EURIZON final Meeting 2024

WP3: Neutrons

FZJ, CEA-LLB, ESS, HEREON, ILL, MTA-EK, TUM, UCA, UNIMIB

18. January 2024

Stefan Mattauch, Forschungszentrum Jülich GmbH

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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History:

CREMLINplus WP3: „PIK“

- **ST 3.1**: High-brilliance cold neutron source; **A. Ioffe**
  FZJ, NRC KI-PNPI, MTA EK, ESS, MAX-IV
- **ST 3.2**: Bi-spectral neutron extraction system; **A. Ioffe**
  FZJ, NRC KI-PNPI, MTA EK
- **ST 3.3**: Development of advanced Very Cold Neutron Source; **O. Zimmer/E. Lychagin**
  ILL, NRC KI-PNPI, JINR, PTI, UCA, UNIMIB, ESS
- **ST 3.4**: General blueprint for the instrumentation at PIK; **Y. Kireenko,** NRC KI-PNPI, FZJ, TUM, HZG, CEA- LLB
- **ST 3.5**: Prototype of advanced polarized neutron diffractometer DiPol for PIK reactor; **A. Goukassov**
  CEA-LLB, NRC KI-PNP
- **ST 3.6**: Establ. the scientific infrastructure (SAC, instrum. Subc.) at the ICNR Task; **S. Grigoriev** NRC KI-PNPI, FZJ
- **ST 3.7**: Instrum. specific education and training programs for engineers and scientists; **S. Grigoriev** NRC KI-PNPI, FZJ, SPSU, HZG, TUM, CEA-LLB, ILL, MTA EK, ESS
- **ST 3.8**: User System; **J. Neuhaus** TUM, NRC KI-PNPI, JINR, ILL
- **ST 3.9:** Coordination between all tasks; **S. Grigoriev**
  NRC KI-PNPI, FZJ, JINR, PTI, SPSU, HZG, TUM, CEA-LLB, ILL, UCA, MTA EK, UNIMIB, ESS

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H2020 Programme

BENEFICIARY TERMINATION REPORT

1.2 EXPLANATION OF THE WORK CARRIED PER WP

WORK PACKAGE 3

Task 3.1: High-brilliance cold neutron source

Optimization studies were carried out within the framework of creating a project for a source of cold neutrons on the HEC-2 channel of the PIK reactor complex, namely, the problems of choosing the optimal location of the channel for placing a parahydrogen source of cold neutrons were solved; selection of materials for the working chamber of the cold neutron source and helium supply tubes; estimates of the energy release for structural elements of the source of cold neutrons.

When developing a source of cold neutrons based on parahydrogen, 4 designs for its implementation were considered. Aluminum was chosen as the wall material. Wall thickness - 8 mm. It has been found that the brightness of the source in a channel 8.2 cm in diameter practically coincides with the brightness of the source in a channel with a radius of 16 cm, but close to the center. The smaller the channel radius, the greater the brightness of the source.

In the framework of this work, the energy release was also calculated for two options for placing a parahydrogen source of cold neutrons in a channel with an inner radius of 8.2 cm. compared to aluminum tubes only.

Task 3.2: Bi-spectral neutron extraction system

A description of the primary design of the bispectral extraction system developed at the HEC-2 of the PIK reactor is made.

Taking into account the available space and the geometry of the neutron guide hall, a solution was proposed for the extraction of neutron beams. The reflectometer has an inclined geometry (0.75°). The neutron guide has a cross section of 6 x 3 cm2 and is placed in the center of one of the cold moderators. The idea of such a design has 2 tasks: avoiding direct visibility and transporting neutrons to the sample with a natural angle. Spin-echo and small-angle neutron scattering have square beam output sections with dimensions of 3 x 3 cm2 and are oriented on different sides relative to the surface of the parahydrogen source of cold neutrons. The three-axis spectrometer, diffractometer, and time-of-flight spectrometer are arranged in such a way that their cross sections are oriented to the surface of both the thermal and cold moderators. The neutron guides have the following sections: 6 x 11 cm2 (TAS), 6 x 9.5 cm2 (BioDiff) and 6 x 9 cm2 (TAS). The right, lower and upper parts of the surface of the thermal moderator are available for placement of leads for instruments implemented within the framework of the PIK Instrument Base project.

Task 3.3: Development of advanced Very Cold Neutron Source

Model calculations of the yield of very cold neutrons have been carried out.

Task 3.4: General blueprint for the instrumentation at PIK

A preliminary design of a neutron guide system based on a parahydrogen neutron source has been developed, namely, the problems of forming requirements for experimental facilities have been solved; simulation of a neutron guide system using the McStas program to determine the optimal characteristics of neutron optics; formulating recommendations for building a neutron-water system at HEC-2.

Based on the results of Monte Carlo calculations and an assessment of the geometric position of the neutron-water hall and its dimensions, a preliminary plan of the instruments located on the HEC-2 and HEC-3 channels was developed.

Task 3.5: Prototype of advanced polarized neutron diffractometer for PIK reactor

Calculations have been made to optimize the position and working area of the monochromator of the DIPOL diffractometer, and the necessary design studies have been carried out for the placement of monochromators and other components of neighboring installations.

Works have been carried out to coordinate the location of experimental setups on the HEC-8 and HEC-9 channels: DIPOL, D3 and DC1 diffractometers.

Numerical simulation of the c-bender-based polarizer for the DIPOL diffractometer has been performed.

A new numerical simulation of the neutron optical path of the DIPOL diffractometer in the McStas environment has been performed.

A set of design documentation has been completed and a DIPOL diffractometer sample unit has been created with the possibility of installing three pairs of leading field coils on it, which ensures the implementation of the XYZ-polarization analysis method.

Task 3.6: Establishing the scientific advisory committees at PIK

The meetings of the specialized subcommittees on spectroscopy, small-angle scattering and reflectometry were held.

November 26, 2021 Second meeting of the subcommittee on spectroscopy. Chairman K. Schmalzl (Julich Research Center).

November 29, 2021 Second meeting of the Subcommittee on Small Angle Scattering and Reflectometry. Chairman A. Ioffe (Julich Research Center).

Task 3.7: Instrument-specific education and training programmes for engineers and scientists

From November 8 to 12, 2021, NRC "Kurchatov Institute" - PNPI, together with St. Petersburg State University, organized and conducted the IV School "Neutron studies of condensed matter" NIKONS-2021. For the first time, the school was held simultaneously and in person at two sites - at the Department of nuclear physics research methods of St. Petersburg State University (Peterhof) and at the NRC “Kurchatov Institute” - PNPI (Gatchina). All lectures and workshops were broadcast online and made available to a wide audience on the Internet.

On December 16 - 17, 2021, on the basis of the National Research Center "Kurchatov Institute" - PNPI, the X School on Polarized Neutron Physics "FPN-2021" was held. The school was held in two formats: full-time (in the conference hall of the 7th building of the PNPI) and online. The FPN-2021 school is designed to intensify the activities of the Russian scientific community in the field of research using polarized neutrons and attract young people to research activities. This year, more than 50 people took part in the work of the school. The NIKONS school has been held for the fourth year already and is designed to provide a wide range of young scientists with familiarity with the methods of neutron scattering in physics and condensed matter research through the prism of numerical modelling of neutron installations using the McStas package. The audience of the school consists of graduate students of natural sciences, graduate students and young specialists who are already conducting experimental research in the field of condensed matter, but are not yet familiar with the methods of neutron scattering. SPbU invited colleagues from the Institute of Metals Physics of the Ural Branch of the Russian Academy of Sciences (Yekaterinburg) to the NIKONS-2021 School to improve the skills and expand the horizons of young employees involved in the development of the concept and design of neutron stations for the compact pulsed neutron source DARIA. In total, 58 participants from 7 organizations registered for the School: NRC “Kurchatov Institute” - PNPI (Gatchina), St. Petersburg State University (St. Petersburg), UrFU (Yekaterinburg), IPM UB RAS (Yekaterinburg), IRM (Yekaterinburg), JINR (Dubna), IKBFU Kant (Kaliningrad).

Task 3.8: User System

The concept of terms of reference for the creation of a beam time distribution system at the International Center for Neutron Research at the PIK reactor was proposed.

Meetings were held with the participation of members of the subcommittee, scientists from the National Research Center "Kurchatov Institute" - PNPI, the Technical University of Munich (TUM), the Joint Institute for Nuclear Research (JINR) and the Leon-Brillouin Laboratory (ILL), the results of which are reflected in the reports, where the structure was provided International Center for Neutron Research.

Task 3.9: Support strategic coordination of PIK

To ensure the full-fledged work of the team of project executors in the context of the novel coronavirus infection pandemic, meetings were held on a regular basis in the format of videoconferences on problem areas.

The WP3 has designed to fulfill the 9 Tasks which are in some parts overlapped and can benefit from the coordination of actions held within them. We coordinate on the regular basis the following actions:

- actions of the community of the Task 3.5 with those of the SC on Neutron diffraction;
- actions of the community of Task 3.7 (specific education) with those of the Task 3.6 (SAC + SC);
- actions of the communities of Task 3.1, Task 3.2 and Task 3.3 with those of the SC on the Neutron optics and moderators.

