ($2\theta_{min} - 2\theta_{max}$)	4°<2θ<168°
Resolution Δd/d	≤ 0.003
Sample size	0.8 x 3 cm^2 [width x height]

D3 – High intensity powder

D3 is a high-aperture powder diffractometer which is designed for structural studies of atomic and magnetic order in polycrystalline materials by thermal neutron diffraction [same as for D1]. This type of experiments requires a high neutron flux on the sample and a large detector solid angle. Instrument monochromator located at 4.5 m from the moderator, have two monochromator take-off angles: 44.22° and 90° (Table 3).

Table 3. Parameters of D3

Instrument	D3
Monochromator type	PG(002), Ge(115)

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Monochromator take-off angle ($2\theta_M$)	44.22°, 90°
Available neutron wavelengths (λ_M), Å	0.82, 1.54, 2.52, 4.74
Angular range of detectors ($2\theta_{min} - 2\theta_{max}$)	4° < 2θ < 132°
Sample size	<0.8 x 3 cm^2

DC1 – Single crystal diffractometer

The DC1 is classic four-circle thermal neutron diffractometer which is designed to investigate the atomic and magnetic structure of crystals [same]. Instrument will be placed at ~ 5.8 m from moderator. The studies will be carried out at one of three fixed wavelengths of thermal neutrons. The wavelength (λ) required in a particular experiment is specified by the choice of the monochromator (Table 4).

Table 4. Parameters of DC1

Instrument	DC1
Monochromator	Cu(220), Ge(311), PG(002)
Monochromator take-off angle ($2\theta_M$)	42°
Available neutron wavelengths (λ_M), Å	0.9, 1.2, 2.4
Sample size	<1 x 1 cm^2

TEX3 – Stress diffractometer

TeX-3 is thermal four-circle diffractometer which is optimized for texture studies on different types of polycrystalline materials. This instrument was a part of the National Program and was transferred from the closed FRG-1 reactor to the PIK reactor. TEX-3 is located at neutron guide hall at HEC-2 channel (future bi-spectral source) (Table 5).

Table 5. Parameters of TEX3

Instrument	TEX-3
Monochromator	Ge (311), HOPG (002)
Monochromator take-off angle ($2\theta_M$)	42°
Available neutron wavelengths (λ_M), Å	1.24, 2.4

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Sample size	0.1 x 0.1 - 1 x 1 cm2

Conclusions:

The instrumental program includes

- 2 thermal powder diffractometers
- 2 thermal 4-circle diffractometers

and miss

- any diffractometer set on a guide
- diffractometer with cold neutrons.

Considering all above instruments existing within the National Programme we believe that reactor PIK and community will benefit from the diffractometer for studies of large biological macromolecules. **Therefore, diffractometer BioDiff is a good choice for bi-spectral source in neutron guide hall.**

4.2. Large scale structures

Large scale structures block of the National Programme includes four instruments:

TENZOR – Polarized SANS

TENZOR is a small-angle polarized-neutron diffractometer which is located at neutron guide hall on HEC-3 channel. It was intended for research of magnetic and nuclear inhomogeneities of nanoscale size structures [2, 3]. TENZOR can perform studies with non-polarized or polarized neutrons and analyse the polarization of the scattered neutron beam (Table 6).

Table 6. Parameters of TENZOR

Instrument	Tenzor
Available neutron wavelengths (λ_M), Å	4.5-20
Sample size	3 x 3 cm^2
Q-range	0.001 Å^{-1}< q < 0.5 Å^{-1}.
Primary flightpath	22.25 m
Secondary flightpath	22.25 m

SONATA – Vertical sample reflectometer

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SONATA is a high flux polarized neutron reflectometer with vertical sample geometry. It has conventional design for studying in thin films and layered structures. Additionally, it has an option of vector polarization analysis [4]. SONATA located at neutron guide hall, cold HEC-3 channel (Table 7).

Table 7. Parameters of SONATA

Instrument	SONATA
Available neutron wavelengths (λ_M), Å	2-25
Q-range	• 1 Å $^{-1}$ (specular scattering) • 0.05 Å $^{-1}$ (nonspecular scattering) • 0.2 Å $^{-1}$(GISANS)
Additional options	• Time-of-flight/constant wavelength • Polarization analysis

SESANS – Spin echo SANS

The SESANS is a spin-echo small angle neutron scattering instrument which is designed for studies of large-scale objects of biology, membrane or porous systems, etc [5]. Accessible size range of structures to be investigated by SESANS covers three orders of magnitude on the size scale: from 100 nm to 40 microns. SESANS is located at neutron guide hall HEC-3 channel (Table 8).

