



CREMLINplus WP 3 Workshop:

"Neutron diffraction - 2021"

8 - 10 June 2021, from 10:00 to 18:00 (GMT+3) every day

Venue: Petersburg Nuclear Physics Institute named by B.P.Konstantinov of NRC «Kurchatov Institute» Address: 188000, Russian Federation, Leningradskaya oblast, Gatchina, 1, mkr. Orlova roshcha Site: https://oiks.pnpi.spb.ru/events/difraction2021



Objectives

The workshop "Neutron Diffraction - 2021" is held to discuss topical scientific problems solved by neutron diffraction methods, new methods in decoding magnetic structures, new methodological and software developments in the processing of experimental neutron diffraction patterns. The workshop addressed the issues of determining and refining crystal and magnetic structures by powder and single crystal neutron diffraction methods, the relationship between structures and the physical properties of materials. The workshop served to coordinate the research of Russian and International scientific teams on diffractometers of the PIK reactor complex.

This workshop was held at PNPI annually, starting in 2013. The last such meeting was organized in 2017. The decision of the management of the NRC "Kurchatov Institute" to resume the workshop "Neutron diffraction" is primarily due to the beginning of the active phase of creating the instrumentation base of the PIK reactor complex. According to the implementation plan, at the end of 2022, a high-resolution powder neutron diffractometer D1 should be created, at the end of 2023 - a 4-circle single-crystal neutron diffractometer DC-1, at the end of 2024 - a high-intensity powder neutron diffractometer D3. In parallel, within the framework of the CREMLINplus project, a DIPOL polarized neutron diffractometer is being developed. A TEX-3 texture diffractometer and a DPN polarized neutron diffractometer have already been assembled and installed on horizontal beams in the PIK reactor hall.

Therefore, the most important goal of the workshop "Neutron Diffraction - 2021" is to discuss the designs of these installations and their individual units, software and electronic support for diffractometers of the PIK reactor, software for processing experimental data, as well as the program of scientific research on them. Another purpose of the workshop is to demonstrate the unique possibilities of using diffraction methods in modern research, to discuss the latest basic scientific results obtained with the use of neutron diffraction in Russia and in the world.









Another important goal of the workshop is, as always, educational. Young scientists, graduate students and students will receive information on the most modern methods for determining magnetic structures from powder and single crystal data.

The scientific program includes the following topics:

- Neutron Diffraction in Solid State Physics;
- Complementarity of diffraction techniques in solid state physics;
- Diffraction of polarized neutrons;
- Fundamental and applied materials science using diffraction research methods;
- World trends in neutron diffractometry. Modern diffraction instrumentation. Instrumentation base of the PIK reactor complex.
- Progress in the mathematical and software solution of magnetic structures by neutron diffraction methods.

The workshop "Neutron Diffraction - 2021" is an event within CREMLINplus WP3 [Collaboration with PIK], Task [Task 3.7: Instrument specific education and training programs for engineers and scientists].

Lead beneficiary: [FZJ]. Related CREMLINplus Deliverable: [MS3.1 Plan for the workshops and schools, dissemination level: public].











Neutron Diffraction - 2021 Program

June 8

10-00 A.I. Kurbakov (NRC KI - PNPI, Gatchina) Opening of the meeting.

Session I. Neutron diffraction in condensed matter physics.

Chairman: I.A. Zobkalo (NRC KI - PNPI, Gatchina)

10-10 **I.V. Golosovsky** (NRC KI – PNPI, Gatchina) "Magnetic structures and phase transition in ferroborate HoFe₃(BO₃)₄. Single crystal neutron diffraction".

10-50 **A. F. Gubkin** (IMP UB RAS, Yekaterinburg) "Magnetic diffuse neutron scattering in intermetallic compound Tb3Ni with short-range magnetic order".

11-30 Tea-coffee break.

11-50 **A.I. Kurbakov** (NRC KI - PNPI, Gatchina) "Features of magnetic ordering in a new chiral magnet MnSnTeO₆".