The Transition:

CREMLINplus WP3: „PIK“

The objective of this work package is to strengthen the scientific and technical cooperation between PIK and European neutron research infrastructures in mutual interests of European and Russian researches. The WP3 will achieve its objective by undertaking research and activities in the following key areas:

- *Joint development of advanced cold neutron sources;*
- *Joint development of the instrumentation concept for reactor PIK;*
- *Establish international bodies at PIK;*
- *Development of the neutron user-based education platform and an user system;*
- *Support strategic coordination of PIK in the whole*

EURIZON WP3: „Neutrons“

- *To strengthen scientific and technical cooperation between European neutron research infrastructures in mutual interests of European researches*
- *Joint development of advanced cold neutron sources and bi-spectral extraction for European neutron sources*
- *Joint development of advanced very cold neutron sources for European neutron sources*
- *Development of advanced polarized neutron diffractometer, paving the path from CEA-LLB via JCNS@MLZ to the ESS*
- *A white paper explaining the tasks of user offices to manage international access to European Research Infrastructures will be developed*

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The Transition:

CREMLINplus WP3: „PIK“

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EURIZON WP3: „Neutrons“

- **ST 3.1**: Development of advanced High-brilliance cold neutron source in combination with Bi-spectral extraction system; **A. Ioffe -** FZJ, MTA EK, ESS, MAX IV
- **ST 3.3**: Development of advanced Very Cold Neutron Source (VCN); **O. Zimmer -** ILL, UCA, Uni Milano-Bicocca, ESS
- **ST 3.5**: Prototype of advanced polarized neutron diffractometer; **A. Goukassov -** CEA/LLB, ESS, ILL, FZJ
- ~~ST 3.8: User System;~~ **J. Neuhaus -** TUM

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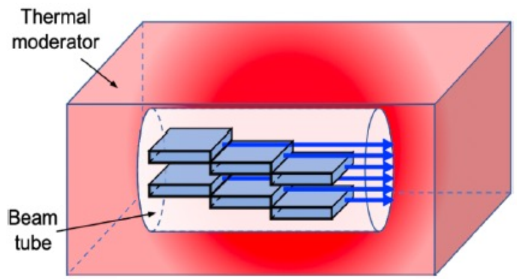
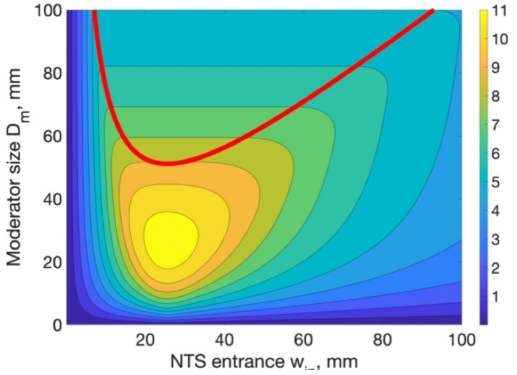
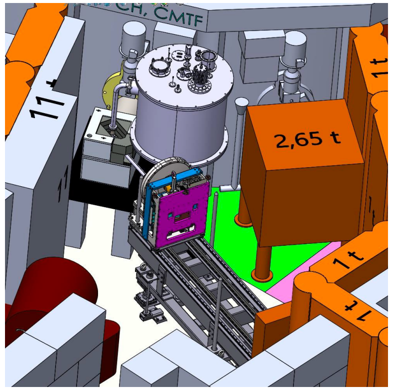
Task 1: Development of advanced high-brilliance cold neutron source in combination with Bi-spectral extraction system (FZJ, MTA EK, ESS, MAX IV, HEREON)



1. Design of high-brilliance and high-flux cold neutron source utilizing high-aspect ratio rectangular para-hydrogen moderators. Prototype.

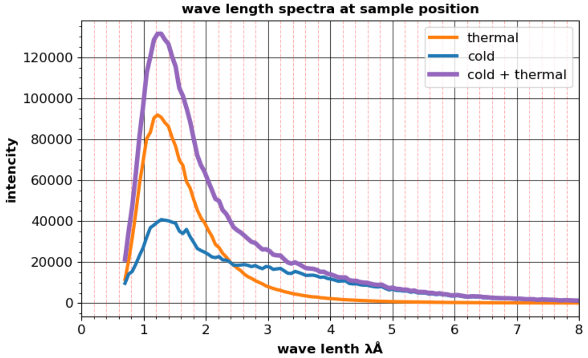


2. General framework based on phase space considerations allowing to estimate the required moderator size based on instrument parameters, such as sample size, angular resolution and collimation distance.



3. Cold Moderator Test Facility (CMTF) at the Budapest Research Reactor is designed, constructed and commissioned. First experiments are carried out.

4. Bi-spectral extraction system fed by combination of cold neutron para-hydrogen moderator and large thermal moderator. Modelling of its expected performance with BEER diffractometer (Hereon).



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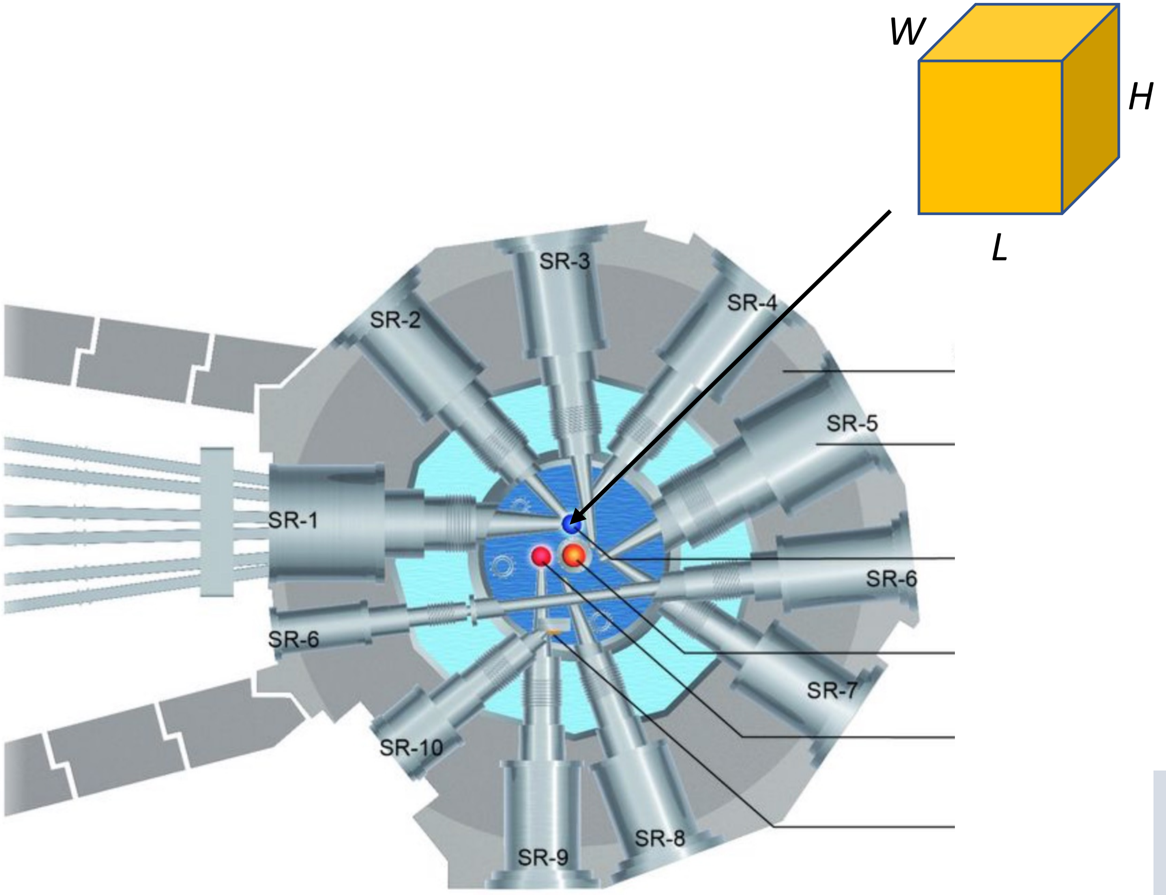
A high neutron flux at the sample of neutron scattering instruments is key for their performance.

Cold neutron source
(hydrogen-reach material)



Given by reactor/accelerator power

Thermal neutrons

Cold neutron source

Neutron instruments

Efficiency of the thermal-to-cold moderation

Gain in efficiency of such conversion is just
the gain in intensity at the sample of neutron instruments.