Table 8. Parameters of SESANS

Instrument	SESANS
Available neutron wavelengths (λ_M)	3.5-12 Å
Measuring range	100 nm - 40 µm
Sample size	1 x 1 cm^2
Instrument length	~8 m

Conclusion:

- Several large-scale instruments are located at the neutron guide hall HEC-3 channel.
- HEC-3 have a conventional LD2 source, so moving existing large-scale instruments on low-dimensional pH2 source at HEC-2 will be highly beneficial to most of it.
- The SANS-instrument MEMBRANA and the reflectometer HARMONY can be set at the HEC-2 channel, the design of which is developed within CREMLINplus project.

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4.3. Spectroscopy

IN1 – Thermal TAS

The IN1 thermal neutron spectrometer is designed to study inelastic neutron scattering on collective excitations in solids (Table 9). It is located in a reactor hall, where the distance between monochromator and moderator is ~6.8 m. IN1 has Rowland geometry design, which greatly increase signal-to-noise ratio [6,7].

Table 9. Parameters of IN1

Instrument	IN-1
Available neutron wavelengths (λ_M)	0.9-2.36 Å
Sample size	1 x 1 cm^2
Available monochromators	PG(002), Cu(200), Si(111)
Polarization option	no

IN2 – Cold TAS

The IN2 cold neutron spectrometer is designed to study, with good energy resolution, low-energy collective excitations in solids by inelastic neutron scattering (Table 10). IN2 placed in neutron guide hall at HEC-3 channel. It has Rowland geometry design [6,7] with polarization analysis options (v-cavity polarizers/analysers).

Table 10. Parameters of IN2

Instrument	IN-2
Available neutron wavelengths (λ_M), Å	1.5-6
Sample size	1 x 1 cm2
Available monochromators	PG(002), Si(111)
Polarization option	Yes (V-cavity types polarizers/analysers)

SEM – Spin echo spectrometer

Add science case for last version of SEM and his parameters.

Conclusion:

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- The National Programme implies the development and construction of three triple-axis, one time-of-flight and one spin-echo spectrometers.
- TOF instrument will generally benefit from bi-spectral source because of broad wavelength range used for experiments.
- While SEM has a good position at HEC-3 channel, its limited range of the available SE time suggests to build additional NSE spectrometer at HEC-2 channel.
- The limited space at HEC-3 channel of the neutron guide hall, the cold triple-axis spectrometer can be placed at HEC-2 channel.
- We suggest the placement of three instruments IN3, IN4 (National Programme), and NSE (developed within CREMLINplus project) at HEC-2 channel.

5. Instruments to be designed within CREMLINplus project

Bellow we discuss instruments to be designed within CREMLINplus project.

5.1. Diffraction

BIODIFF – Diffractometer for biology studies

The BioDiff type diffractometer (Fig. 2) is a monochromatic single-crystal diffractometer optimized for determining the structure of large biological macromolecules such as proteins or DNA. It has a similar design to existing diffractometer at FRM II reactor [8]. In such biomolecules, hydrogen plays a crucial role: for example, protons are responsible for substrate binding and take part in proton transfer reactions in the catalytic cycle of many enzymes. Such often free protons in general cannot be detected by X-ray structure detection, but they are especially important for understanding reactions in the active centre of proteins. The device allows the incoming neutron wavelength to be varied to adapt to the size of the biomolecule under study. The detector is constructed of neutron sensitive cylindrical plates covering half of the full solid angle around the sample and can be equipped with a CCD camera (Table 11).

