Neutron Scattering Instruments of IBR-2 Reactor for Condensed Matter Research. Current State and Recent Results

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Modernized IBR-2 High Flux Pulsed Reactor (FLNP JINR)

Operational since 1984

2007 - 2010: modernization shutdown

2010 – 2011 Physical and power start-up completed

2012 – Regular operation renewed

Information: [http://flnp.jinr.ru/34/](http://flnp.jinr.ru/34/)

Technical parameters of IBR-2M

<table>
<thead>
<tr>
<th>Parameter</th>
<th>IBR-2</th>
<th>IBR-2M</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal neutron flux in pulse, n/cm²/c</td>
<td>5 \cdot 10^{15}</td>
<td>5 \cdot 10^{15}</td>
</tr>
<tr>
<td>Average power, MW</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Power in pulse, MW</td>
<td>1850</td>
<td>1850</td>
</tr>
<tr>
<td>Fuel</td>
<td>PuO₂</td>
<td>PuO₂</td>
</tr>
<tr>
<td>No. fuel elements</td>
<td>78</td>
<td>69</td>
</tr>
<tr>
<td>Max. fuel burn up, %</td>
<td>6,5</td>
<td>9</td>
</tr>
<tr>
<td>Repetition rate, Hz</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Pulse width, μs</td>
<td>215</td>
<td>240</td>
</tr>
<tr>
<td>RPM of movable reflector blades</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- main</td>
<td>1500</td>
<td>600</td>
</tr>
<tr>
<td>- auxiliary</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>- No. of satellite pulses</td>
<td>4</td>
<td>1</td>
</tr>
</tbody>
</table>

Pelletized cryogenic moderator of IBR-2
IBR-2M Spectrometers Complex

Diffractometers:
HRFD, DN-12, FSD, SKAT/Epsilon

Reflectometers:
REMUR, REFLEX

Small Angle Scattering Spectrometer: YuMO

Inelastic Neutron Scattering Spectrometers:
NERA-PR, DIN-2PI

New Instruments:
DN-6, GRAINS, NRT

Reconstruction:
DN-2 – RTD,
REFLEX - SESANS

2011: 11 instruments in operation
2014: 14 instruments in operation
The priority directions of fundamental research:

- Nanoscale physics

- Physics and Chemistry of Functional Materials

- Physics and Chemistry of Complex Liquids and Polymers

- Physics of Soft Condensed Matter
The priority directions of applied research:

- Structural characterization of functional materials used in different (nano)technologies

- Non-destructive control of residual stresses and internal organization of bulk materials and products

- Texture analysis of geomaterials and constructional materials
User Programme at IBR-2 instruments:

Two calls of proposals per year with deadlines 15 April and 15 October

Applications are collected via web-site http://ibr-2.jinr.ru

200 applications from 16 countries were received in 2013
**Diffraction (fundamental research)**

**HRFD**
- Precise structural studies of crystalline materials using reverse TOF method, $\Delta d/d \sim 0.001$

**DN-2**
- Reconstruction to real-time diffractometer (RTD)

**DN-12**
- Studies of structure and dynamics of condensed matter under extreme conditions ($P \sim 7$ GPa)

**DN-6**
- In operation since 2012
- Structural studies at ultrahigh pressures (up to 30-50 GPa)
High Resolution Fourier Diffractometer

Neutron flux at sample position: $10^7$ n/cm$^2$/s

Resolution at $d = 2$ Å, $2\theta = 152^0$: $\Delta d/d = 0.0008$

D-spacing range in high resolution mode: 0.7 - 4 Å

$I(\omega, t) \sim \int_0^\infty \sigma(\tau) \cdot R[(\tau - t), \omega] \, d\tau$
DN-12 Spectrometer for Studies of Microsamples

- Neutron flux at sample position: \(2 \times 10^6\) n/cm\(^2\)/s
- Resolution at \(d = 2\) Å, \(2\theta =90^\circ\): \(\Delta d/d = 0.02\)
- D-spacing range: 0.8 - 13 Å
- Pressure range: 0 – 7 GPa
- Temperature range: 10 – 300 K

Circular Detector consists of 16 \(^3\)He counters

Pressure cell with sapphire anvils

Pr\(_{0.52}\)Sr\(_{0.48}\)MnO\(_3\)

- Intensity, arb. units
- d-spacing, Å

- Pressure cell with sapphire anvils

![Diagram of DN-12 Spectrometer](image-url)
Diffractometer DN-6 for studies of microsamples under extreme conditions