12-30 **A.M. Balagurov** (FLNP JINR, Dubna) "New possibilities of neutron diffraction in the analysis of the structure and microstructure of metal alloys". 13-10 *Lunch*.

Session I. Neutron diffraction in condensed matter physics. Continuation.

Chairman: **A.M. Balagurov** (FLNP JINR, Dubna)

14-30 **D. P. Kozlenko** (FLNP JINR, Dubna) **on - line** "Neutron diffraction at ultrahigh pressures at the IBR-2 pulsed reactor".

15-10 **A.N. Korshunov** (NRC KI - PNPI, ESRF, Grenoble, France) **on - line** "Order and disorder in a triangular magnet CuSb2O₆".

15-40 **A.A. Vaulin** (IMP UB RAS, Yekaterinburg) "Diffraction studies of the crystal and magnetic structure in the binary intremetallide Ho₇Rh₃".

16-00 Tea-coffee break

16-20 **E.K. Nigmatullina** (NRC KI - PNPI, Gatchina) "Phantom" atoms "and thermal motion in fullerene C60, X-ray and neutron diffraction".

16-40 **A.E. Susloparova** (NRC KI - PNPI, Gatchina) "Neutron diffraction study of low-dimensional frustrated tellurates of the family A_2MnTeO_6 ".









17-00 **I.A. Bobrikov** (FLNP JINR, Dubna) "Temperature-induced phase transitions on the surface and in the bulk of the Fe₂₇Ga magnetostrictive alloy".

17-30 **B. Mukhametuly** (FLNP JINR, Dubna) "Prospects of neutron radiographic and diffraction studies at the WWR-K reactor of the INP (Almaty, Kazakhstan)".

June 9

Session I. Neutron Diffraction in physics of condensed state. Continuation.

Chairman: A. I. Kurbakov (NRC KI - PNPI, Gatchina)

10-00 **A. Senyshyn** (Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany) **on-line** "Neutron diffraction and its role in the studies of Li-ion batteries".

11-00 **M. Avdeev** (ANSTO, Australia) **on-line** "Neutron diffraction at the Australian Neutron Scattering Center: instrument base, user program, and recent research examples".

11-50 Tea-coffee break

12-10 **A.N. Pirogov** (IMP UB RAS, Yekaterinburg) "Crystal structure and magnetic state of rare earth compounds based on TbNi₅".

12-50 I.A. Zobkalo (NRC KI - PNPI, Gatchina) "Features of the HoFeO $_3$ magnetic phase diagram".

13-30 *Lunch*.

Session I. Neutron Diffraction in physics of condensed state. Continuation.

Chairman: A. I. Kurbakov (NRC KI - PNPI, Gatchina)

14-50 **T.I. Ivankina** (FLNP JINR, Dubna) **on-line** "Texture and anisotropy of the properties of rapakivi granites: to the problem of destruction of architectural monuments of St. Petersburg".

15-20 **A. Goukassov** (LLB, Saclay, France) **on-line** "Advances and trends in modern neutron diffraction on single crystals".

16-10 Tea-coffee break

16-30 **Yu.A. Kibalin** (NRC KI - PNPI, Gatchina, LLB, Saclay, France) **on-line** "Investigation of magnetic anisotropy in single crystals and powders using the CrysPy library for analysis of polarized neutron diffraction data".

17-00 **V. Pomiakushin** (LNS, PSI, Switzerland) **on-line** "Superspace Magnetic Structure and Topological Charges in Weyl Semimetal CeAlGe".

June 10

Session I. Neutron Diffraction in physics of condensed state. Continuation

Chairman: Yu.P. Chernenkov (NRC KI - PNPI, Gatchina)

10-00 **G. D. Bokuchava** (FLNP JINR, Dubna) "Time-of-flight neutron Fourier stress diffractometry at the IBR-2 reactor for solving materials science problems".