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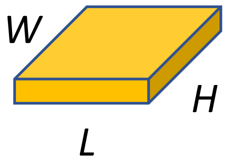
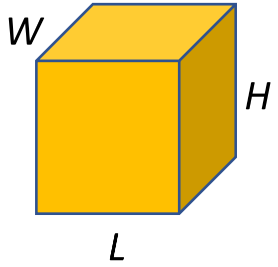
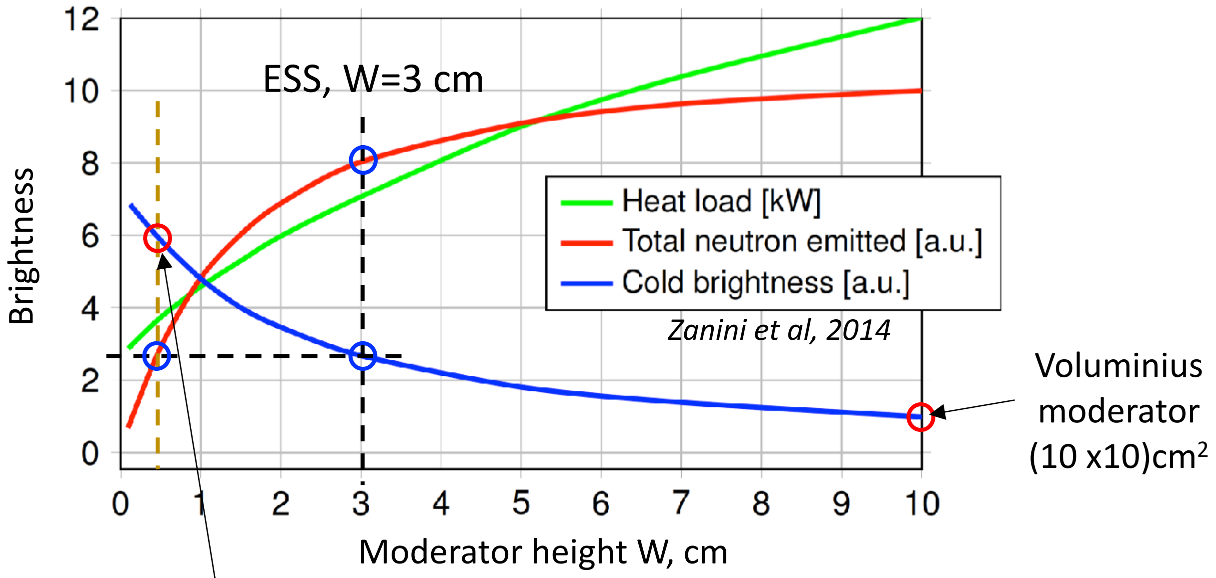
Flat moderators vs. voluminous moderators





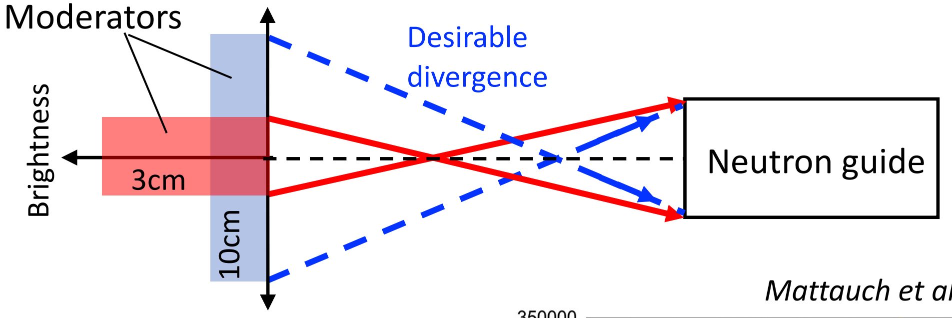
1. Gain in brightness by costs of intensity losses:



W=0.5 cm

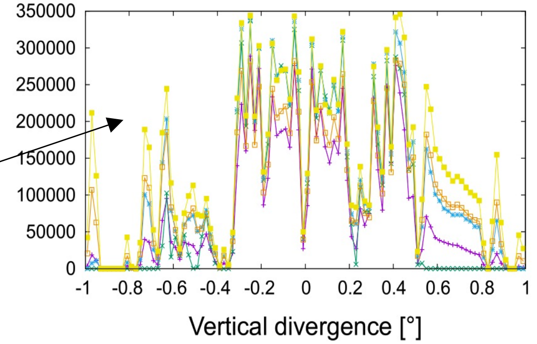
(+) another gain in brightness,
(-) 5x intensity drop
(-) even worth divergence profile

2. Under-illumination of neutron guide by small moderator



Mattauch et al, 2017

“Gothic” structure of beam divergence



=> Partial solution: multichannel guides (losses in intensity)

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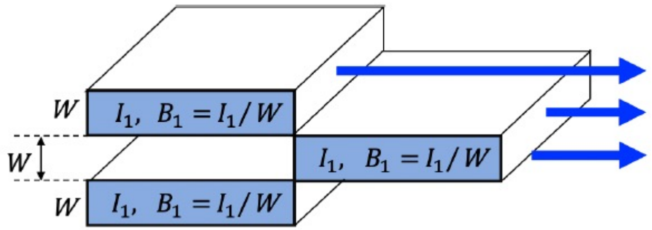
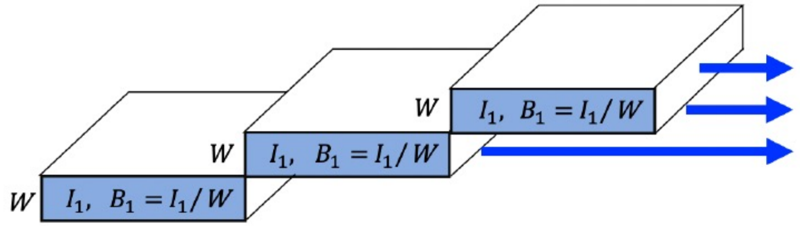
Staircase arrangement of rectangular moderators



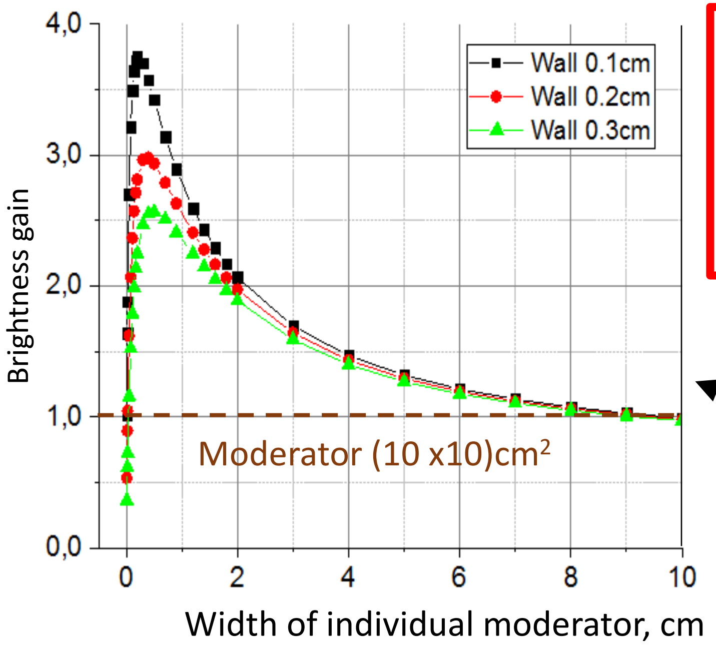


A.Ioffe, P.Konik, K.Batkov

http://arxiv.org/abs/2311.15389

Brightness gain of individual moderator

(relative 10cm moderator)



Such moderator assemblies:

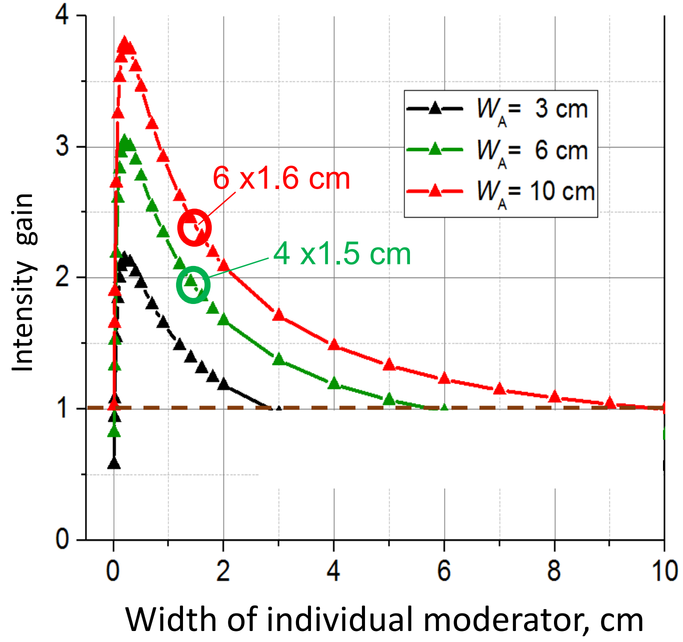
a significant gain

both in brightness and in intensity

relative to commonly used voluminous moderators

Intensity gain of moderator assembly

(relative 10cm moderator)



