Programme Advisory Committee for Condensed Matter Physics

47th meeting (22 – 23 January, 2018)

Pavel Alekseev

Agenda of the 47th PAC meeting

Monday, 22 January 2018

9.30	1. Opening of the meeting	D. L. Nagy (5 min.)
	2. Implementation of the recommendations of the previous PAC meeting	D. L. Nagy (20 min.)
	of the User Programme at the IBR-2 spectrometers in 2015–2017	(20 min.)
	Coffee break	
	10. Scientific reports:	
	10.1. "Cultural heritage research using neutron imaging at the IBR-2 reactor"	I. Saprykina (25 min.)
	10.2. "Planar graphene tunnel field-effect transistor: effect of edge vacancies on performance"	V. Katkov (25 min.)

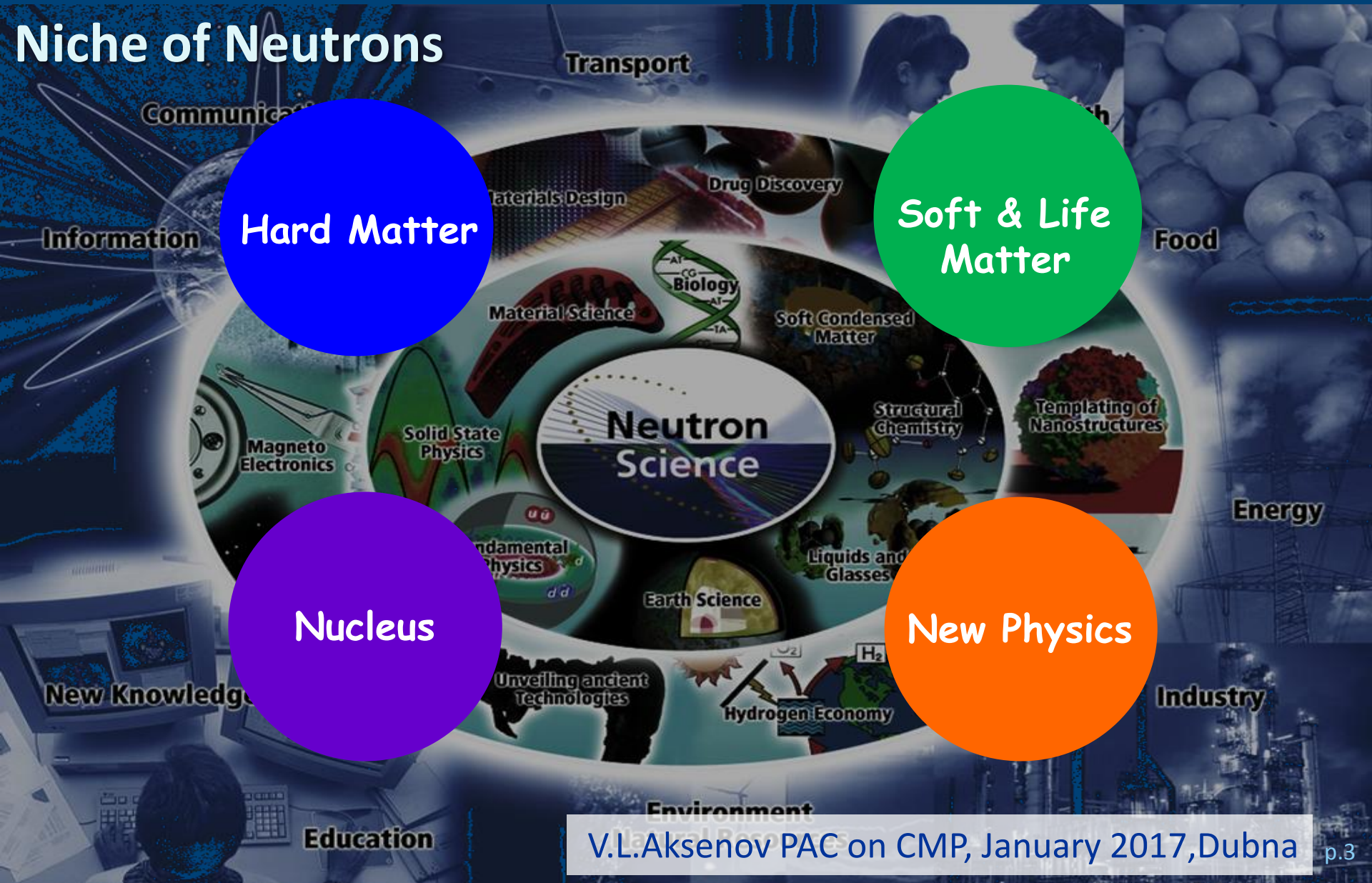
Tuesday, 23 January 2018

9.00	11. Meeting of the PAC members with the JINR Directorate	(1 h)
10.00	12. Information about the International Conference "Condensed Matter Research at the IBR-2" (Dubna, 9–12 October 2017)	T. Ivankina (15 min.)

Highlights of the PAC-CMP meeting:

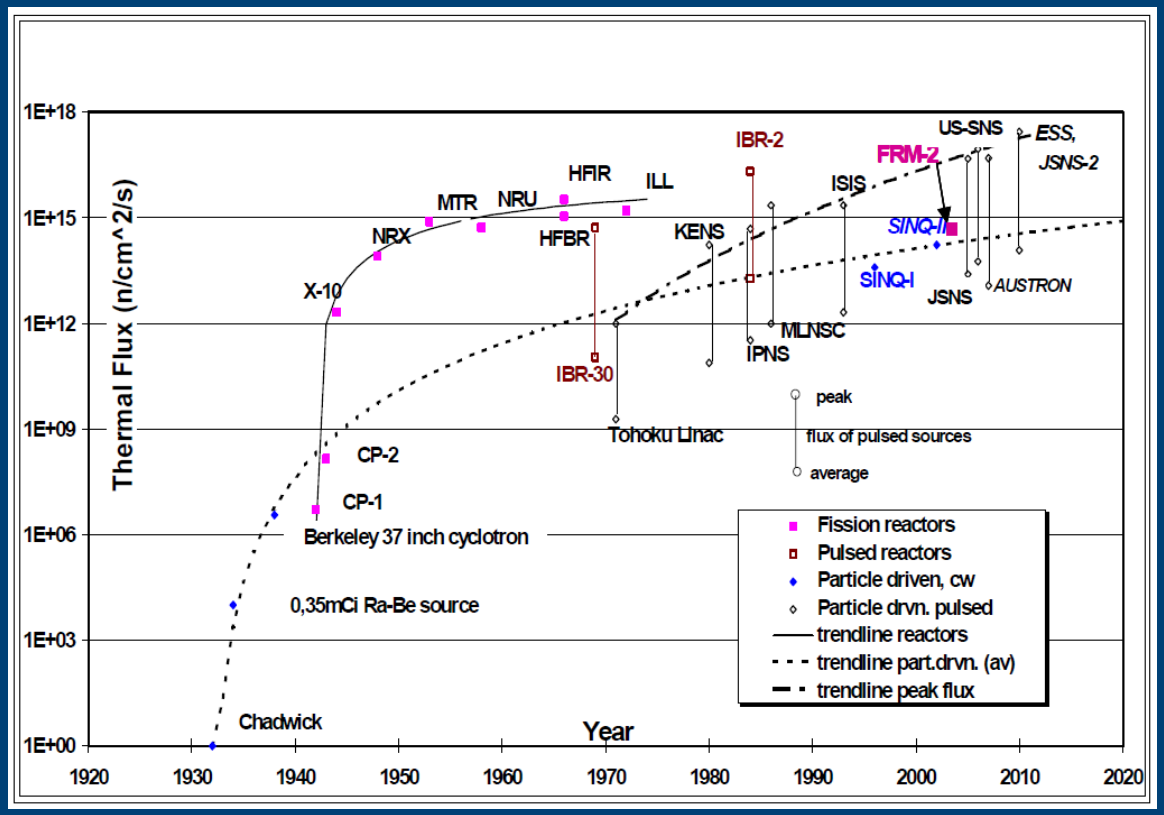
- ✓ **Discussion of the scientific case for a new source of neutrons at JINR**
- ✓ **Cooperation between JINR and the National Synchrotron Radiation Centre SOLARIS**
- ✓ **FLNP User Programme and information on IBR-2 instruments**