- Intensity gain: 12 times (compared to DN-12)
- Pressure range: 30-50 GPa
- Temperature range: 4–300 K

Neutron diffraction studies of structural phase transition in \( \text{PbMg}_{1/2}\text{W}_{1/2}\text{O}_3 \) perovskite under pressure (proposal from Institute of Physics, Azerbaijan), published in Phys. Solid State (2014)

Neutron diffraction patterns of \( \text{Fe}_3\text{O}_4 \) sample measured in DAC at \( P = 5.5 \) and 23 GPa
Diffraction (applied research)

**FSD**

Determination of residual stresses in construction materials, industrial materials and factory-made goods using RTOF method

$\Delta d/d \sim 0.002$

**SKAT**

Texture analysis of geological materials (rocks, minerals) and constructional materials

**EPSILON-MDS**

Residual stress analysis in geological materials (rocks, minerals)

High resolution due to long flight path $L \sim 105 \text{ m}$

$\Delta d/d \sim 0.003-0.004$

Major modernization focused on replacement of neutron guides was finished by 2012
YuMO - SANS
A study of structural characteristics of nanostructured materials, biological objects, polymers

REMUR
Reflectometer with polarized neutrons

REFLEX
Reflectometer with polarized neutrons
A study of structural properties of thin films and layered nanostructures
Reconstruction into Spin Echo Small Angle Neutron Scattering Spectrometer

GRAINS
Multifunctional reflectometer

A study of structural properties of liquid and soft matter interfaces
YuMO Small Angle Scattering Spectrometer

1 – two reflectors;
2 – zone of reactor with moderator;
3 – chopper;
4 – first collimator;
5 – vacuum tube;
6 – second collimator;
7 – thermostate;
8 – samples table;
9 – goniometer;
10-11 – Vn-standard;
12 – ring-wire detector;
13 – position-sensitive edetector "Volga";
14 – direct beam detector.

$L_1 = 17.8$ m, $L_2 = 13.2$ m

Neutron flux at sample position: $4 \cdot 10^7$ n/cm$^2$/s

Q-range: $7 \cdot 10^{-3}$ - 0.5 Å$^{-1}$

Q-resolution: 5-20 %

Typical measurement time: 1 h
REMUR - Reflectometer with polarized neutrons

1 - Moderator
2 - Double Disk Background Chopper
3 - Collimators
4 - Cross-type Collimator
5 - Small-Angle Scattering Mode Polarizer
6 - Adjustable Platforms
7 - Spin-Flipper
8 - Variable Diaphragms
9 - Sample Position
10 - Electromagnet
11 - Fan Polarization Analyzer
12 - Position-Sensitive Detector
13 - Control and operative visualization/analysis
14 - Data Acquisition
15 - Data Transfer

Neutron flux at sample position: $3 \times 10^4$ n/cm²/s

$\lambda$-range: 0.9 - 10 Å⁻¹

$\theta$ range: 1-100 mrad

$\Delta\lambda/\lambda$: 2 %

Reflection coefficients from $12\times[\text{Fe}(35\text{ Å})\text{Cr}(4.4 \text{ Å})/\text{Gd}(50 \text{ Å})]$
Inelastic Neutron Scattering

NERA-PR

Vibrational spectra of molecular crystals

DIN-2PI

Lattice dynamics, atomic dynamics of liquids and amorphous materials

DN-12

Vibrational spectra of hydrogen-containing materials under pressure up to 5-10 GPa
NERA-PR – Inelastic Neutron Scattering Spectrometer in Inverted Geometry

Neutron flux at sample position:
\[ 4 \times 10^6 \text{n/cm}^2/\text{s} \]

Energy transfer range:
0-500 meV

1 - Moderator
2 - Background Choppers
3 - Ni Guide Tube
4 - Detector for High Intensity Diffraction
5 - Detector for High Resolution Diffraction
6 - He3 Detectors (INS and QNS)
7 - Single Crystal QNS Analyzer
8 - Pyrolytic Graphite INS Analyzer
9 - Be-Filters
10 - Collimators
11 - VME control and operative visualization/analysis
12 - VME Station (OS/9) Data Acquisition
13 - EtherNet Data Transfer

Major modernization focused on replacement of neutron guide was finished by 2012
DIN-2PI – Inelastic Neutron Scattering Spectrometer in Direct Geometry

Neutron flux at sample position: \(4 \times 10^6 \text{n/cm}^2/\text{s}\)

2\(\theta\) range: 5-135°

Incident neutron energy range: 1-300 meV

Energy resolution: \(\Delta E/E = 4-10\%\)