10-30 **M. M. Murashev** (NRC "Kurchatov Institute", Moscow) **on-line** "Visualization of the diffraction contrast between the ferritic and martensitic phases of steel by neutron radiography".

10-50 **M.A. Semkin** (IMP UB RAS, Yekaterinburg) "Study of the crystal and magnetic structure of antiferromagnets Li(Ni,Co)PO₄ by methods of time-of-flight diffraction and diffraction of monochromatic neutrons".

11-00 *Coffee, tea.*









11-30 **V. Hutanu** (Institute of Crystallography, Aachen University and JCNS at MLZ, Germany) **on-line** "Diffraction methods using polarized neutrons".

12-30 **M.S. Plekhanov** (IMP UB RAS, Yekaterinburg) "Studies of the local and defect structure of proton-conducting oxides by PDF analysis".

12-50 **I.D. Karpov** (NRC "Kurchatov Institute", Moscow) **on-line** "Conceptual design of a neutron diffractometer for the study of internal stresses at the PIK reactor".

13-10 **V.T. Em** (NRC "Kurchatov Institute", Moscow) **on-line** "Instrument base of stress diffractometry and prospects for its development in Russia".

13-30 *Lunch*.

Session II. Instrument base of PIK

Chairman: I.A. Zobkalo (NRC KI - PNPI, Gatchina)

14-40 S.V. Gavrilov (NRC KI - PNPI, Gatchina) "DPN Polarized Neutron Diffractometer".

15-00 A.E. Sokolov (NRC KI - PNPI, Gatchina) "TEX-3 texture diffractometer".

15-20 **V.A. Ulyanov** (NRC KI - PNPI, Gatchina) "High-resolution powder diffractometer D1". 15-40 *Coffee, tea.*

16-00 I. V. Golosovsky (NRC KI - PNPI, Gatchina) "Polarized neutrons and diffraction on polycrystals. Powder diffractometer D3".

16-20 I.A. Zobkalo (NRC KI - PNPI, Gatchina) "DiPol Polarized Neutron Diffractometer".

16-40 V.A. Polyakov (NRC KI - PNPI, Gatchina) "Single-crystal diffractometer DC-1".

17-00 Discussion

17-30 Closing of the meeting

Nº	Surname	Name	Organization
1.	Altynbaev	Evgeny	NRC KI - PNPI
2.	Avdeev	Maxim	ANSTO
3.	Balagurov	Anatoly	FLNP JINR
4.	Beskrovnyy	Anatoly	FLNP JINR
5.	Bobrikov	Ivan	FLNP JINR
6.	Bokuchava	Gizo	FLNP JINR
7.	Bykov	Alexei	NRC KI - PNPI
8.	Chernenkov	Yuri	NRC KI - PNPI
9.	Dyachkov	Maxim	NRC KI - PNPI
10.	Em	Vyacheslav	NRC "Kurchatov Institute"

Participants







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Connecting Russian and European Measures for Large-scale Research Infrastructures

N⁰	Surname	Name	Organization
11.	Gavrilov	Sergey	NRC KI - PNPI
12.	Golosovsky	lgor	NRC KI - PNPI
13.	Grigoriev	Sergey	NRC KI - PNPI
14.	Gubanova	NadezhdaArtem	NRC KI - PNPI
15.	Gubkin	Andrey	IMP UB RAS
16.	Gukasov	Arsen	LLB
17.	Hutanu	Vladimir	Institute of Crystallography, Aachen University and JCNS at MLZ
18.	Ivankina	Tatiana	FLNP JINR
19.	Karpov	Ivan	NRC "Kurchatov Institute"
20.	Kibalin	lurii	LLB
21.	Kireenko	Yuri	NRC KI - PNPI
22.	Kopitsa	Gennady	NRC KI - PNPI
23.	Korshunov	Artem	NRC KI - PNPI, ESRF
24.	Kozlenko	Denis	FLNP JINR
25.	Kurbakov	Alexander	NRC KI - PNPI
26.	Likholetova	Elena	NRC KI - PNPI
27.	Matveev	Vasily	NRC KI - PNPI
28.	Mekawy	Abdelrahman Mohamed	Alexandria university
29.	Mukhametuly	Bagdaulet	FLNP JINR
30.	Murashev	Michael	NRC "Kurchatov Institute"
31.	Nigmatullina	Evgeniya	NRC KI - PNPI
32.	Pavlov	Konstantin	NRC KI - PNPI
33.	Pavlova	Anastasia	NRC KI - PNPI
34.	Pirogov	Alexander	IMP UB RAS