Development of the scientific case for a new source of neutrons at JINR



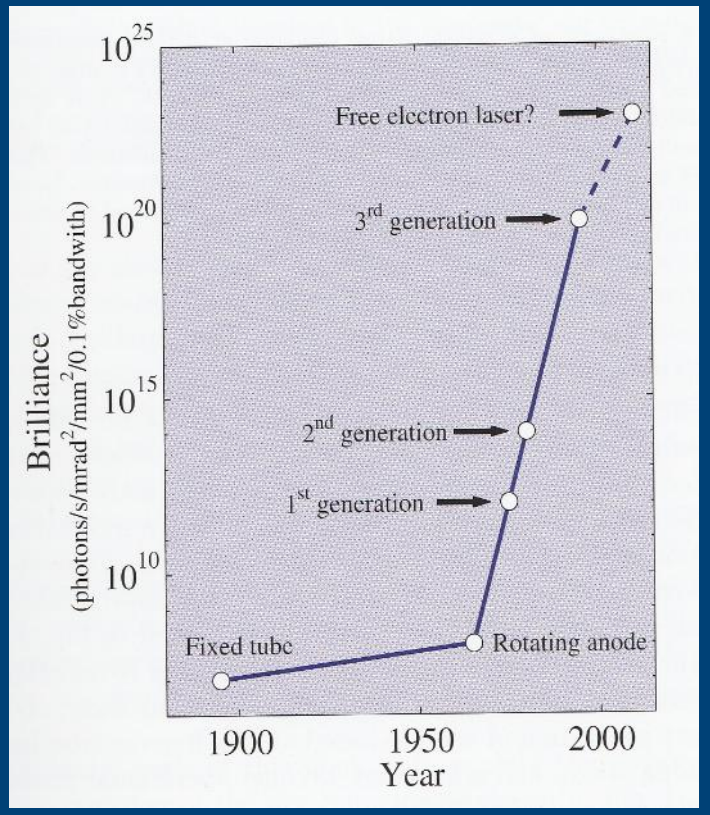
Flux Advancements

Neutron sources



Report of a technical meeting held in Vienna, 18–21 May 2004 , IAEA-TECDOC-1439 (2005).

X-ray sources



J. Als-Nielsen, D. McMorrow, Wiley (2001)

Parameters in Focus

- flux@sample [$n/cm^2/s^1$] $>10^8$
- background <5-10%
- frequency 5-10 Hz
- wavelengths 1-20 Å
- resolution <5%
- pulse width 200-400 µs vs. ~10 µs

Diff.+SANS+Refl. Inelastic

Efficiency Determining Factors

- neutron optics
- spectrometer performance (resolution, background)
- data collection speed

The PAC was informed by the FLNP Directorate that a preliminary activity to elaborate a scientific case has been started by internal and external experts

Starting points of this work include:

- physics of condensed matter using nuclear methods is aligned well with the scientific program of JINR
- (pulsed) neutron sources at JINR fit within the neutron source landscape geographically and historically

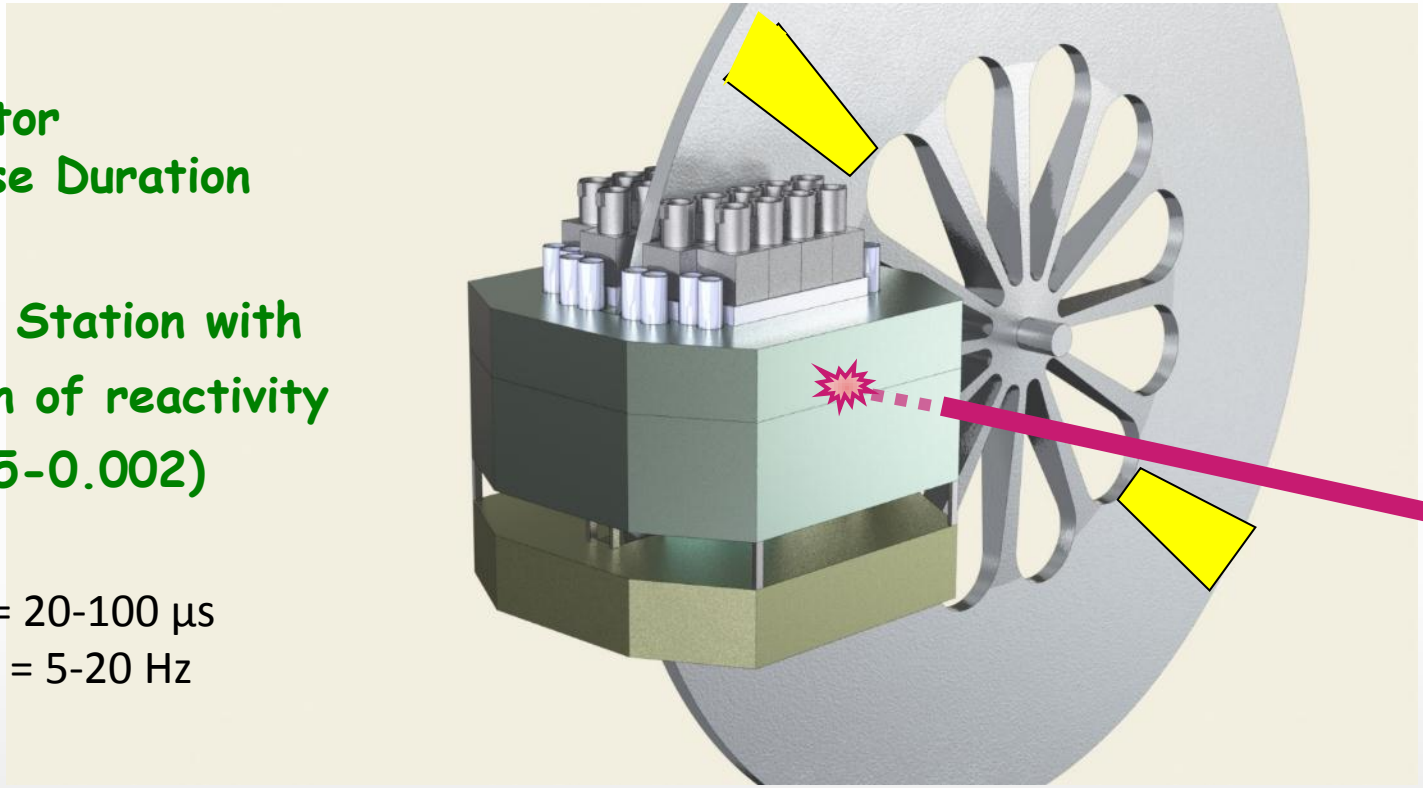
PAC recommendation

The PAC supports the activities of FLNP in this direction and appreciates the attention being paid to the requirements of scientific community in a context of modern sciences. The design of the future source must take into account the role of neutron experiments that is changing in accordance with the landscape of relevant scientific facilities.

Recommendation. The PAC supports the ongoing discussions on the scientific case of the new source and recommends their continuation in close connection with the scientific plans of FLNP. In particular, potential instruments should be considered in developing this scientific case.

"Neptun" Superbooster (DNS-4)

Linear p-Accelerator
with Variable Pulse Duration
+
Multiplying Target Station with
periodic modulation of reactivity
(subcriticality 0.05-0.002)



Ep =1.2 GeV, Δt = 20-100 μs
I max = 50 mA , ν = 5-20 Hz
W ≤ 100 kW

Multiplying target:

Modulation of reactivity

Neptunium subcritical system

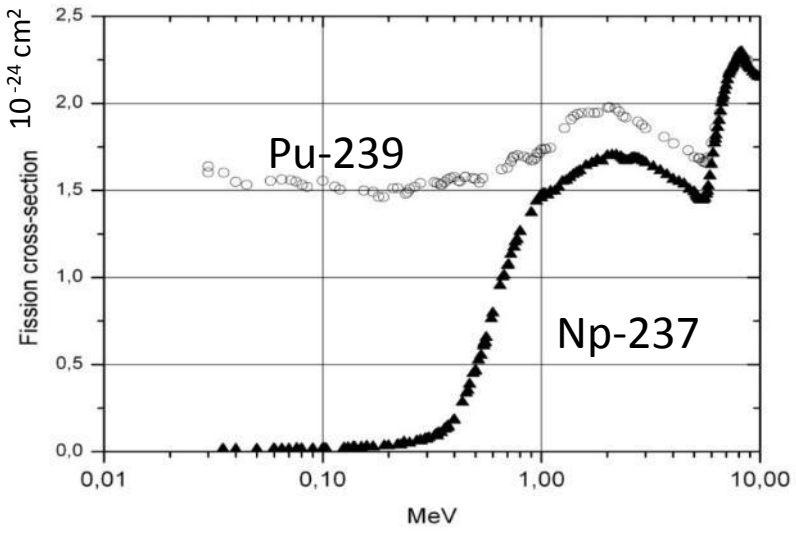
Long pulse ≤ 300 μs

Short pulse 20 μs

W = 10-15 MW

by V. Aksenov

Why Neptunium-237?