Significant brightness and intensity gains for assemblies of 4 and 6 individual moderators

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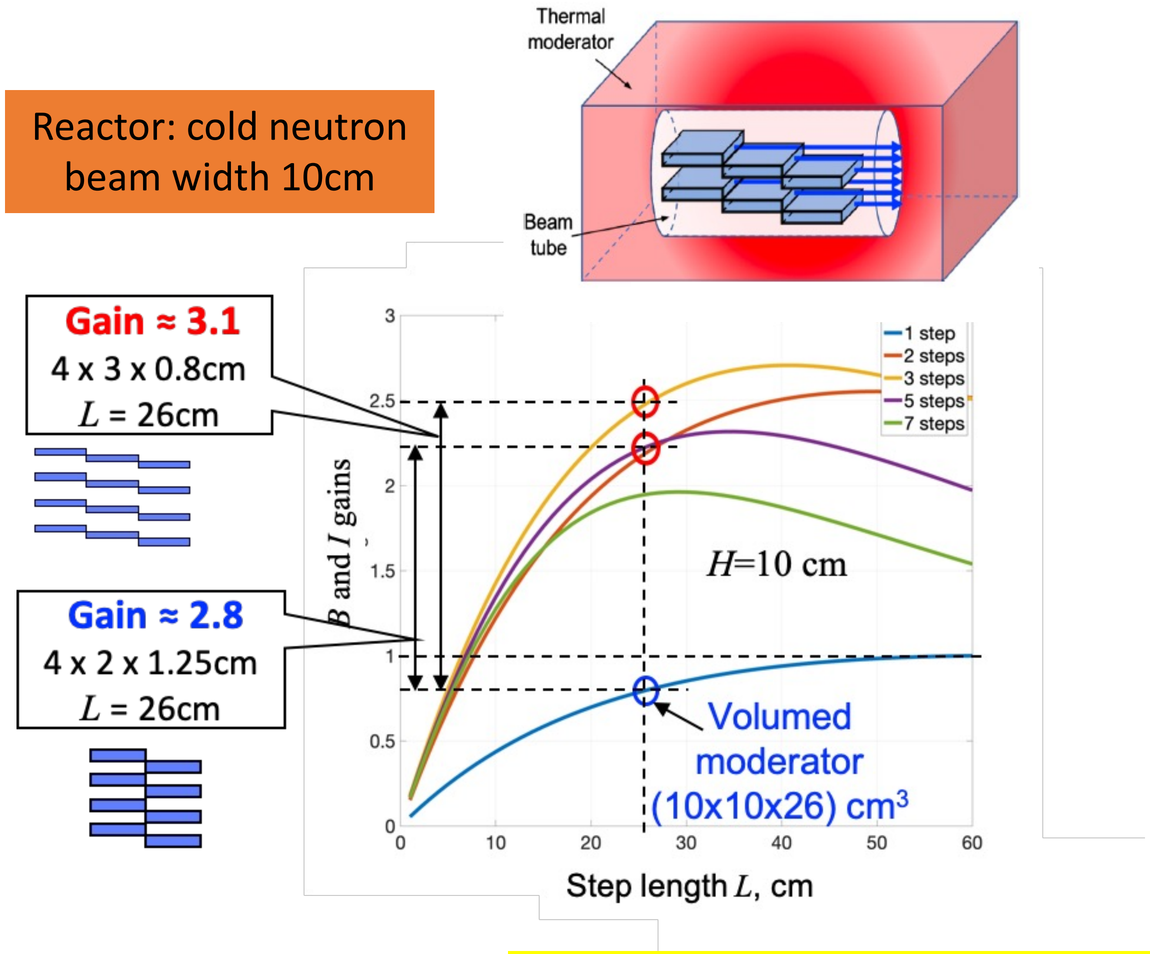
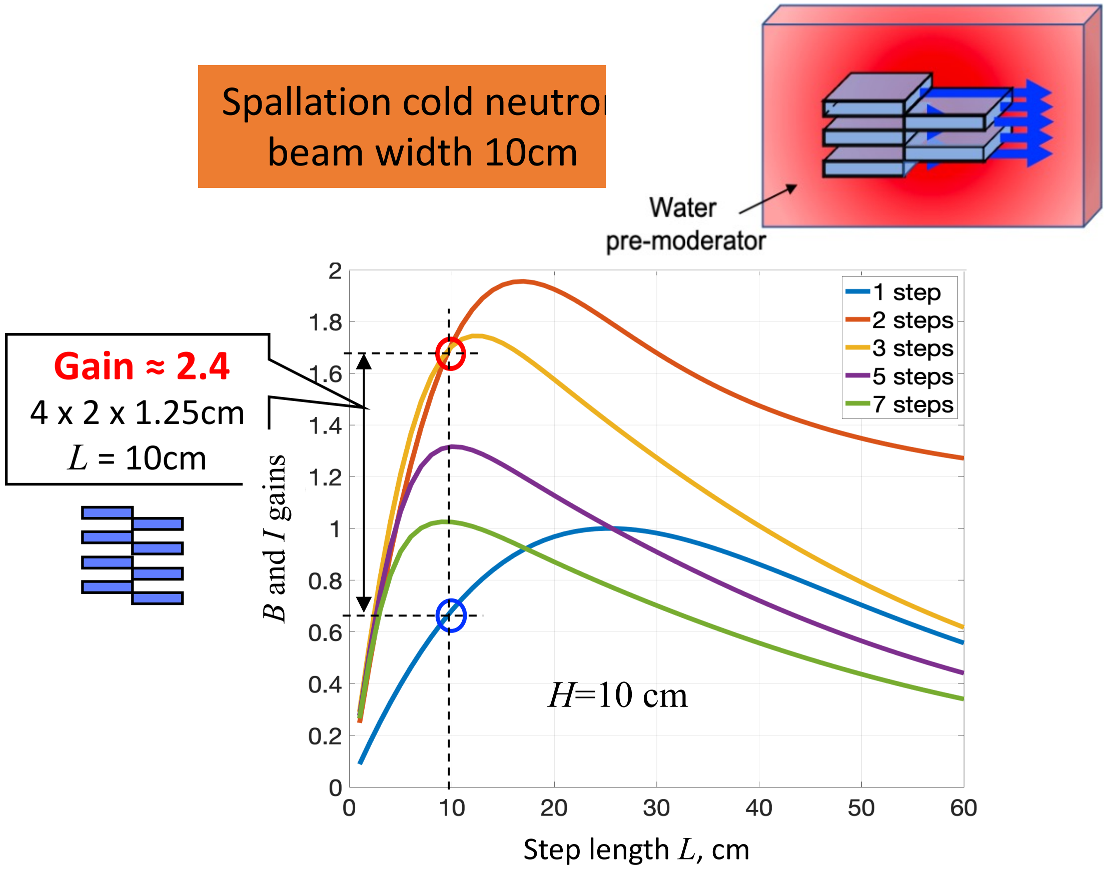
A novel cold neutron source with higher intensity and brightness: up to 2.5 -3 times more than any para-hydrogen-based cold neutron source with equal cold neutron beam cross-section made of a single moderator (flat or voluminous).





Great interest from new projects (HBS, CSNS-II, RANS@RIKEN)