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Nº	Surname	Name	Organization
35.	Plekhanov	Maxim	IMP UB RAS
36.	Poliakov	Vladimir	NRC KI - PNPI
37.	Pomyakushin	Vladimir	Laboratory for Neutron Scattering and Imaging LNS, Paul Scherrer Institute PSI, Switzerland
38.	Pshenichnaya	Angelina	NRC KI - PNPI
39.	Pshenichny	Kirill	NRC KI - PNPI
40.	Senishin	Anatoly	Heinz Maier-Leibnitz Zentrum, Technische Universität München
41.	Sikolenko	Vadim	FLNP JINR
42.	Skanchenko	Daria	NRC KI - PNPI
43.	Sokolov	Alexei	NRC KI - PNPI
44.	Sumnikov	Sergey	FLNP JINR
45.	Susloparova	Anna	NRC KI - PNPI
46.	Syomkin	Michael	IMP UB RAS
47.	Syromyatnikov	Vladislav	NRC KI - PNPI
48.	Ulyanov	Vladimir	NRC KI - PNPI
49.	Usmanov	Oleg	NRC KI - PNPI
50.	Vasiliev	Andrey	NRC KI - PNPI
51.	Vaulin	Artem	IMP UB RAS
52.	Yashina	Ekaterina	NRC KI - PNPI
53.	Yeast	Kirill	NRC KI - PNPI
54.	Yuzvyuk	Maria	NRC KI - PNPI
55.	Zobkalo	lgor	NRC KI - PNPI

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Workshop Organisers

Program Committee

Chairman: A.I. Kurbakov, Doctor of Physical and Mathematical Sciences (NRC "Kurchatov Institute" -PNPI, Gatchina)

Members of the Program Committee: A.M. Balagurov, Doctor of Physical and Mathematical Sciences (FLNP JINR, Dubna) V.T. Um, Doctor of Physical and Mathematical Sciences (SRC KI, Moscow) I.V. Golosovsky, Doctor of Physical and Mathematical Sciences (NRC "Kurchatov Institute" -PNPI, Gatchina) I.A. Zobkalo, Ph.D. (NRC "Kurchatov Institute" - PNPI, Gatchina) Yu.P. Chernenkov, Ph.D. (NRC "Kurchatov Institute" - PNPI, Gatchina)

Organizing Committee

Chairperson: Gubanova Nadezhda (NRC "Kurchatov Institute" - PNPI, Gatchina)

Members of the organizing committee:

Dyachkov Maxim: technical support (NRC "Kurchatov Institute" - PNPI, Gatchina) Skanchenko Daria: technical support (NRC "Kurchatov Institute" - PNPI, Gatchina) Pshenichny Kirill: technical support (NRC "Kurchatov Institute" - PNPI, Gatchina) Usmanov Oleg: technical support (NRC "Kurchatov Institute" - PNPI, Gatchina) Kuga Natalia: financial issues (NRC "Kurchatov Institute" - PNPI, Gatchina) Lukin Alexander: technical support (NRC "Kurchatov Institute" - PNPI, Gatchina) Travina Olga: economic issues (NRC "Kurchatov Institute" - PNPI, Gatchina)

«GoodFoodOrlik» Ltd company organized lunches and coffee breaks.

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