Fission threshold 0.4 MeV

* Np^{237} is a product of atomic power plants; $T_{1/2} = 2.14 \cdot 10^6$ years

5 advantages over Pu-239, each quite important :

* I. Short life time of prompt neutrons τ_{Np} = 10 ns

τ_{Pu} (IBR-2) > 65 ns.

Optimal multiplication factor $M = \frac{\theta_{eff}}{\tau}$

2. Lower background between pulses (due to lower effective delayed neutron fraction)

3. Potential for reactivity modulation by VOID

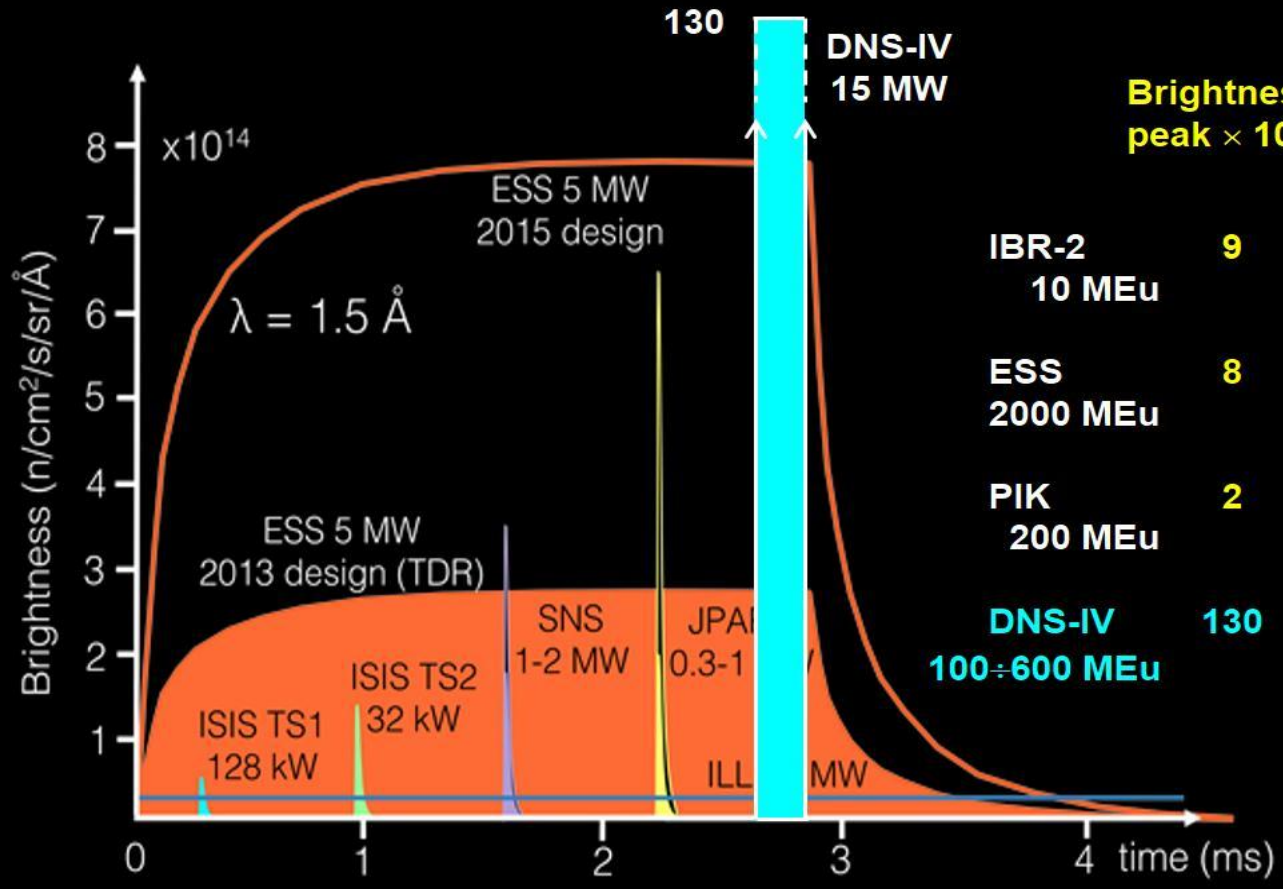
(hydrogen is effective absorber of fast neutrons)

4 Facility operation time to fuel reloading is as long as 10-20 fold of that for plutonium core

5. Not nuclear weapon material

by V. Aksenov

Dubna Neutron Source of the Fourth Generation



	Brightness, peak × 10^{14}	Flux density, time aver.	Flux density, peak
IBR-2 10 MEu	9	0.1	58
ESS 2000 MEu	8	2	75
PIK 200 MEu	2	10	10
DNS-IV 100÷600 MEu	130	3	800

Data $\times 10^{14}$ $[n \cdot cm^{-2} \cdot s^{-1}]$

Single-pulse source brightness as a function of time at wavelenght of 1.5 A at ESS, ILL, SNS, J-PARC and ISIS Target Stations 1 and 2. In each case, the thermal moderator with the highest peak brightness shown. (Source: ESS)

Shabalin E.P., Rogov A.D., Komyshev G.G., Ananiev V.D., Aksenov V.L. (2016) JINR P3-2016-90

PAC discussion

If successfully implemented, such a source (superbooster) will take one of the world's leading positions among the high-flux pulsed sources which will be in operation in the mid of the current century.

Nevertheless, taking a univoque position by the PAC in the matter of the physical scheme of the new neutron source would be premature at this stage. In particular, concerns about the facility background (signal to noise) were raised during the discussion.

For selecting the optimal physical scheme, all reasonable options should be carefully analysed and compared with each other by an expert group properly representing the potential user community both from national and topical point of view.

Suggested timeline

The suggested timeline of the preparatory phase of JINR's new neutron source with estimated deadlines includes:

- establishing an international working group (IWG) in 2018;
- organizing international workshops by FLNP and scientifically coordinated by the IWG from 2018 until the conceptual design report will be concluded;
- publishing a short (up to 50 pages) kick-off document elaborated by the IWG on the idea of the new facility until mid-2019;
- elaborating and publishing a detailed scientific case until early 2020;
- elaborating a detailed conceptual design report until the end of 2020;
- elaborating the administrative and financial model for the construction, commissioning, operation and decommissioning phases until 2021;
- taking decision on the construction of the new facility until 2023.

The PAC recommendation

Recommendation. The PAC considers the subcritical assembly of ^{237}Np with a mechanic reactivity modulation controlled by a pulsed proton accelerator (superbooster) to be a possible conception of the future neutron source. At the same time, the PAC recommends continuing the work of studying other options with a clear analysis of the parameters of the new source in terms of strengths, weaknesses, opportunities and threats with respect to the envisaged long-term user programme. Instrument background should be considered in the design of the source.

Cooperation between JINR and the National Synchrotron Radiation Centre SOLARIS

The PAC heard with interest the report on the concept of the JINR Synchrotron Radiation Laboratory at the SOLARIS synchrotron of the Jagiellonian University in Kraków, presented by V. Shvetsov.