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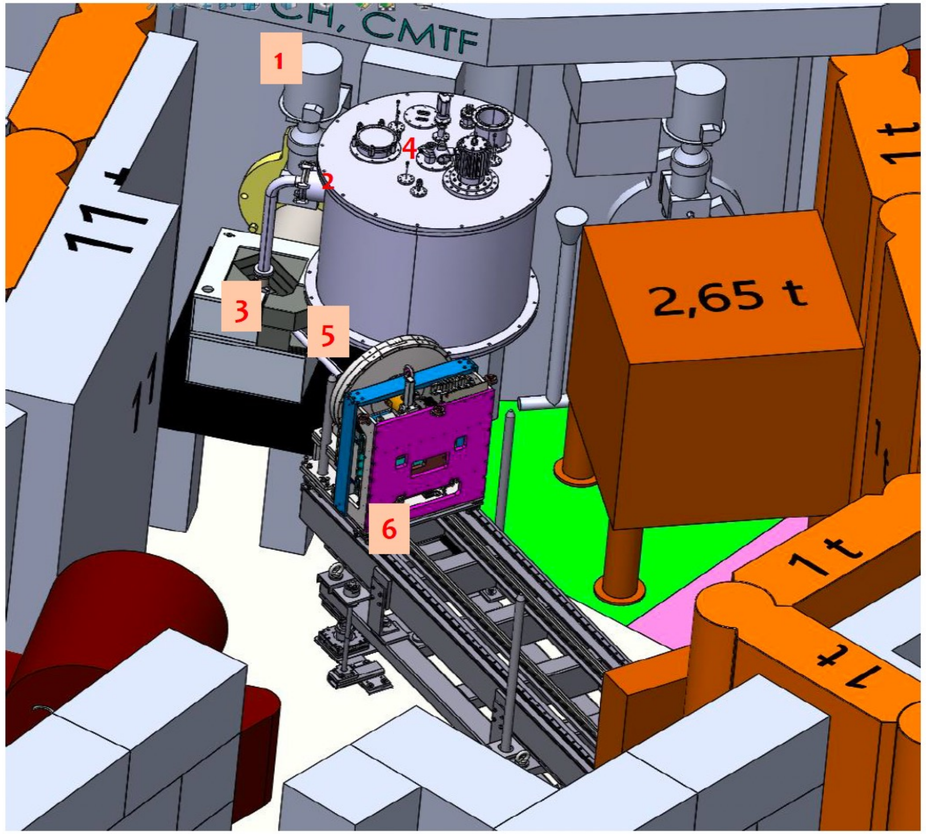
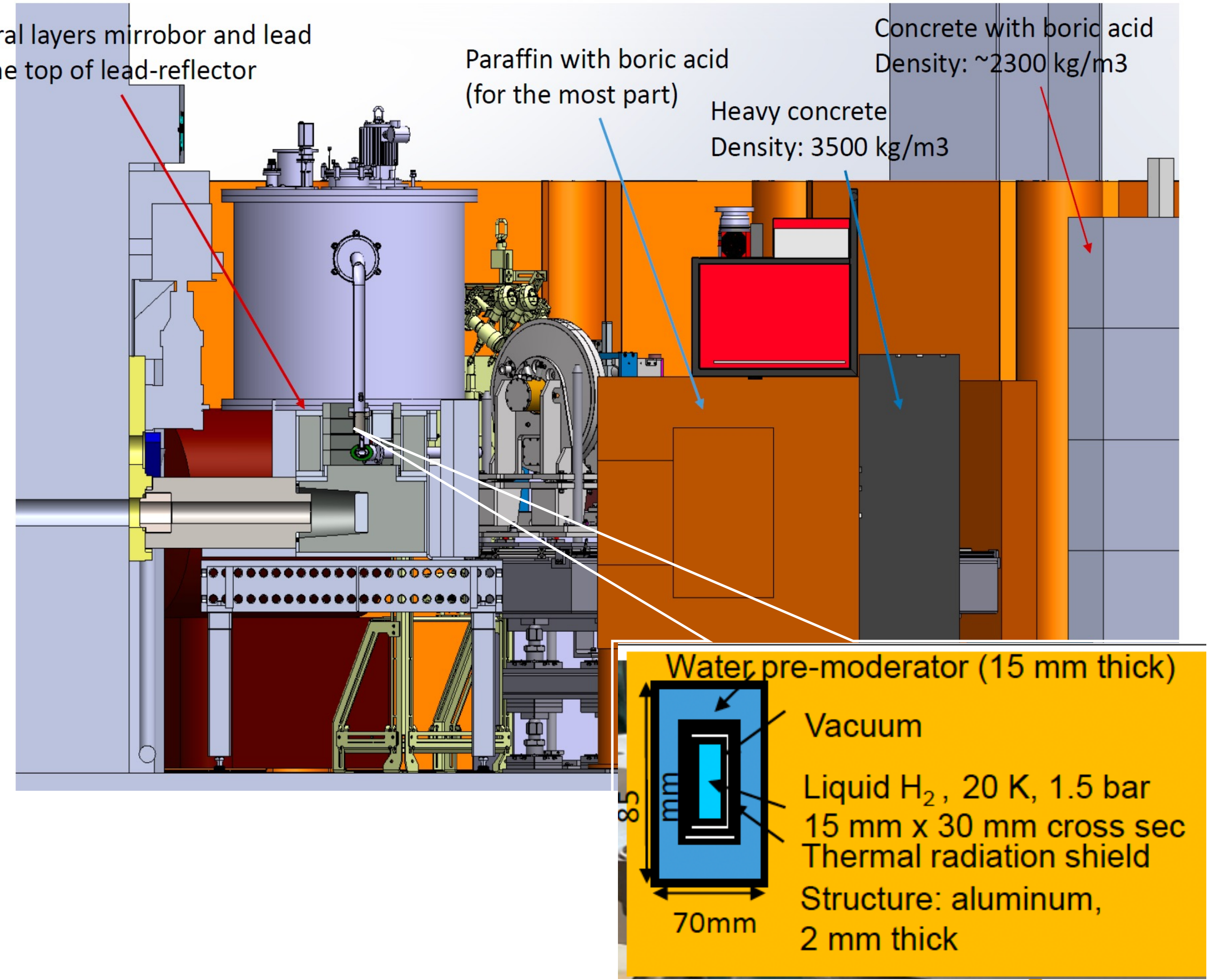
Cold Moderator Test Facility (CMTF) at the Budapest Research Reactor

Centre for Energy Research

CMTF construction

BNC Budapest Neutron Centre





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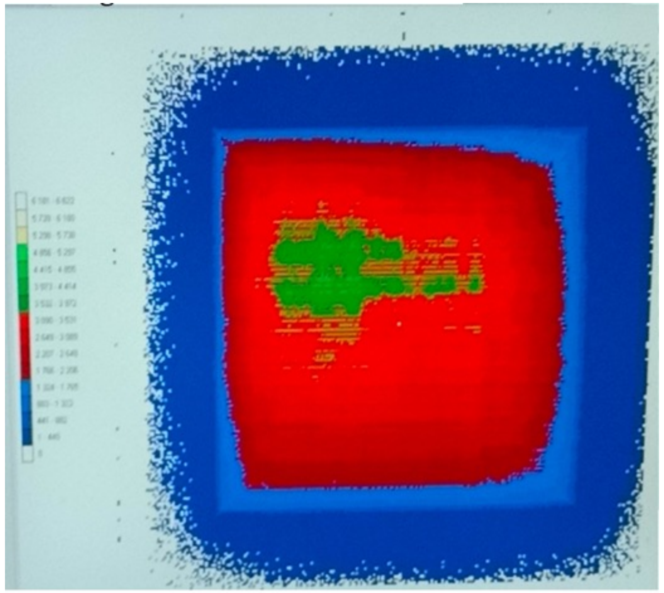
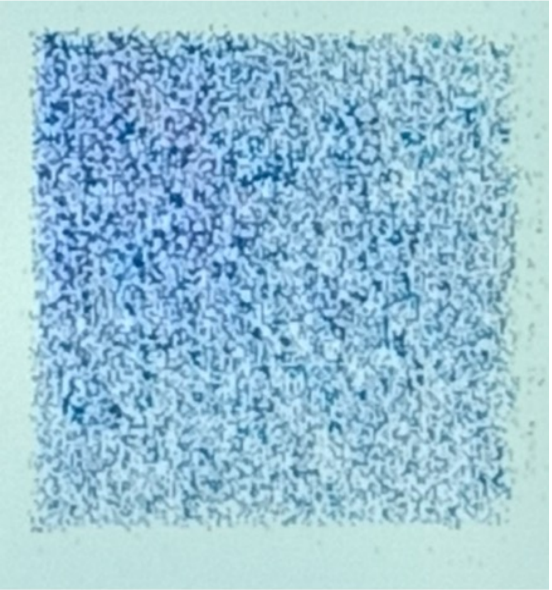
Cold Moderator Test Facility (CMTF) at the Budapest Research Reactor

2D image on the He-3 detector from the moderator (empty H-cell, premoderator vessel filled with water)



Background at closed beam



Cryostat with moderator chamber

Planned experiment (December 2023) didn’t take place because of the unexpected reactor shutdown: lack of reactor personal (COVID)

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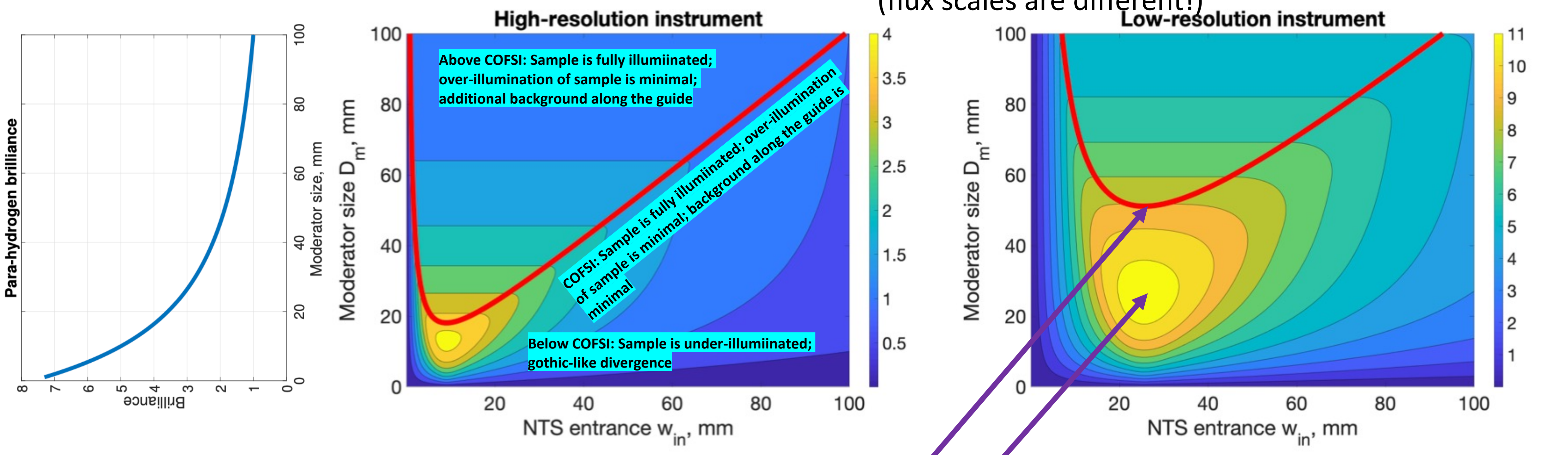
One moderator serving two instruments

(flux scales are different!)