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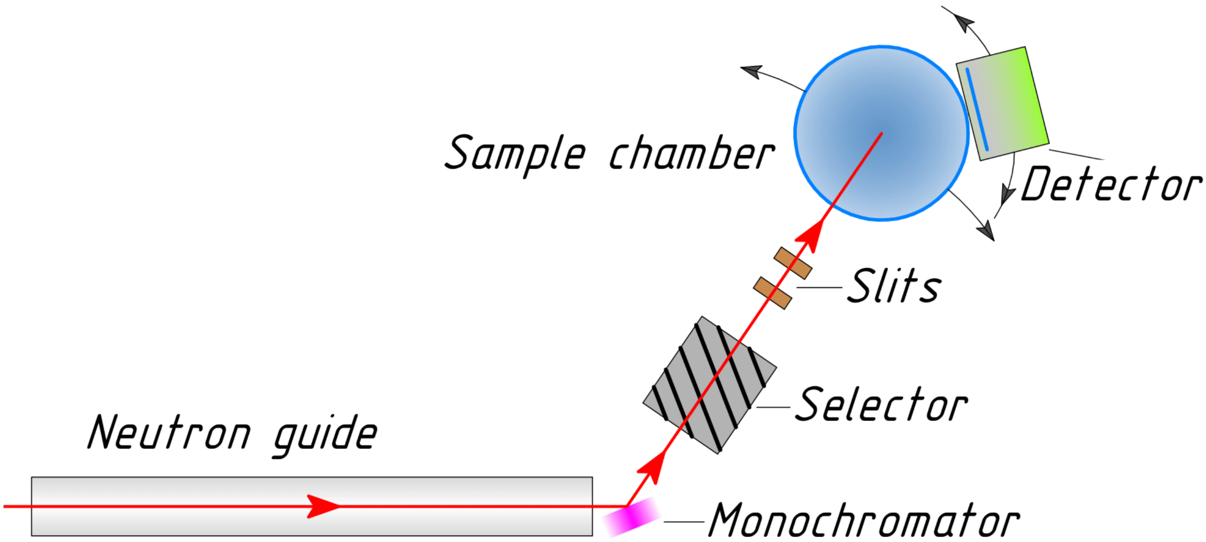

Fig. 2. BIODIFF instrument layout

Table 11. Parameters of BIODIFF

Instrument	BioDiff/diffractometer
Available neutron wavelength (λ_M), Å	2.4-6
Sample size	1 x 1 cm^2
Monochromator	PG(002)
Location	Neutron guide hall (HEC-2)

5.2. Large scale structures

MEMBRANA-2 – SANS Diffractometer

Membrana-2 is a small-angle diffractometer for studying of different subatomic, molecular, and supramolecular structures such as biological polymers, macromolecules, fullerenes, etc. It has a very wide possible range of momentum transfers which can be done in one measurement (Table 12). Membrana-2 can work in two modes: monochromatic mode with the possibility of changing the wavelength and in polychromatic mode using the time-of-flight technique. A typical setup is shown in Fig. 3.