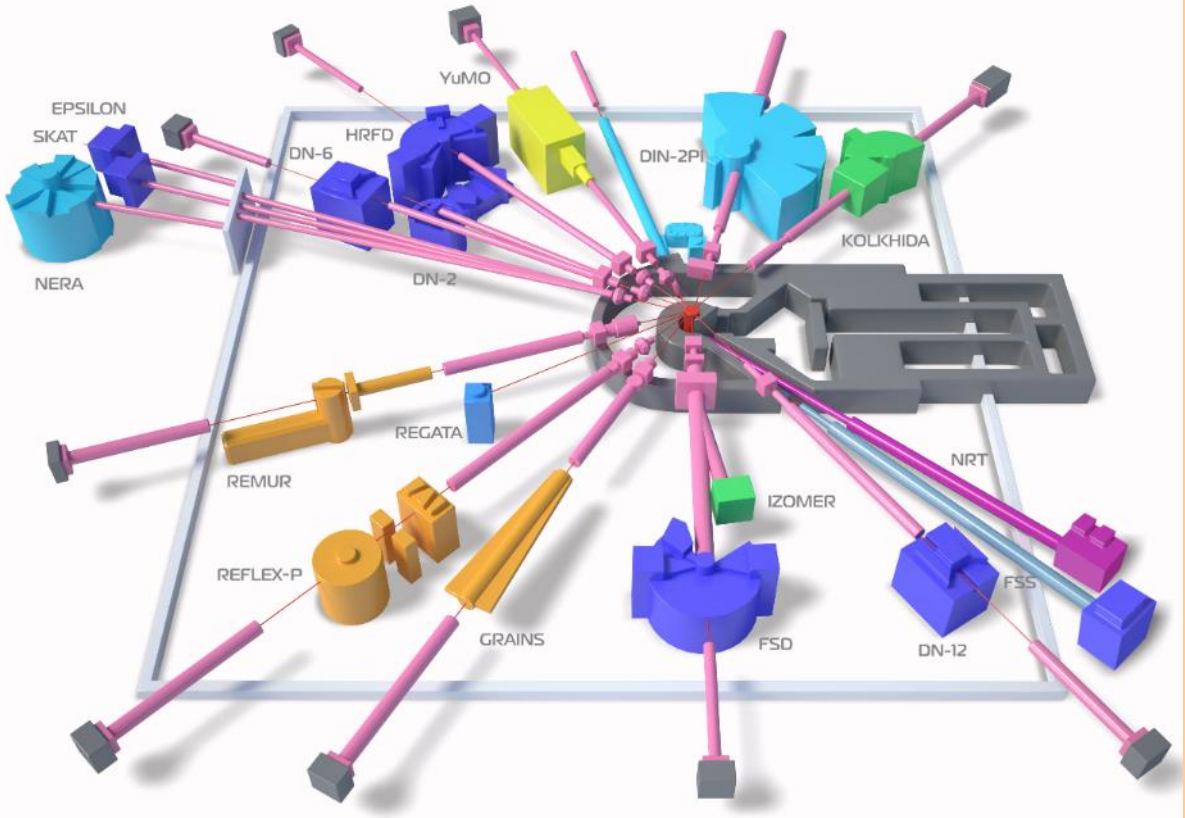
PAC recommendation

The PAC considers fruitful the idea of establishing a synchrotron radiation laboratory belonging to JINR in one of the Member States. The PAC supports this idea and believes that its implementation will significantly enhance the experimental capabilities of the JINR teams working in the field of condensed matter physics at the Institute. Therefore it invites the directorates of JINR Laboratories to elaborate the details of envisaged cooperation based on a more detailed scientific case and in terms of well-established user demands and the existing synchrotron radiation landscape.

Recommendation. The PAC recommends that the JINR Directorate, together with the Jagiellonian University, form a working group of representatives of both organizations with the participation of interested representatives of scientific centres of JINR Member States, and provide it with the necessary support in order to develop the concept of the laboratory and a forward-looking scientific programme. Relevant materials should be presented at the next PAC meeting in June 2018.

Status reports on upgrades of IBR-2 instruments

IBR-2M Spectrometers Complex



2011:
11 instruments in operation

2018:
15 instruments in operation

Diffractometers:

HRFD, DN-6, RTD, DN-12, FSD, SKAT/Epsilon, FSS

Reflectometers:

REMUR, REFLEX, GRAINS

Small Angle Scattering Spectrometer: YuMO

Inelastic Neutron Scattering Spectrometers:

NERA, DIN-2PI

Radiography and Tomography: NRT

New Instruments:

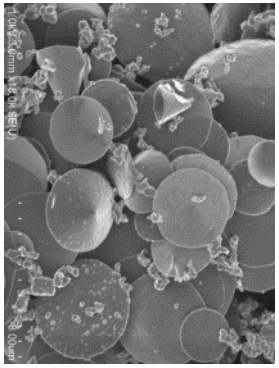
DN-6, GRAINS, NRT, FSS

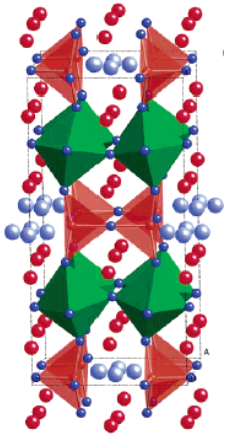
Reconstruction:

REFLEX – SESANS

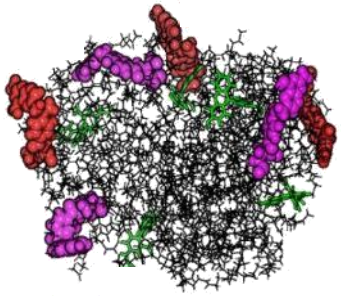
The priority directions of fundamental research :

- Nanoscale physics

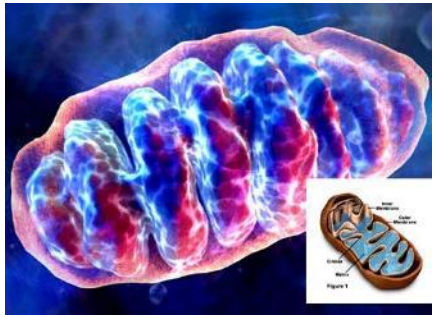




- Physics and Chemistry of Functional Materials



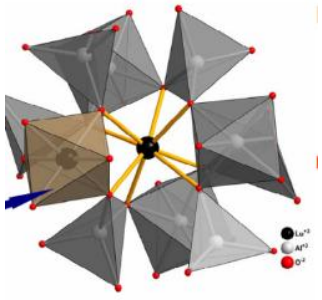
- Physics and Chemistry of Complex Liquids and Polymers



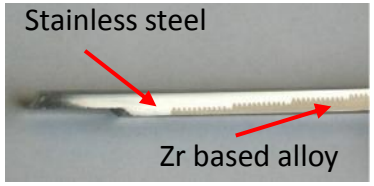
- Physics of Soft Condensed Matter

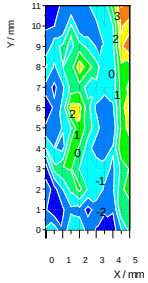
The priority directions of applied research:

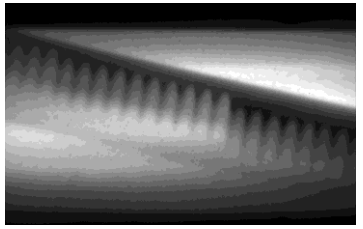
- **Structural characterization of functional materials used in different (nano)technologies**



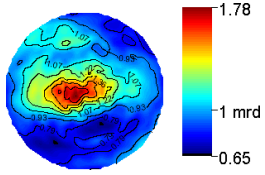
- **Non-destructive control of residual stresses and internal organization of bulk materials and products**

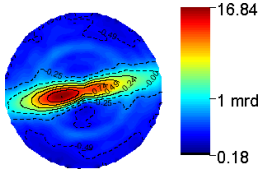






- **Texture analysis of geomaterials and constructional materials**





PAC recommendation

The PAC appreciates the significant upgrade of the IBR-2 spectrometers and development of new instruments, resulting in improvement of their parameters and extension of research areas, as well as making them more attractive for potential users. The development plans take into account specific features of the IBR-2 reactor (high flux, long pulse, availability of cryogenic moderator) and will assure the maintenance of the parameters of the instruments at the level comparable with other leading research centres in the world, as well as further extension of research areas and improvement of research quality.

Recommendations. The PAC recommends further development of IBR-2 instruments taking into account the current trends in the progress of neutron scattering techniques.

High-pressure neutron diffractometer DN-6 for investigation of microsamples under extreme condition: recent results

New focusing guide design (2016-2017)

Design: vertical parabolic tapered neutron guide

Guide profile:

-Profile (hor./vert.): parallel/parabolic tapered (linar appr.)