	HR instrument	LR instrument
Optimally and fully illuminated sample	$D_{opt} = 18$ mm $\Phi_s = 3.8$	$D_{opt} = 51$ mm $\Phi_s = 9$
Under-illuminated sample; maximal sample flux	$D_{opt} = 13$ mm $\Phi_s = 4.1$	$D_{opt} = 25$ mm $\Phi_s = 11.5$

<u>Best solution is close to D_{opt}=18 mm:</u>

- HR instrument reaches best performance
- LR instrument gets very high (not maximum) flux
- LR instrument sample under-illumination does not compromise its operation

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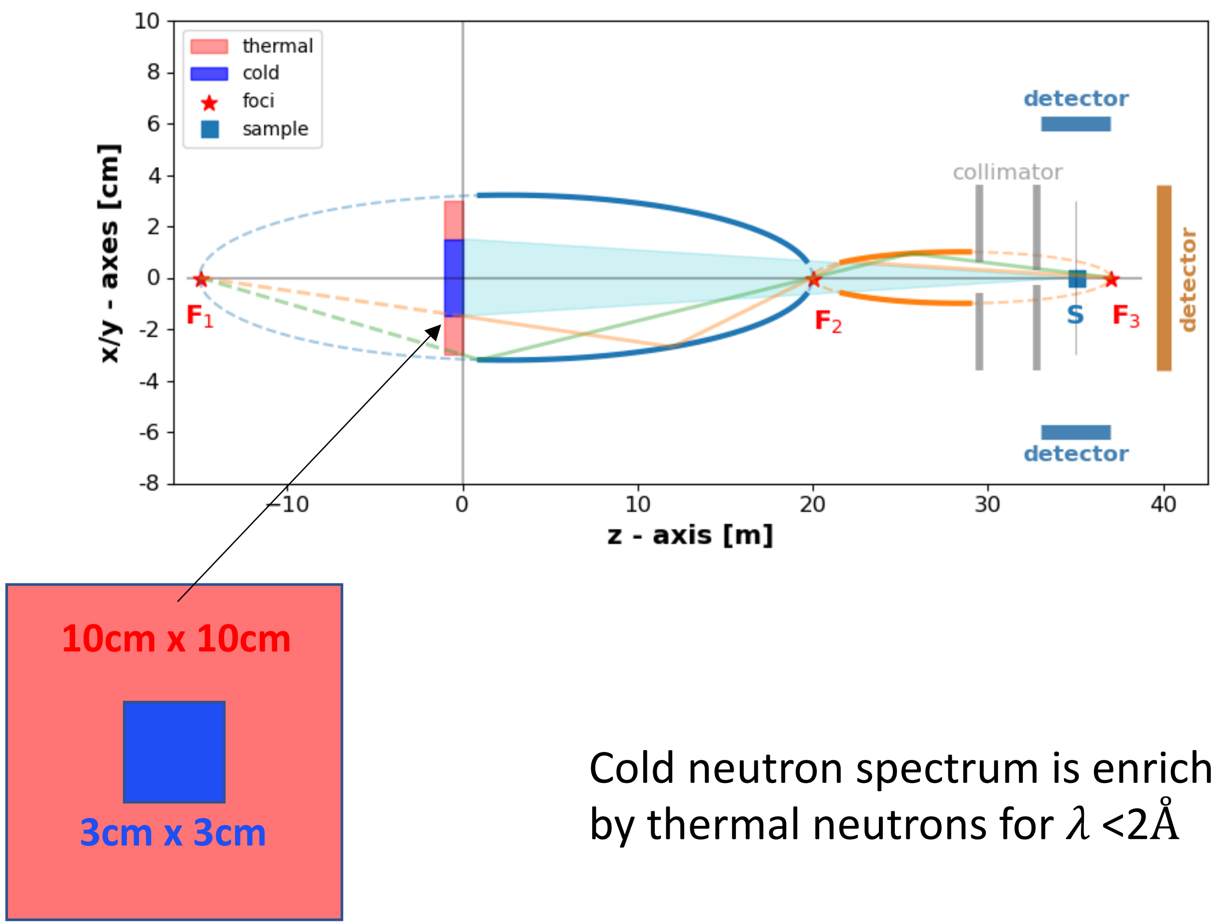
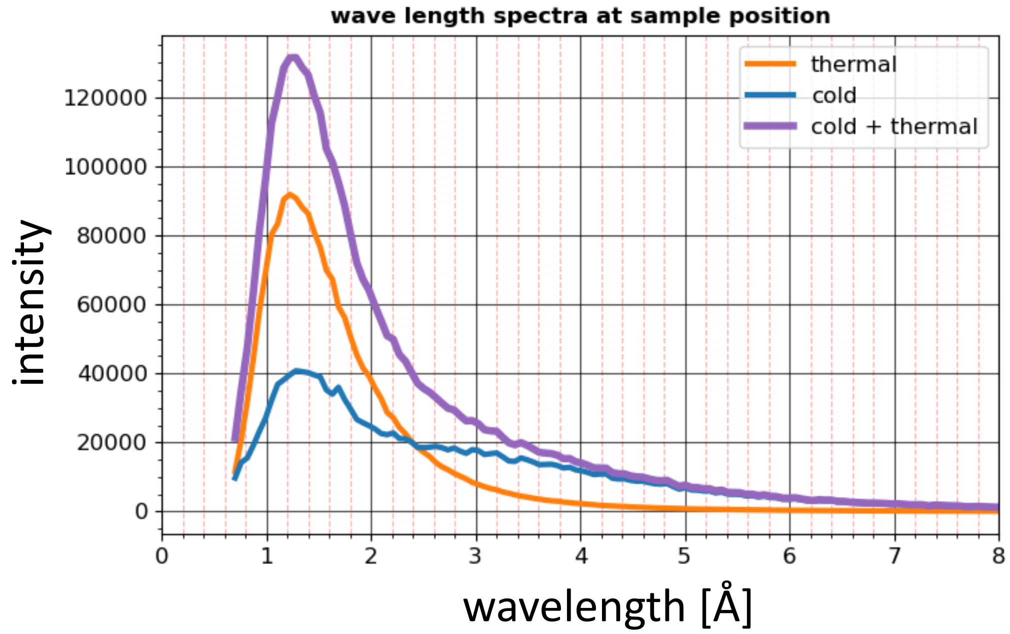
Bi-spectral extraction for diffraction instrument



Modelling of its expected performance with BEER like diffractometer (Hereon).