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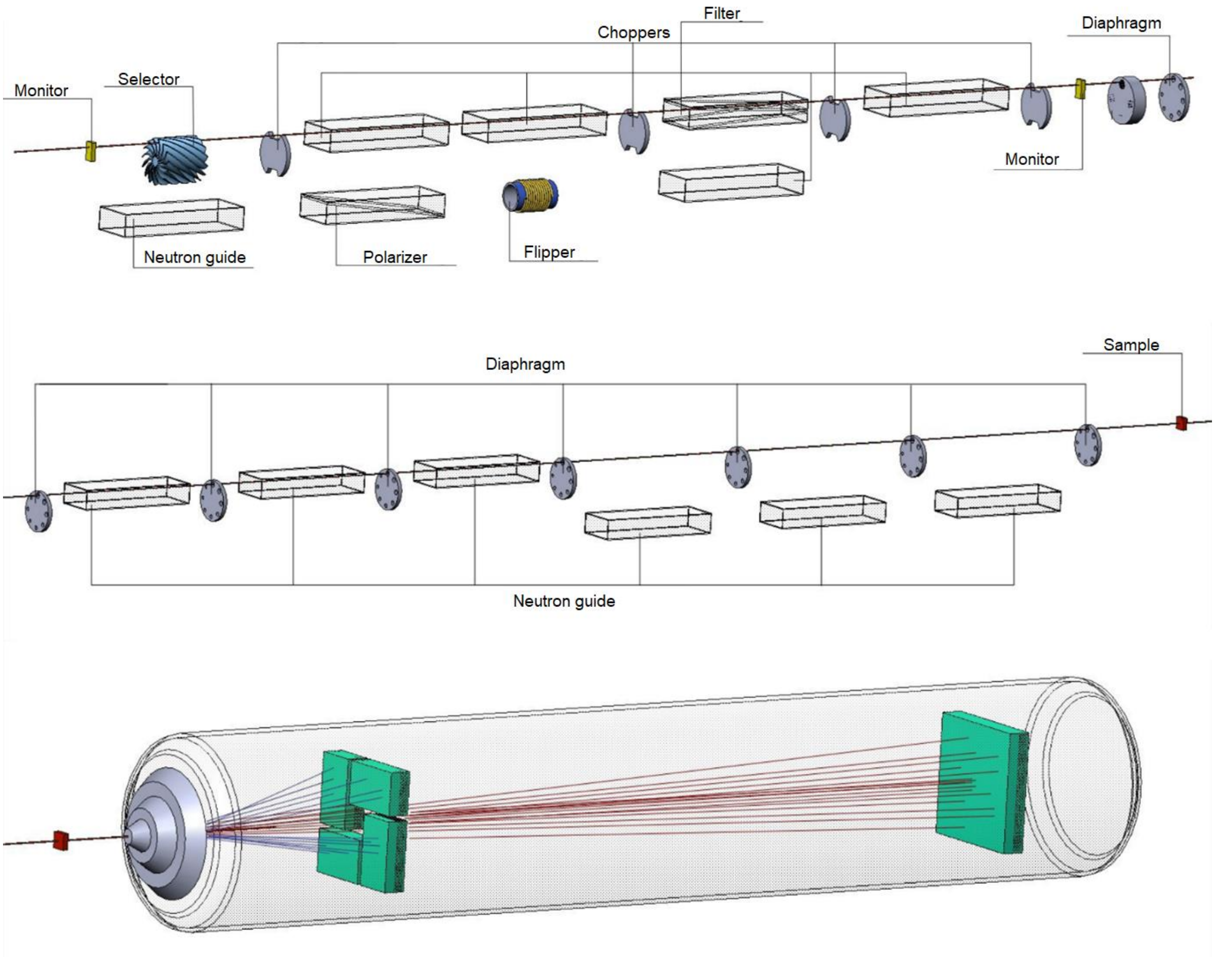

Fig. 3. MEMBRANA Instrument layout

Table 12. Parameters of MEMBRANA

Instrument	Membrana/SANS
Available neutron wavelength (λ_M), Å	4.5-20
Q-range	0.0007 $Å^{-1}$< q < 0.7 $Å^{-1}$
Sample size	1.5 x 1.5 cm^2
Location	Neutron guide hall (HEC-2)

HARMONY – Polarized reflectometer

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HARMONY is a neutron reflectometer (Fig. 4) which is designed both for studies of soft matter physics (including liquids, liquid crystals, membranes, polymers, complex solutions, etc.) and for studies of magnetic and non-magnetic solid-state nanostructures. HARMONY have horizontal sample with possibility of reflection from the sample both above and below (Table 13).

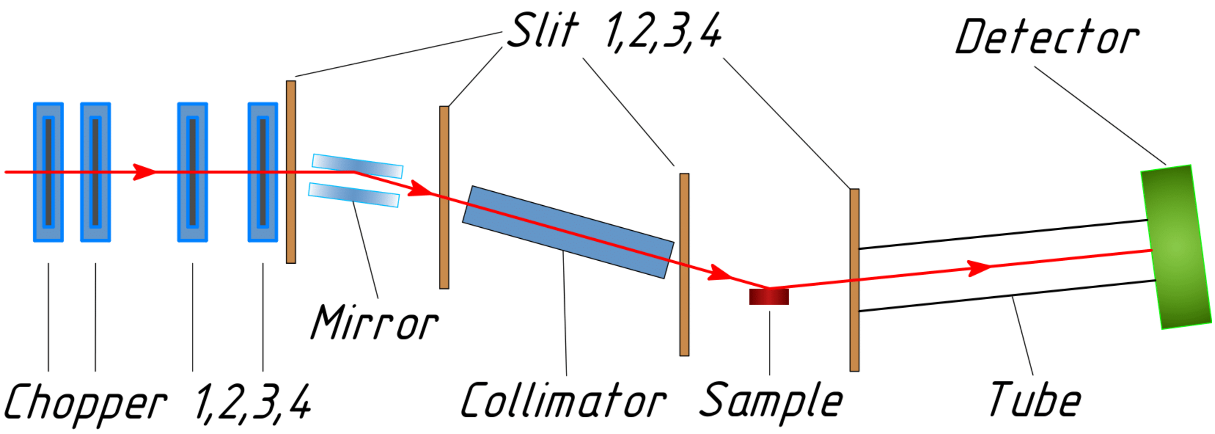

Fig. 4. HARMONY Instrument layout

Several features describe available options of this instrument:

1) Reflectometry of polarized neutrons in the mirror and non-mirror scattering mode with polarization analysis;

2) Reflectometry of non-polarized neutrons in the mode of mirror and non-mirror scattering;

3) Small-angle scattering in sliding geometry (GISANS) can be considered as an option.

The analogue of the HARMONY reflectometer is the well-known high-flow time-of-flight neutron reflectometer FIGARO [9]. HARMONY will be unique instrument since unlike FIGARO it will use full neutron polarization analysis using a new type of polarizer and a fan multichannel polarization analyser. In addition, HARMONY will use a more advanced new type of neutron beam interrupter.

Table 13. Parameters of the reflectometer HARMONY

Instrument	Harmony/reflectometer
Available neutron wavelength (λ_M)	2-20 Å
Sample size	0.01 x 1 cm2 – 0.4 x 10 cm^2
Q-range	Solid samples: Q_z~0.005-0.5 $Å^{-1}$; Liquid samples: Q_z~0.005-0.35 $Å^{-1}$

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Polarization	~96%
Location	Neutron guide hall (HEC-2)

5.3. Spectroscopy

IN3 – triple-axis spectrometer with polarization analysis

The polarized neutron spectrometer IN3 is designed to study collective excitations in solids by inelastic neutron scattering. Spectrometer uses a Rowland focusing scheme in which the source, monochromator, and sample are located on the same circle. For this purpose, the "virtual source" principle is used, i.e., a slit is placed at a small distance from the monochromator which serves as a virtual neutron source (Figure 5). Parameters of instruments are shown below in Table 14.

Table 14. Parameters of IN3

Instrument	IN-3
Available neutron wavelength (λ_M)	0.9-2.36 Å
Sample size	1 x 1 cm^2
Available monochromators	PG(002), Si(111)
Polarization	Fully polarized neutron beam
Location	Neutron guide hall (HEC-2)