Cross section:

-Entrance: 180.00 mm(h)x 15.00 mm(w)

-Exit: ~60 mm (h)x 15.00 mm(w)

Reflectivity:

-Top/bottom R_{ave}=92%

-Sides R_{total}~99,5%

First three units:

Coating: Ti/Ni

-Top/bottom m=3

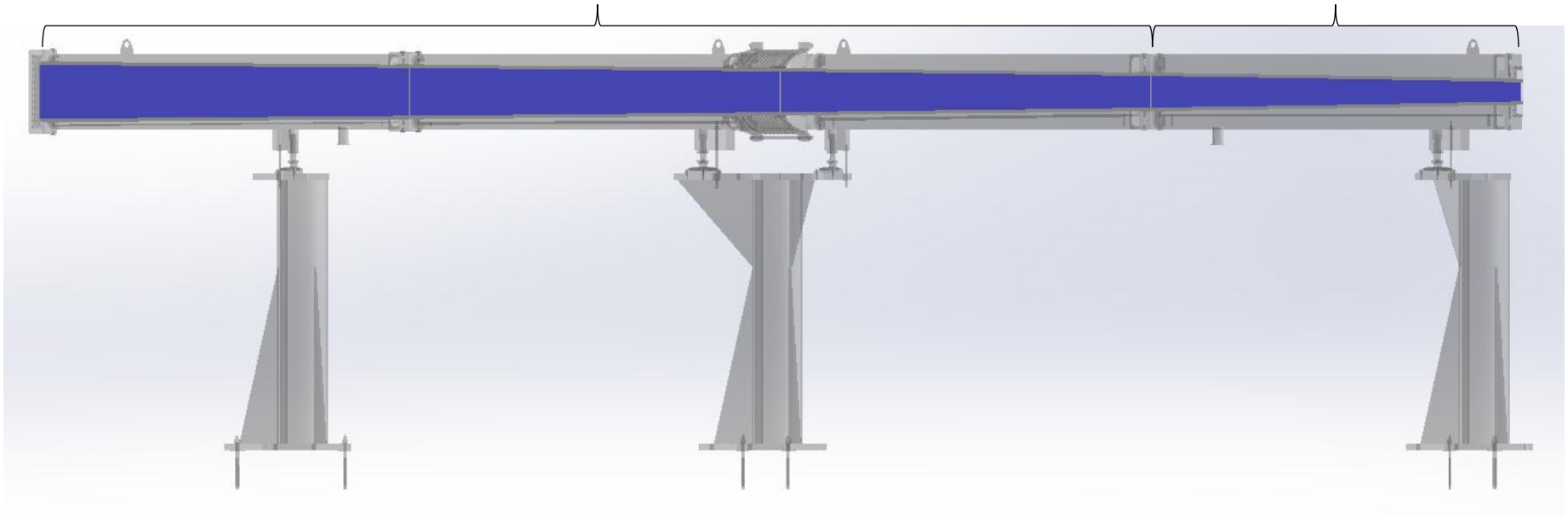
-Sides m=1

Last unit:

Coating: Ti/Ni

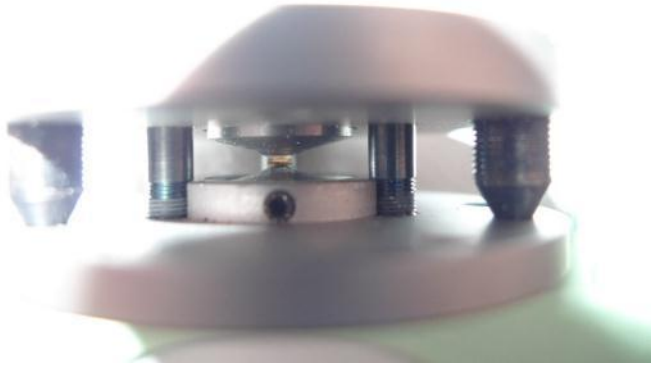
-Top/bottom m=5

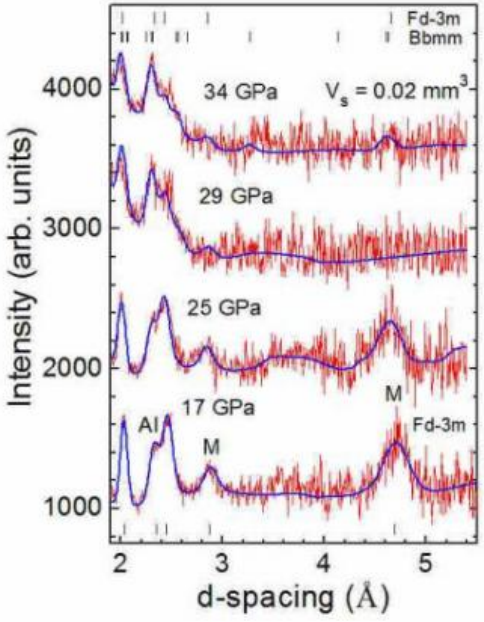
-Sides m=1



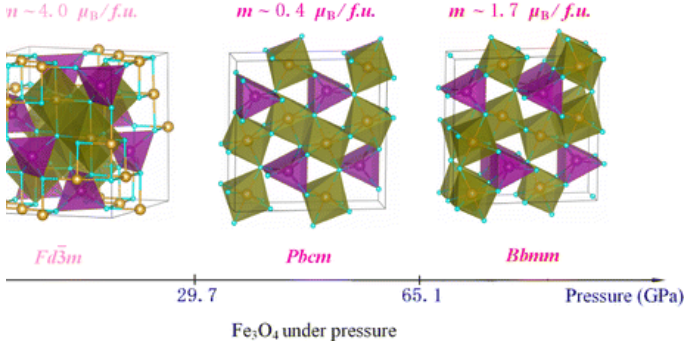
DN-6 diffractometer: experiments with diamond anvil cell

Culet size – 0.8 mm
Volume – 0.02 mm^3
Pressure - 35 GPa
Exposition time – 48 h

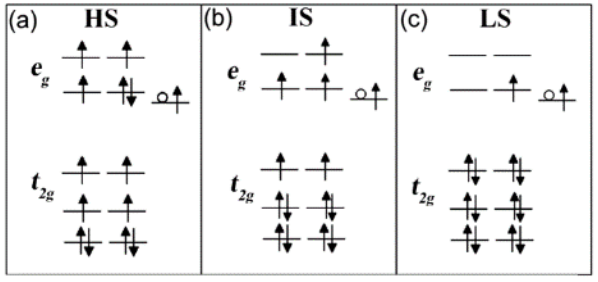




Neutron diffraction patterns of Fe_3O_4 sample measured in DAC up to 35 GPa



Chem. Soc., **2012**, *134* (33), pp 13780–13786



PRL **100, 045508 (2008)**

PAC recommendation

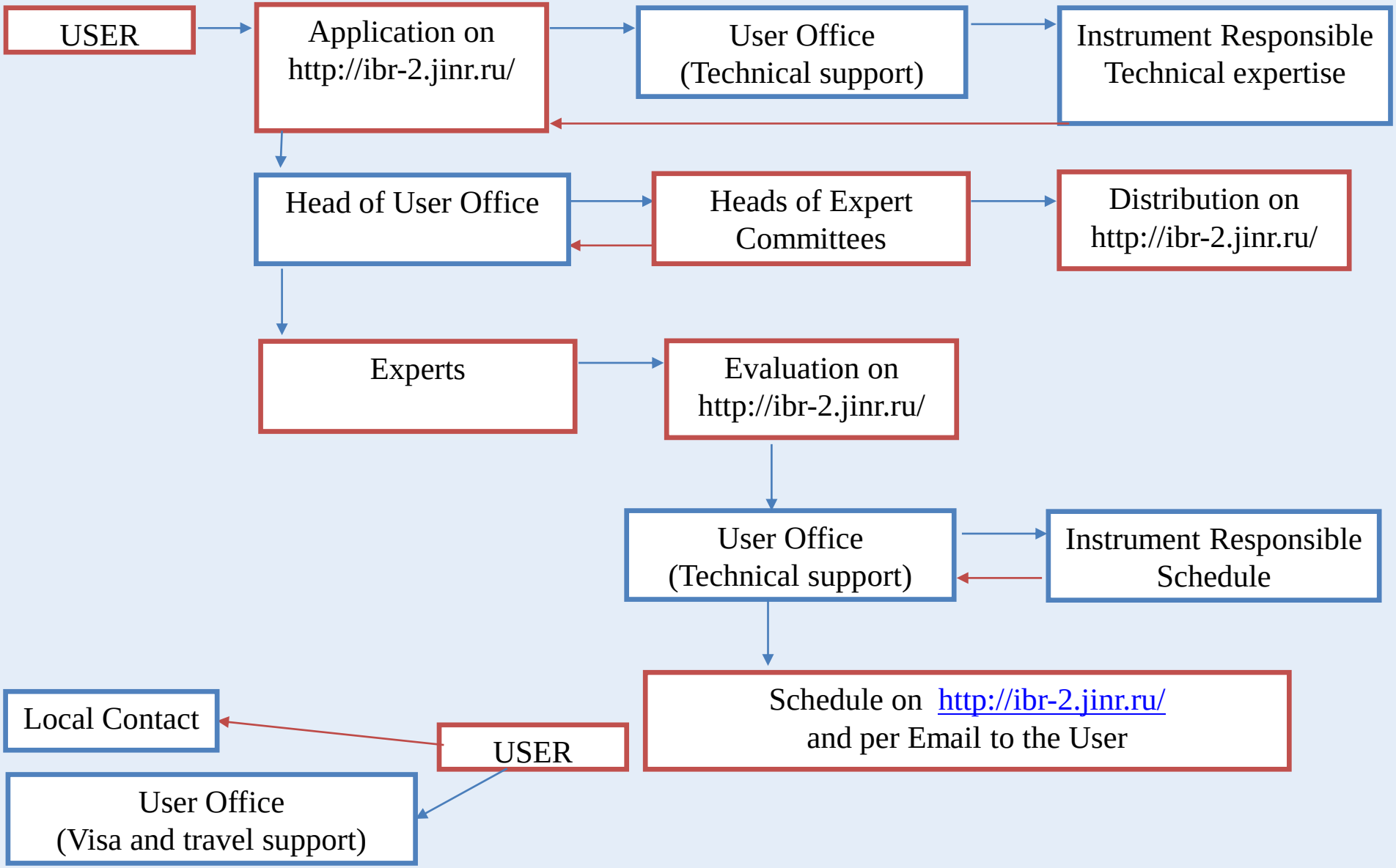
The PAC notes the ongoing work to improve this instrument, which is a first-priority task in developing the IBR-2 spectrometer complex. The neutron flux on the sample has been increased by replacing part of the neutron guide with the neutron beam focusing system. Full-scale experiments are underway with high-pressure diamond anvil cells of various configurations. The PAC finds it reasonable to consider the possibility of further increasing both the neutron flux and the solid angle of the facility's detector system.