Cold neutron spectrum is enriched by thermal neutrons for λ <2Å



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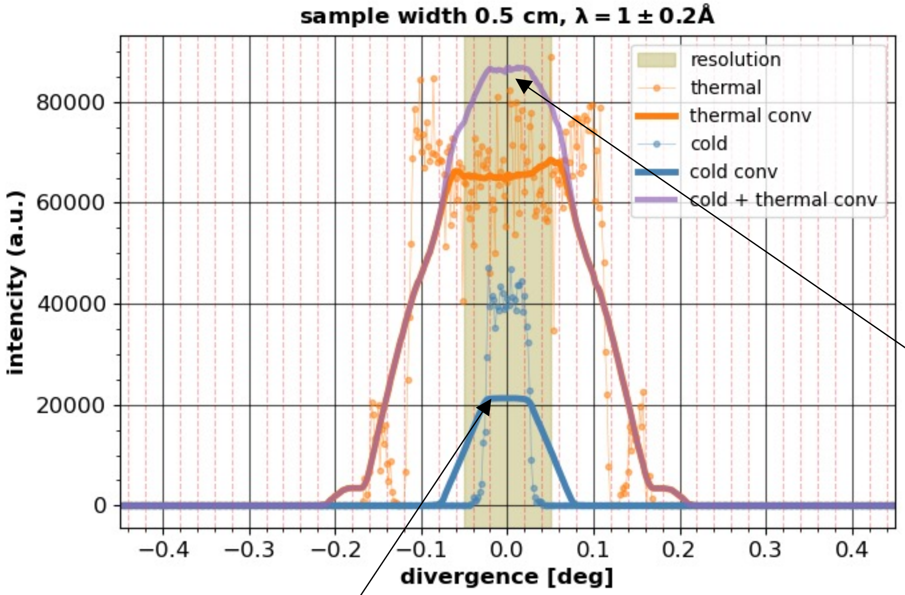
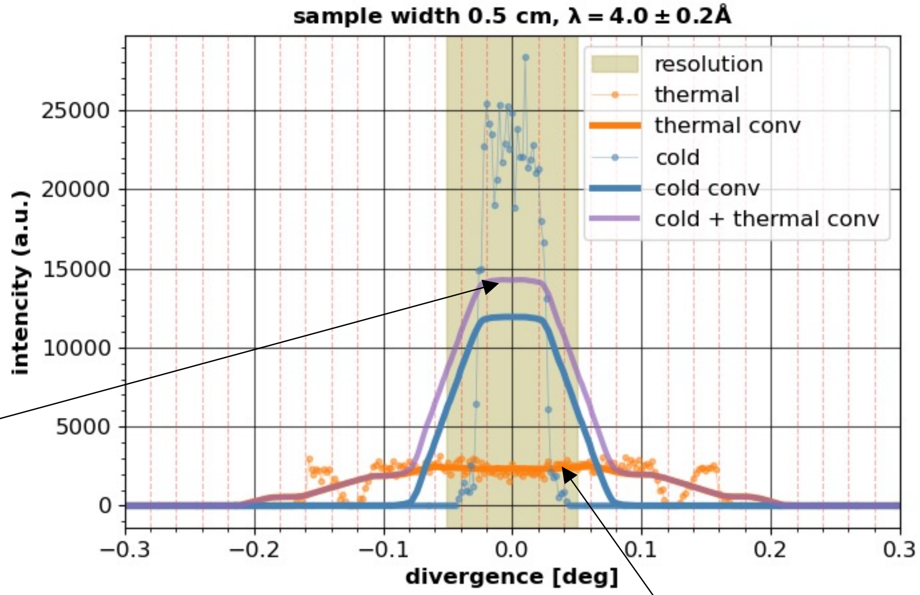
Bi-spectral extraction for diffraction instrument

Beam on the sample convoluted with resolution function (FWHM=0.2°)

Thermal neutrons: λ = 1 Å



Cold neutrons: λ = 4 Å



With bi-spectral extraction

Only cold neutron source

Only thermal neutron source

Gain in intensity by factors

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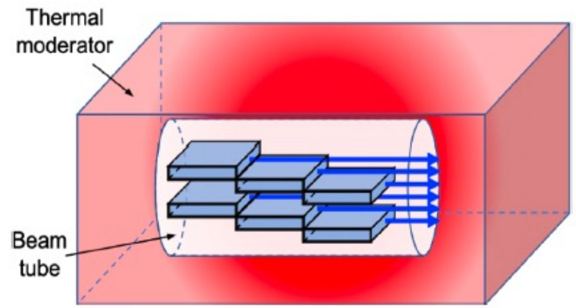
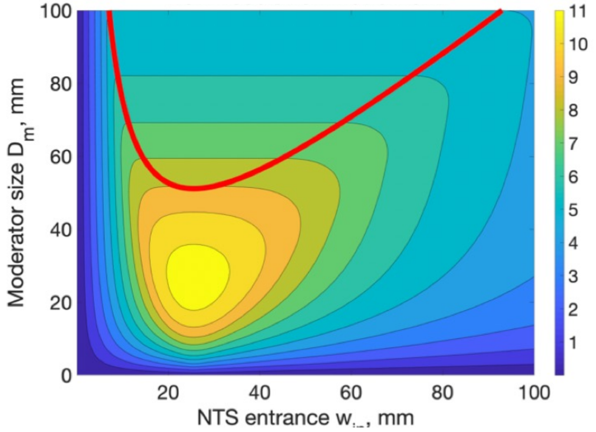
WP3: Task 1



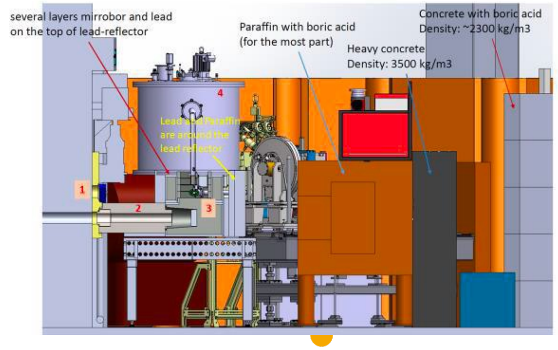
Publications:

1. Petr Konik, Alexander Ioffe. ”**A new method to find out the optimal neutron moderator size based on neutron scattering instrument parameters”,** Nuclear Instruments and Methods in Physics Research Section A, Volume 1056, 2023,B168643, https://doi.org/10.1016/j.nima.2023.168643.11.



2. Alexander Ioffe, Petr Konik, Konstantin Batkov. “**High-brightness and high-flux cold neutron source utilizing high-aspect ratio rectangular para-hydrogen moderators“,** November 2023, DOI: [10.48550/arXiv.2311.15389](https://doi.org/10.48550/arXiv.2311.15389)

Submitted to Nuclear Instruments and Methods in Physics Research Section A



Presented at ICNS-2022 (Argentine), ECNS-2023 (Germany) and ICANS-2023 (China)

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Task 3.3: Development of advanced Very Cold Neutron Source (VCN); O. Zimmer - ILL, UCA, Uni Milano-Bicocca, ESS

Development of reflectors based on fluorinated detonation nanodiamonds (F-DNDs) for very cold neutrons (VCNs) and cold neutrons (CNs), **Valery Nesvizhevsky**

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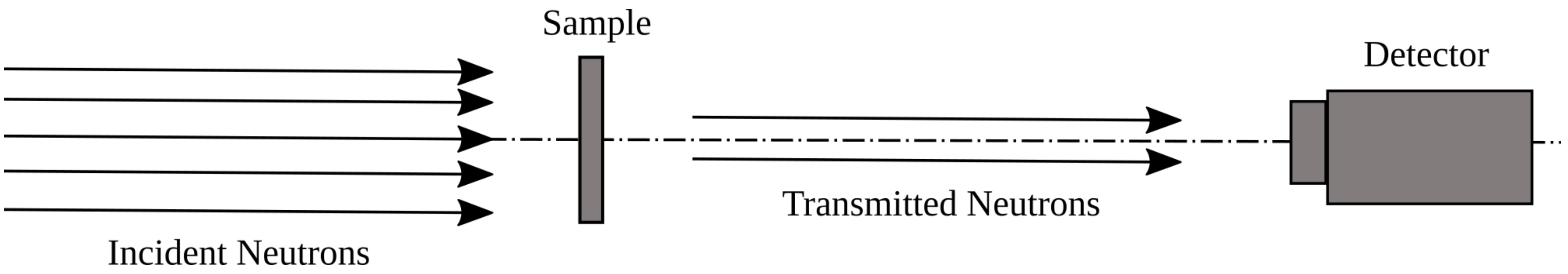
Neutron transmission Experiments

- Determination of the total cross section throughout the CN & VCN range
- Transmission experiments at **ILL** (PF1B, PF2|VCN) & **PSI** (BOA)

$$T = \frac{Z_{sample}}{Z_{empty}} = \exp\left(N_V\ d\ \sigma_{tot}\right), \quad \sigma_{tot} = \frac{1}{N_V d} \cdot \ln\left(\frac{1}{T}\right)$$



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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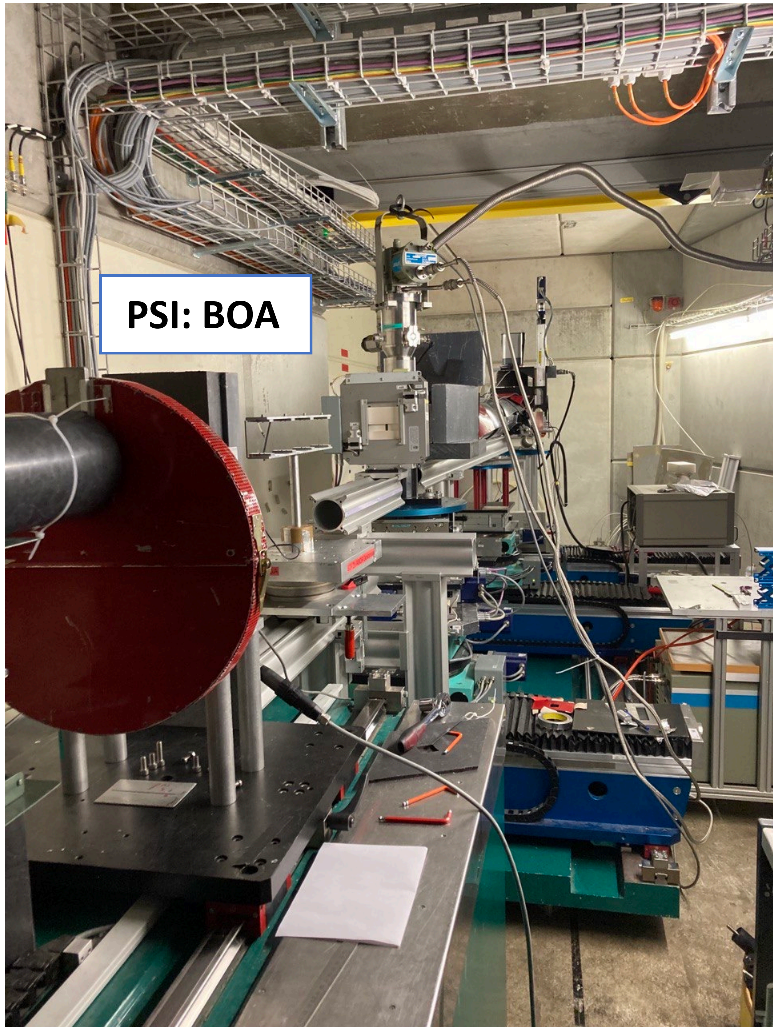
Setups at PF2 | VCN & BOA