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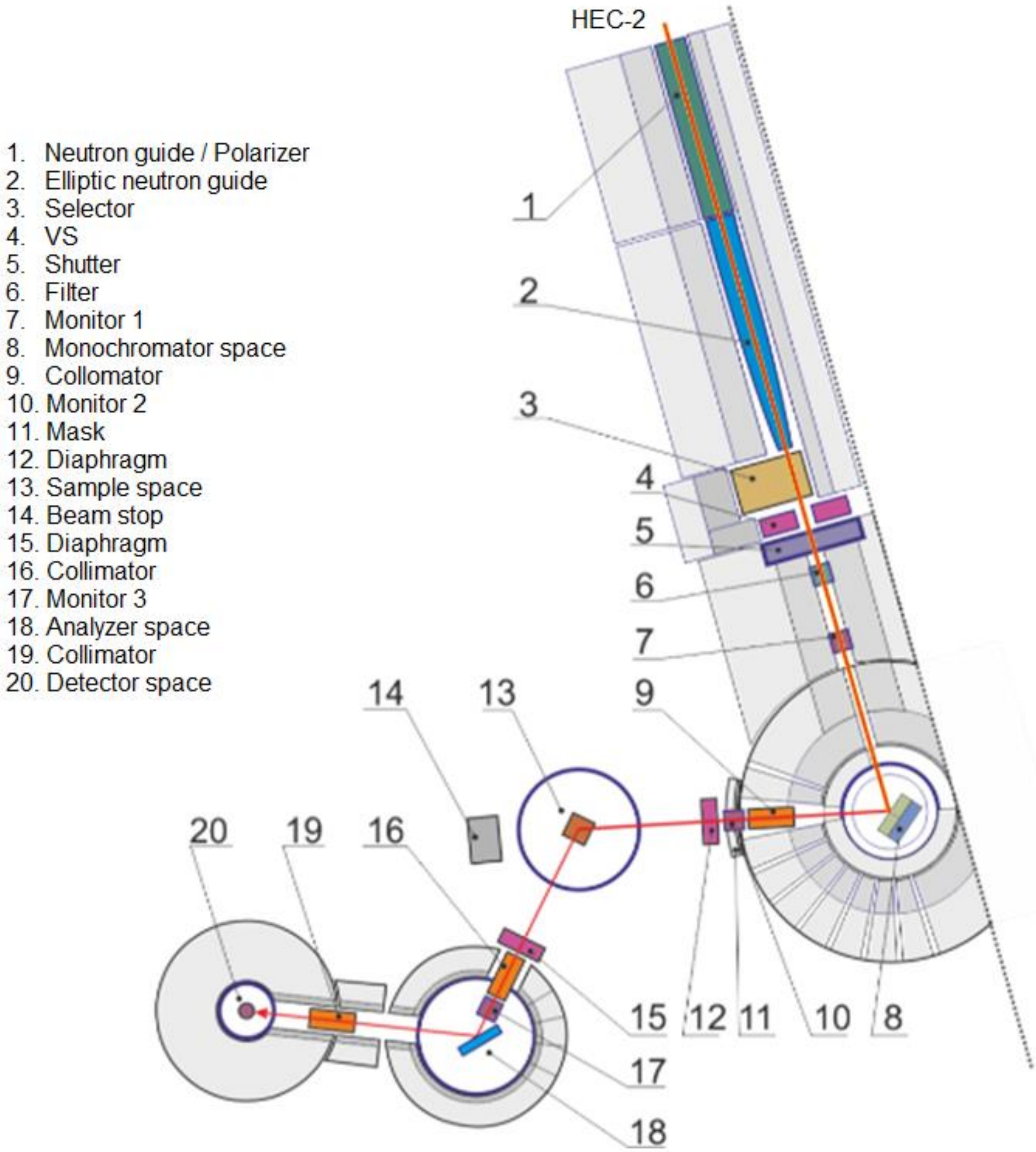

Fig. 5. TAS instrument layout

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IN4 – TOF

IN4 is time-of-flight spectrometer of direct geometry (TOF, Fig6) which is designed for inelastic neutron scattering in various materials, solids, liquids, polymers. The TOF instrument of direct geometry is superior to the spectrometer of inverse geometry in terms of the amount of area available for scanning in Q-E space. In particular, the range of transmitted pulses for the former type is much wider.

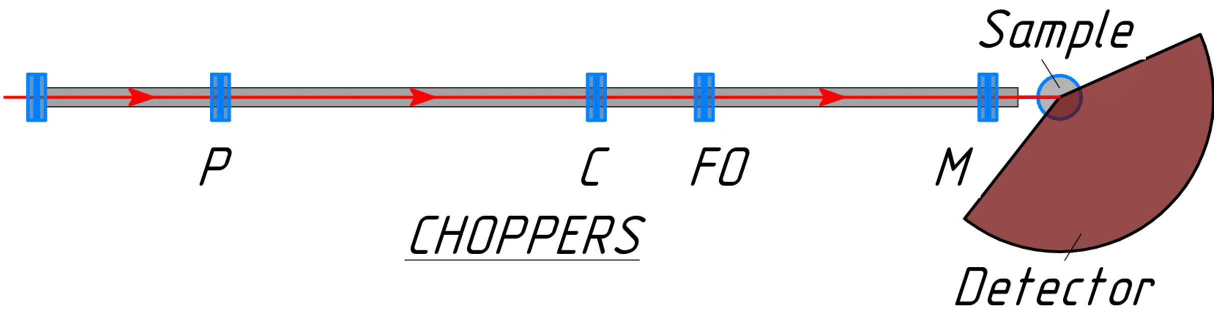

Fig6. IN4 instrument layout

Table 15. Parameters of IN-4

Instrument	IN-4/TOF
Available neutron wavelength (λ_M), Å	2-12
Sample size	<3 x 3 cm^2
Type of TOF	Direct geometry
Detector size	1 m2
Location	Neutron guide hall (HEC-2)

Spin Echo

The operation of the spin-echo spectrometer is based on coding the ultra-small change in neutron energy when neutrons are scattered in the Larmor precession phase of the neutron spin in the magnetic field. A typical instrument sketch is presented in Fig. 7.