Recommendation. Taking into account that the DN-6 diffractometer becomes one of the world-leading instruments for neutron scattering studies of matter under extreme conditions, the PAC recommends that further development of DN-6 and its introduction to the User Programme remain one of the first-priority activities at FLNP.

FLNP User Programme

The PAC took note of the comprehensive report presented by D. Chudoba on the progress in implementing the FLNP User Programme, including details about the organization of the assessment of proposals and the statistics of their realization during 2015–2017.

User Programme - INFORMATION



User Programme - STATISTICS

Reactor operation for physics experiments

2015

- 9 cycles (7 – water moderator, 2 cryogenic moderator)
- 2646 hr

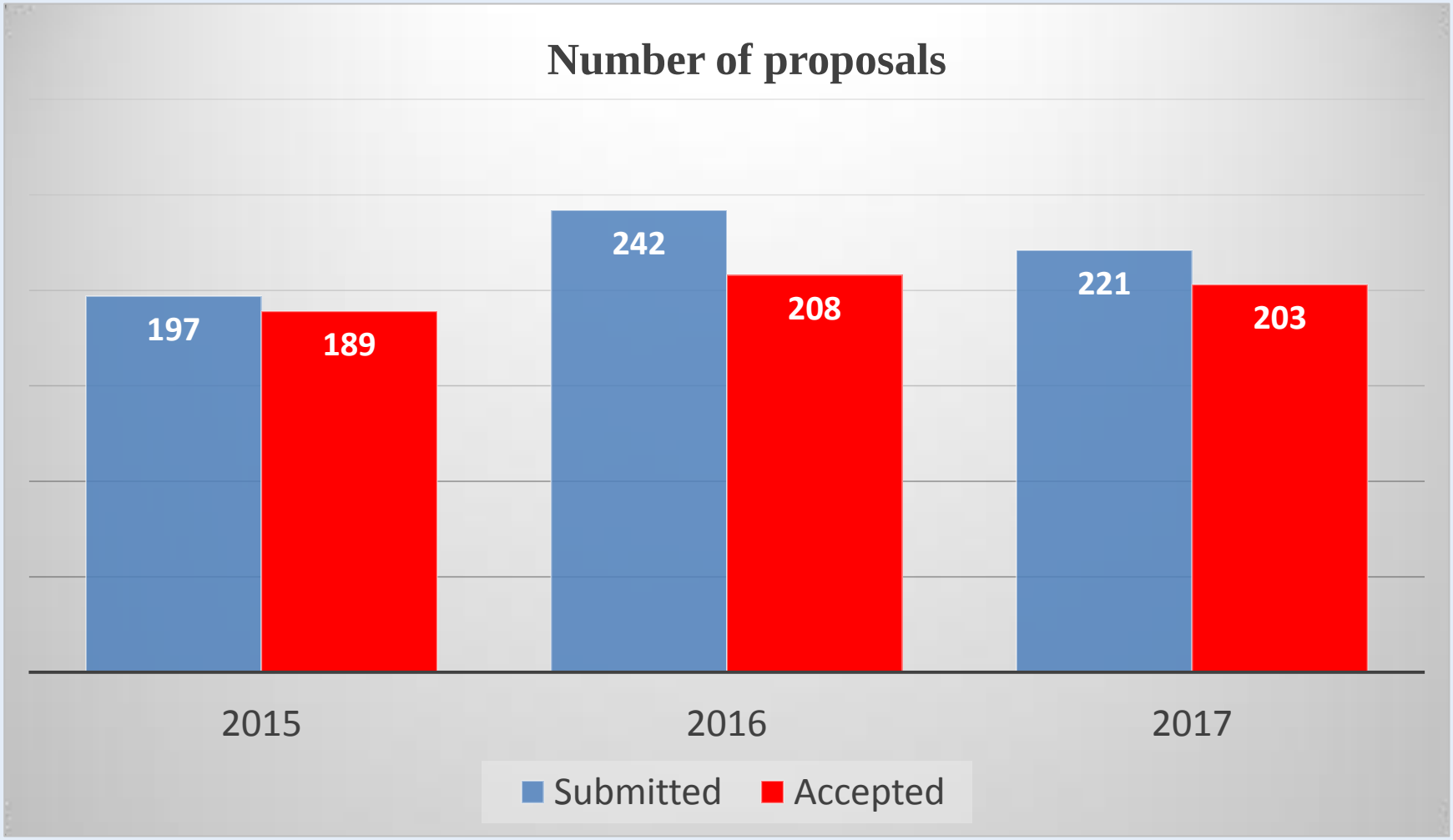
2016

- 8 cycles (7 – water moderator, 1 cryogenic moderator)
- one cycle - canceled due to technical reasons
- 2447 hr