Installation of neutron concentrator gives an order of magnitude increase of neutron flux at sample position

FWHM of incoherent QENS peak in liquid Ga
Instrument for neutron imaging at 14 beamline of IBR-2M: Current State

- Biological shielding
- Vacuumed collimator
- CCD Camera Videoscan
- CCD-based detector and sample position
IBR-2M Spectrometers Complex: Further Developments
RTD diffractometer for real-time studies

Adjustable neutron beam diaphragm for the RTD diffractometer 20x105mm

Ring-shaped helium backscattering detector on the RTD diffractometer

Fedotov V.K., Sholin I.A., Beskrovnii A.I., Sheverev S.G.
FSS diffractometer, beamline 13

Stress rig

+air heaters

FSS chopper
Spin Echo Small Angle Neutron Scattering Spectrometer in construction on the Basis of REFLEX Reflectometer

Time gradient magnetic fields
Overview of recent scientific results
Real-time studies of structural changes in Li-based accumulators during charging and discharging processes with high resolution

Evolution of neutron diffraction patterns of Li accumulator with LiFePO$_4$+xV working substance during three cycles of charging-discharging

I.A. Bobrikov et al., J. Power Sources (2014)
The pressure induced changes in magnetic structure of RCo$_2$

Exploring the nature of Itinerant Electron Metamagnetism phenomena in RCo$_2$

Non-magnetic R-ions

$M_R=0$

$M_{Co}=0$

Magnetic R-ions

$M_{Ho} \sim 9.5 \mu_B$

$M_{Co} \sim 1 \mu_B$

Tuning the magnetic interaction by pressure

JINR - Babes-Bolyai University (Romania)

DN-12 neutron diffractometer

The suppression of ordering of Co moments

E.Burzo et al., J. Alloys and Compounds (2014)
Structural organization of nanodiamonds in liquid dispersions

Continuous spatial transition of carbon states in detonation diamonds liquid dispersions from crystalline diamond ($sp^3$-hybridization) inside particles to graphite-like state ($sp^2$-hybridization) on surface

Experimental curves of small-angle neutron scattering from liquid dispersions of detonation nanodiamonds (DNA) measured with the contrast variation (a). A schematic view of a DNS cluster in liquid dispersions with an enlarged schematic representation of its basic structural unit - a particle composed of crystalline diamond and graphene shell (b). Various approximations to this shell are considered. A continuous diffusive profile (green solid line) gives the best fits to the experimental curves (c).

Shape memory effect:
1. $H_0 = 206 \text{ kA m}^{-1}$; non-stretched
2. $H_0 = 206 \text{ kA m}^{-1}$; stretched by 80% and then unloaded retains its shape for hours.

SIEL elastomer with Fe microparticles and nanoparticles

Deformation of a membrane (D/h=10) in uniform transversal magnetic field $H_0$

- $H_0 = 50 \text{ kA m}^{-1}$
- $H_0 = 80 \text{ kA m}^{-1}$
- $H_0 = 110 \text{ kA m}^{-1}$

The studies of the effect of Ca\(^{2+}\) concentration on the thickness of the lipid bilayers possibly explain why calcium, causing a partial fusion of the single vesicles in the range of \(0.3 \text{mM} \leq C_{Ca} \leq 2 \text{mM}\), is a necessary component in the final stages of the exocytosis.
Experimental and theoretical study of molecular dynamics and crystal structure of hexafluorophosphate (ESP-PF6) и tosylate (ESP-TOS) salts of alkylcoumarine derivatives – photoinitiator compounds.

JINR - Jagiellonian University and University of Technology (Krakow, Poland)

Inelastic neutron scattering spectra, results of theoretical modeling and crystal structure of ESP-PF6 (а) и ESP-TOS (b).
Residual stress in surveillance Charpy specimens, recovered by electron (EBW) and laser (LBW) beam welding

Collaboration: Institute of Electronics of BAS(Sofia, Bulgaria)
FLNP JINR (Dubna, Russia), NECSA Ltd. (Pretoria, South Africa)

by Gizo Bokuchava (FLNP JINR) with colleagues: submitted to Nuclear Engineering and Design

Charpy test specimens

Electron beam welding

Neutron diffraction (211) reflection broadening at weld seam locations during x-scan

Typical neutron diffraction spectra
Neutron imaging of Seimchan meteorite
Neutron imaging of natural heritage objects

Paleontological Institute of RAS and Paleontological Museum (Moscow)

Protosequoia cone (cretaceous period)
Thank You for Your Attention!