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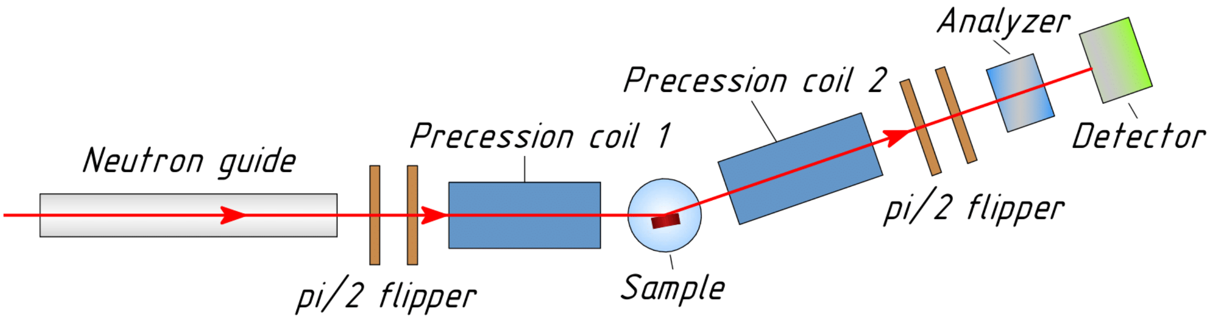

Fig. 7. NSE instrument layout

The neutron spin-echo spectrometry (NSE) method has the highest energy resolution achievable with neutron spectrometers. The method is used mainly in quasi-elastic scattering experiments to study relaxation processes located on the energy scale around zero transmitted energy. In contrast to other methods of inelastic neutron scattering, such as triaxial spectroscopy or time-of-flight spectroscopy, NSE measures the intermediate scattering function S(Q, t) at a point in inverse space, Q, depending on the relaxation time of the process under study, t. The range of measured values of relaxation times $10^{-12} < t < 10^{-7}$ s covers the dynamic scale from microscopic timescales of atomic collisions and spin exchange to macroscopic times of slow relaxation processes of large molecules and atomic conglomerates. In contrast to other experimental methods that provide dynamic information, such as µSR, NMR, ESR, Mössbauer spectroscopy or magnetometric susceptibility measurements, NSE simultaneously gives access to microscopic information via the value of the transmitted momentum, Q, in backward space. Thus, NSE can act as a link between the listed integral methods and microscopic, i.e., traditional neutron spectrometry - triaxial and time-of-flight.

The limitation of the traditional neutron spectrometry is a compromise between intensity and resolution: the better the energy resolution is required, the more neutrons not satisfying high monochromatization requirements ($\Delta\lambda/\lambda \leq 0.03$) have to be discarded, the lower the total intensity of the beam, and vice versa, the higher the intensity, the worse the monochromatization of the beam, the worse the energy resolution becomes. This drawback is deprived of the spin-echo spectrometry method since the energy resolution is mainly determined by the magnetic field integral of precession in its path and the beam monochromatization can be as bad as desired (traditionally $0.1 \leq \Delta\lambda/\lambda \leq 0.25$) giving an order or more increase in intensity.

With such resolution the large-scale slow dynamics of soft substances and biomolecules can be studied, the temperature fluctuations of surface-active membranes in microemulsions, the dynamics of polymer chains in melts, the movement of thermally activated domains in proteins can be studied.

Table 16. Parameters of Neutron Spin Echo instrument.

Instrument	NSE

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Available neutron wavelength (λ_M), Å	4.5-20
Sample size	<3 x 3 cm^2
Velocity selector	$0.1\ Å^{-1} < q < 10\ Å^{-1}$
Location	Neutron guide hall (HEC-2)

6. Summary and Conclusion

While the National Programme at reactor PIK consists of several first-class neutron instruments, the development of the bi-spectral neutron source gives a new opportunity to develop some instruments missing within the National Programme and to locate some of the instruments of the National Programme at the newly developed HEC-2 channel provided with the new bi-spectral neutron source (developed within the CREMLINplus project). Our proposition is to adjust to HEC-2 the following instruments of the National Programme (IN-3, IN-4, HARMONY, MEMBRANA) and to develop two new instruments (BioDiff and NSE) as a part of the CREMLINplus project.

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