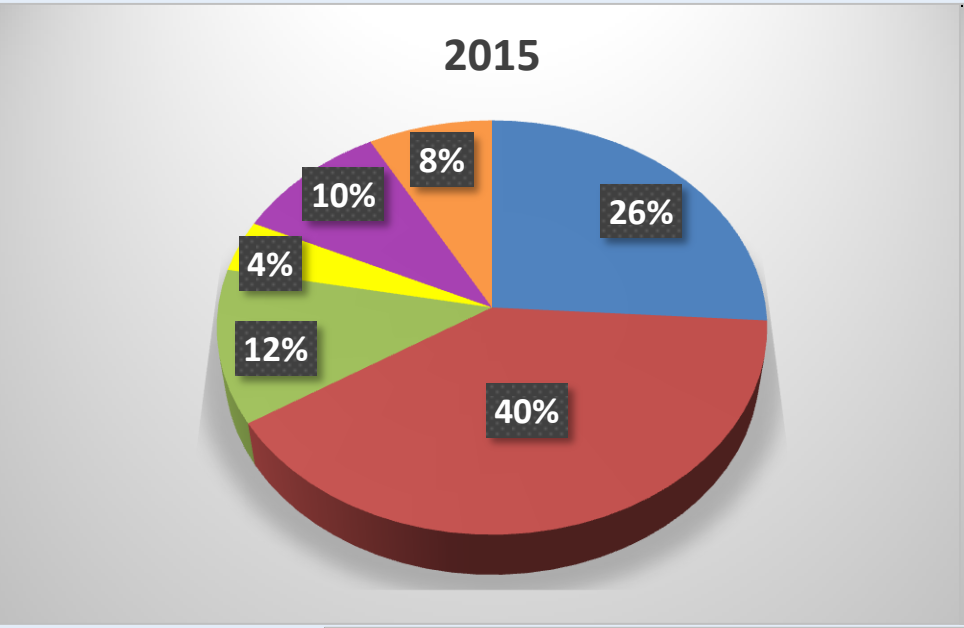
2017

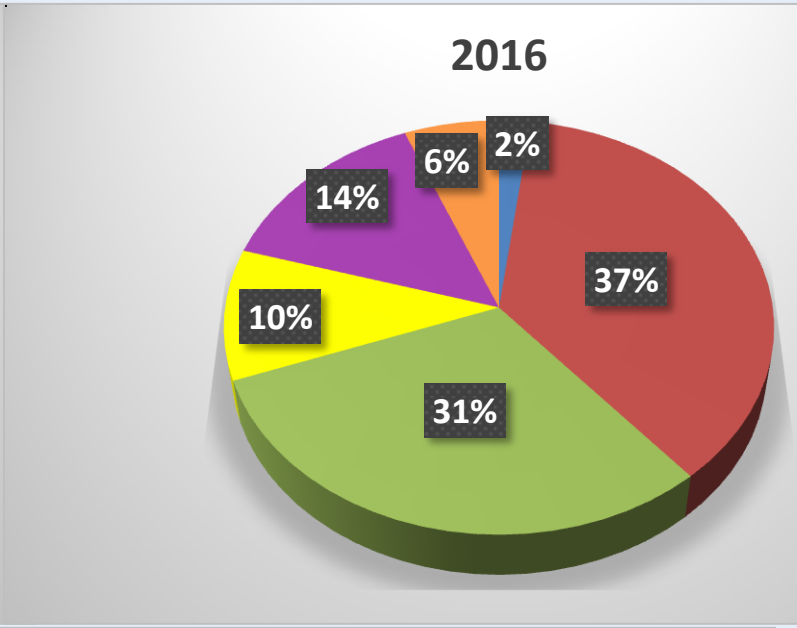
- 9 cycles (8 – water moderator, 1 cryogenic moderator)
- 2471 hr

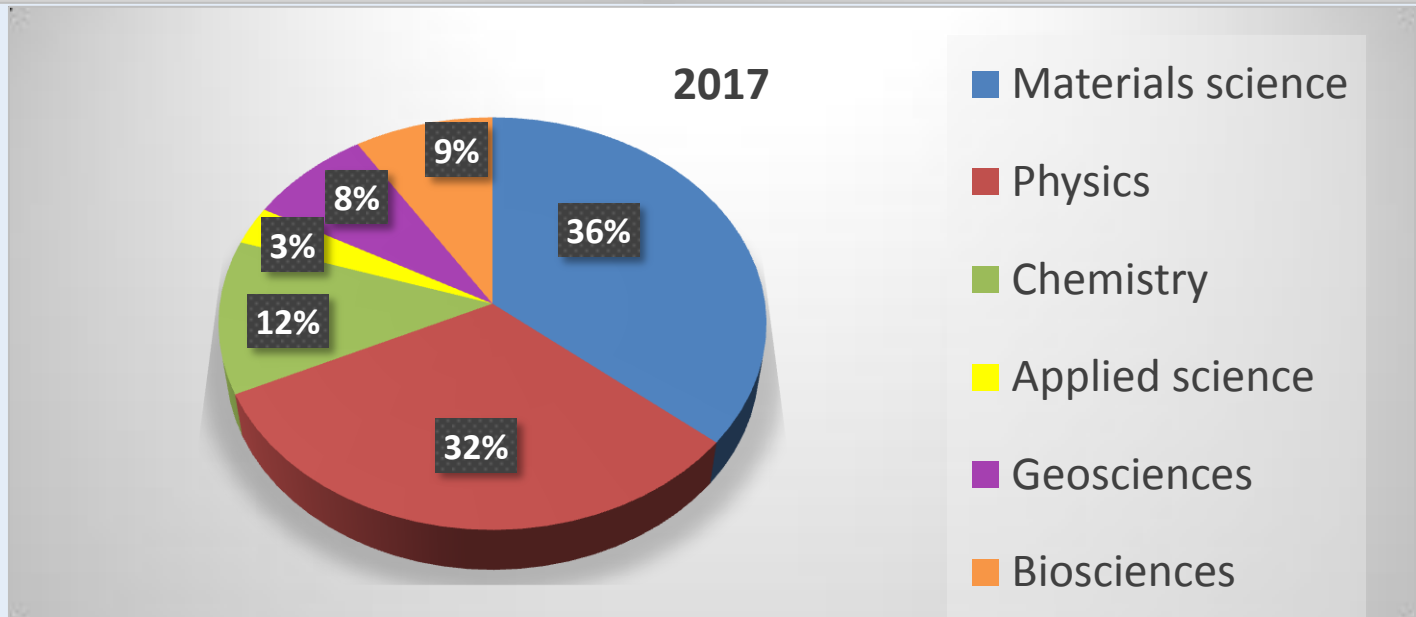
User Programme - STATISTICS



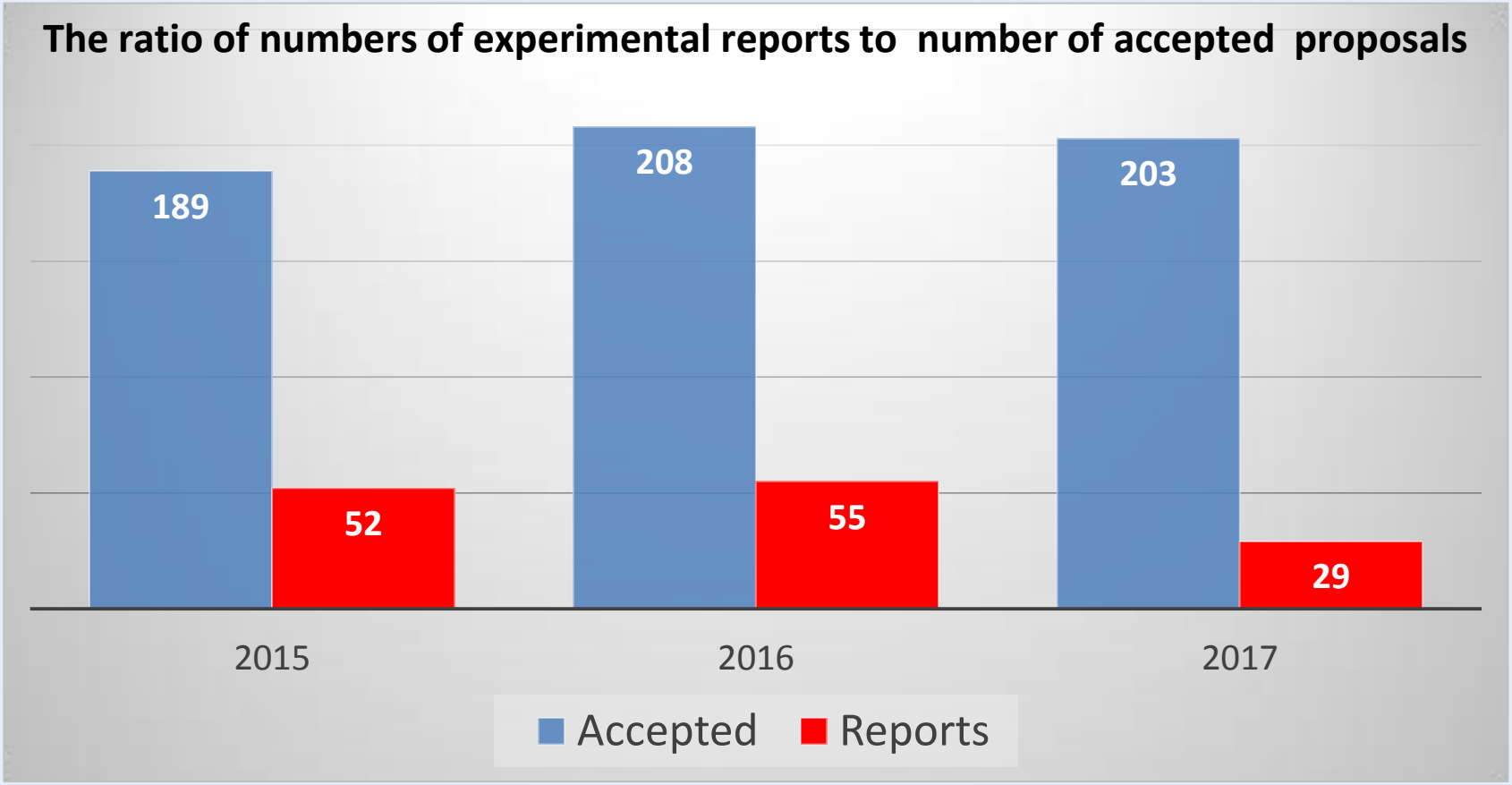
User Programme - STATISTICS







User Programme - STATISTICS



Experimental report policy

Following the recommendation of the FLNP JINR Scientific Council, **Experimental reports are now mandatory for all experiments within 3 months after the experiment has been performed**.

PAC recommendations

The PAC highly appreciates the efforts of the FLNP Directorate and the FLNP User Office to run the User Programme at an internationally highly recognized level. At the same time, technical shortcomings of the proposal assessment web applications were identified as a bottleneck of the evaluation process.

Recommendation 1. The PAC considers the FLNP User Programme to be the key instrument of securing the position of IBR-2 as one of the leading neutron sources in the world and encourages the FLNP Directorate to further support this highly important activity. The PAC recommends that the FLNP Directorate upgrade the IBR-2 proposal assessment web application to a professional system supporting the work of proposers, reviewers and the FLNP management and that it consider entrusting this task to the Laboratory of Information Technologies.

Recommendation 2. The PAC recommends that the FLNP User Office strictly insist on submitting experimental reports by all successful proposers as the necessary feedback.

Scientific reports

The PAC heard with interest scientific reports

“Cultural heritage research using neutron imaging at the IBR-2 reactor” by I. Saprykina

and

“Planar graphene tunnel field-effect transistor: effect of edge vacancies on performance” by V. Katkov.

Poster presentations

The PAC reviewed 24 poster presentations by young scientists in fields of condensed matter physics and information technology.

Best poster: “Fullerene-based complexes in solutions for anticancer therapy and neurodegenerative diseases” by O. Kyzyma.

Two other high-quality posters:

“Investigation of the crystal and magnetic structure of nanostructured complex oxides of transition metals in a wide pressure and temperature range” by N. Belozerova and

“Clusterization aspects of fullerenes C_{60} and C_{70} in toluene/N-methyl-2-pyrrolidone mixture according to SANS, SAXS and DLS data” by T. Nagorna.

Recommendation. The PAC recommends the poster “Fullerene-based complexes in solutions for anticancer therapy and neurodegenerative diseases” to be reported at the session of the Scientific Council in February 2018.

Next meeting of the PAC

The next meeting of the PAC for Condensed Matter Physics will be held on **14–15 June 2018.**

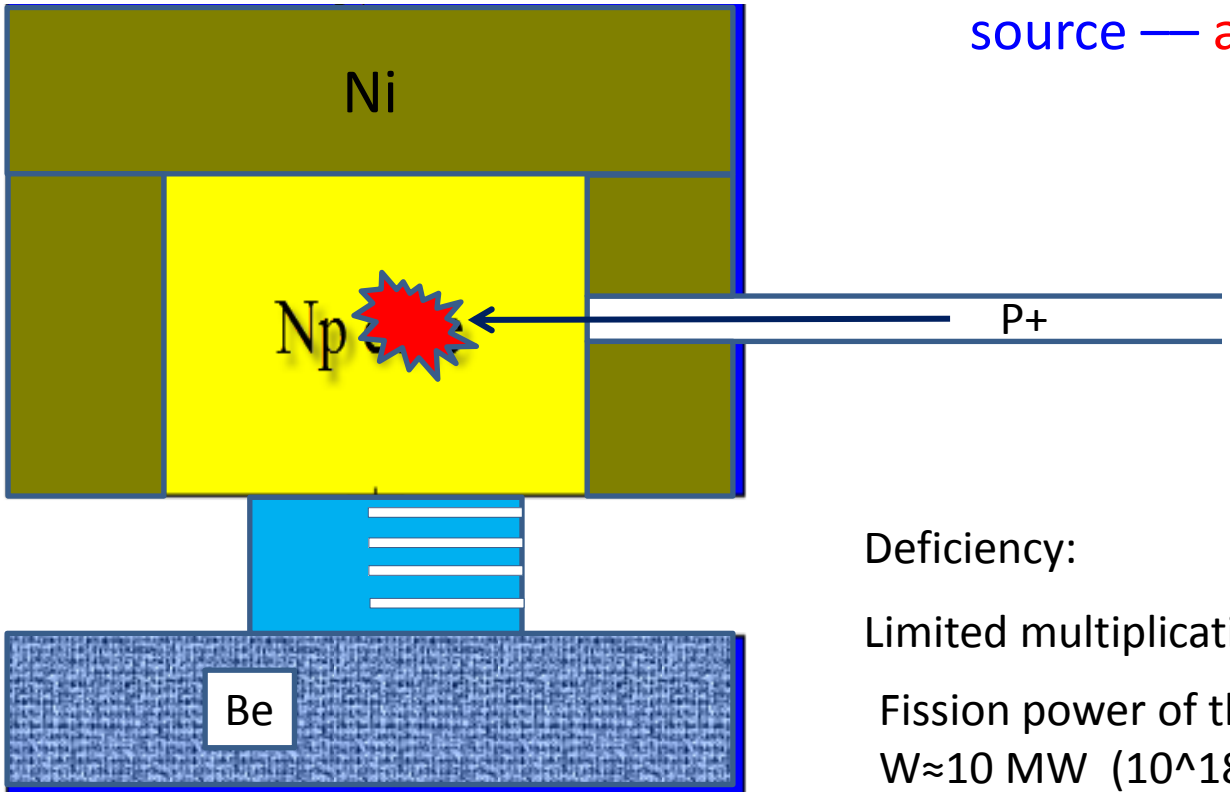
Its tentative agenda will include:

- Information by the PAC Chairperson on the report at the next session of the Scientific Council, and the implementation of the recommendations of the current PAC meeting;
- Information by the JINR Directorate on the sessions of the Scientific Council (February 2018) and of the Committee of Plenipotentiaries (March 2018);
- Reports and recommendations on themes and projects to be completed in 2018;
- Discussion of the progress of the scientific case for JINR's new neutron source;
- Discussion on the cooperation between JINR and the National Synchrotron Radiation Centre SOLARIS;
- Progress in implementing the FLNP User Programme;
- Status reports on the upgrades of FLNP instruments in the context of the JINR Seven-year plan;
- Information on the update of the JINR Seven-year plan by the Laboratories involved in condensed matter research;
- Information about scientific meetings;
- Scientific reports;
- Poster session.

Thank you for your attention

The PAC appreciated the report "A 20-year forward look at JINR's high-flux pulsed neutron source" presented by V. Aksenov.

Basic arrangement of Np booster (without reactivity modulator)



The PAC took note of the principles of construction and the parameters of a neutron source — a superbooster.

Proton linear accelerator 1.2 GeV

Deficiency:

Limited multiplication factor – 25.

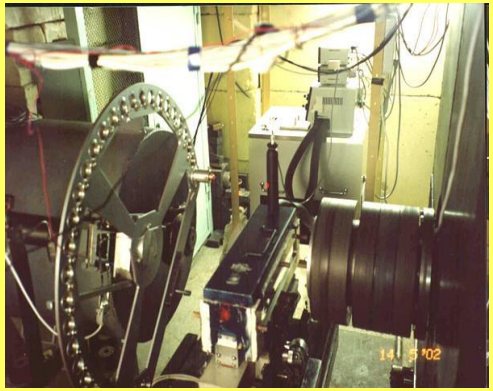
Fission power of the target W≈10 MW (10^18 n/s) at Ipeak ≥ 0.5 A (?!) – unreal

by V. Aksenov

	Moderator type	Peak differential neutron flux 10^{14} n/см^2/s/sr/Ă (Brightness)	Peak neutron flux , 2π eqv. 10^{14} n/см^2/s	Time averaged flux 2π equivalent. 10^{14} н/см^2/с
IBR-2	Grooved, wide	**9**	58	**0.09**
	Grooved, height 4.5 см	12	77	0.16
J-Park	Coupled	10	65	0.3
ESS	Butterfly height 6 см	8	50	2.0
	Height 3 см	**12**	**75**	**3.0**
PIK, Russia	Stationary, D_2O moderator	1.6	12	**12**
DANS	Grooved	**130**	**800**	**2.0**

by V. Aksenov

YuMO - SANS



A study of structural characteristics of nanostructured materials, biological objects, polymers

REMUR

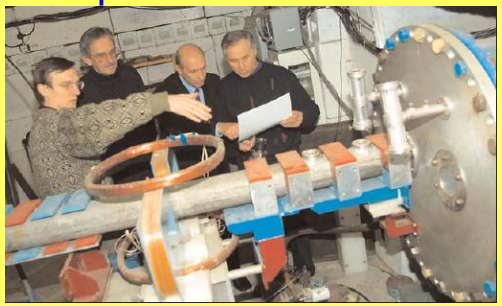
Reflectometer with polarized neutrons

A study of magnetization profile, magnetic and structural properties of layered nanostructures

Small Angle Neutron Scattering and Reflectometry

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