- PF2/VCN at ILL: 20 Å < λ < 80 Å
- BOA at PSI: 3 Å < λ < 23 Å
- Sample length in beam: 4 & 2 cm
- Measurements at 5 K / 20 K

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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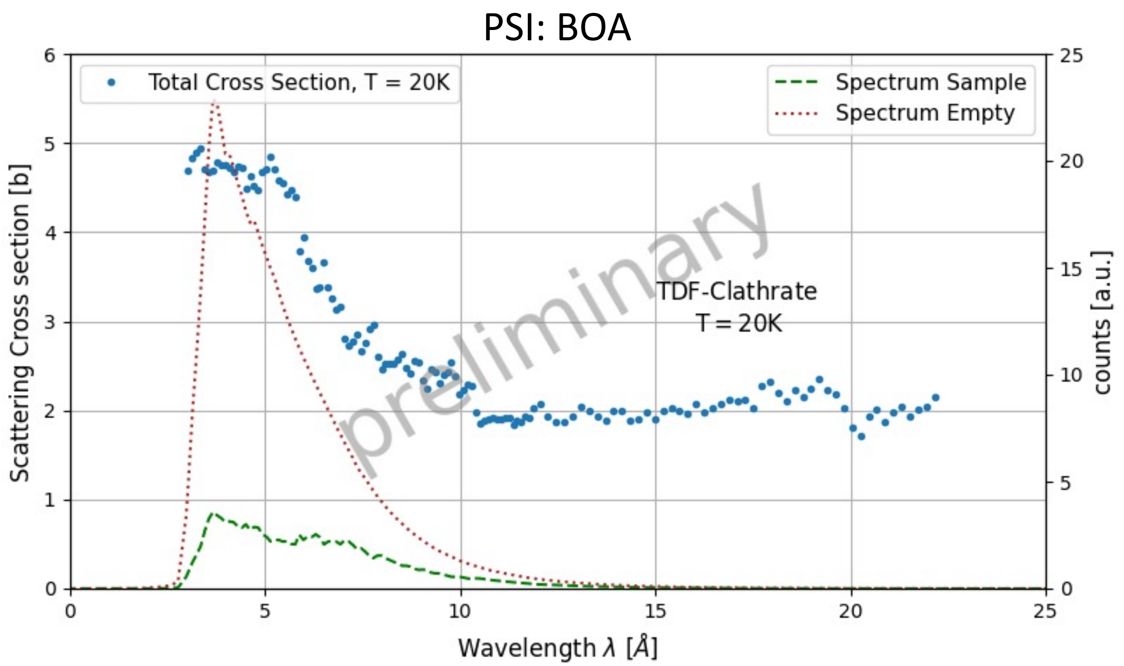
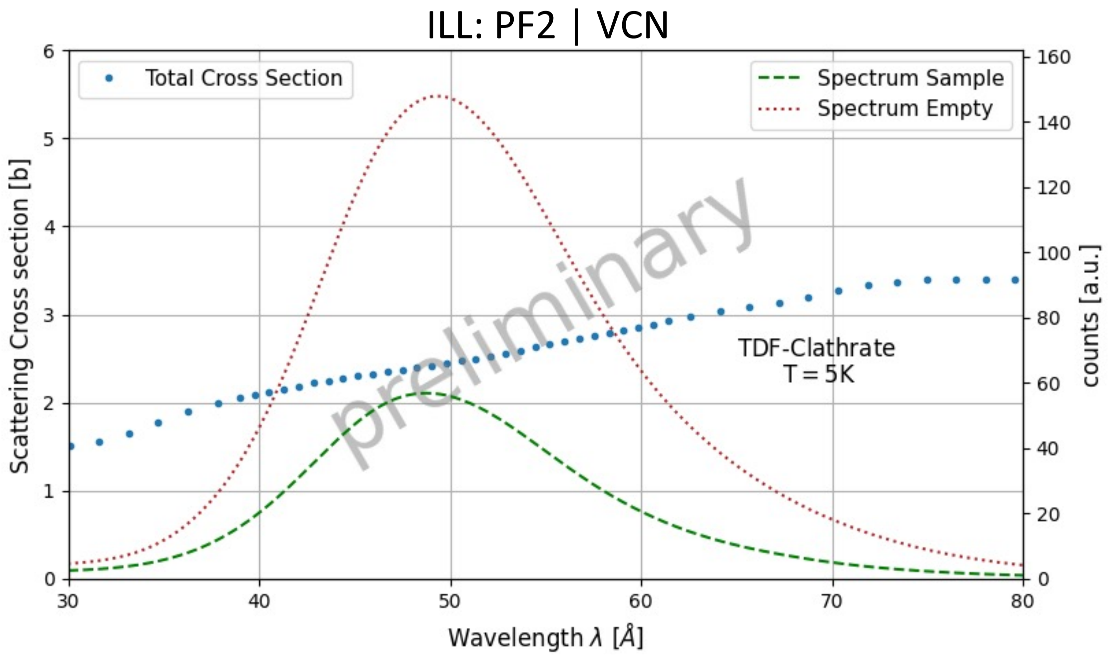
Results PF2 | VCN & BOA

- Observation of the Bragg edges of Type-II Clathrate Hydrates in the CN range (left)
- The cross section in the VCN range is dominated by σ_{inc} of Deuterons (right)





This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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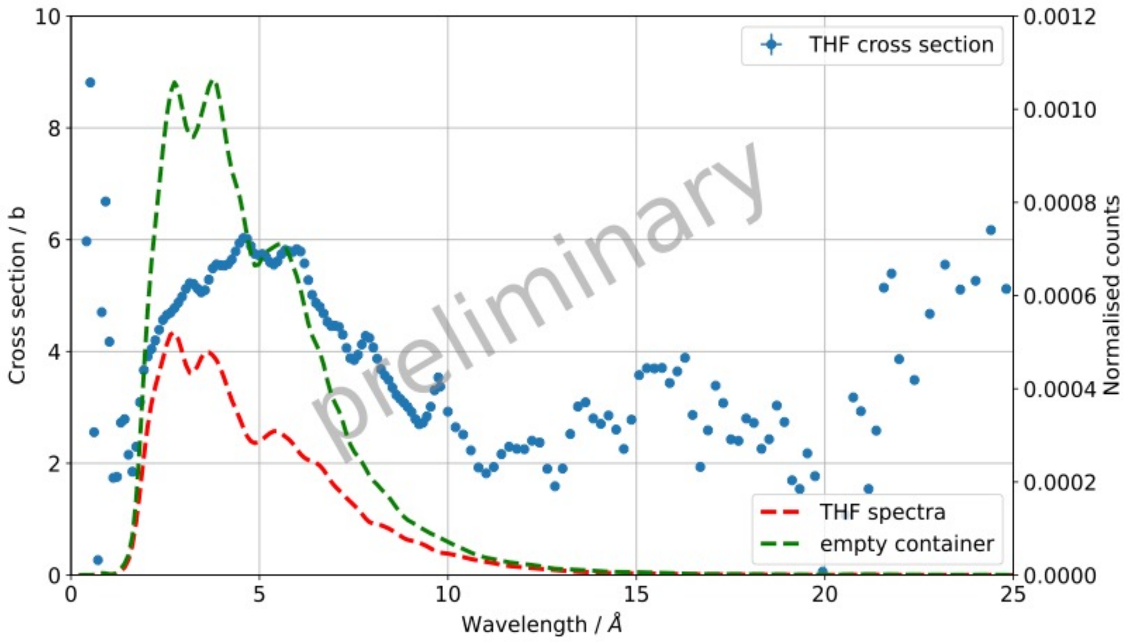
Setup & Results of additional measurements at PF1B

- Wavelength calibration with 4 points
- Calibration samples: graphite, aluminium, iron
- Chopper offset determined with γ-photons of Gd-paint
- Follow up experiment with better resolution:
  beam time at ILL allocated in March 2024



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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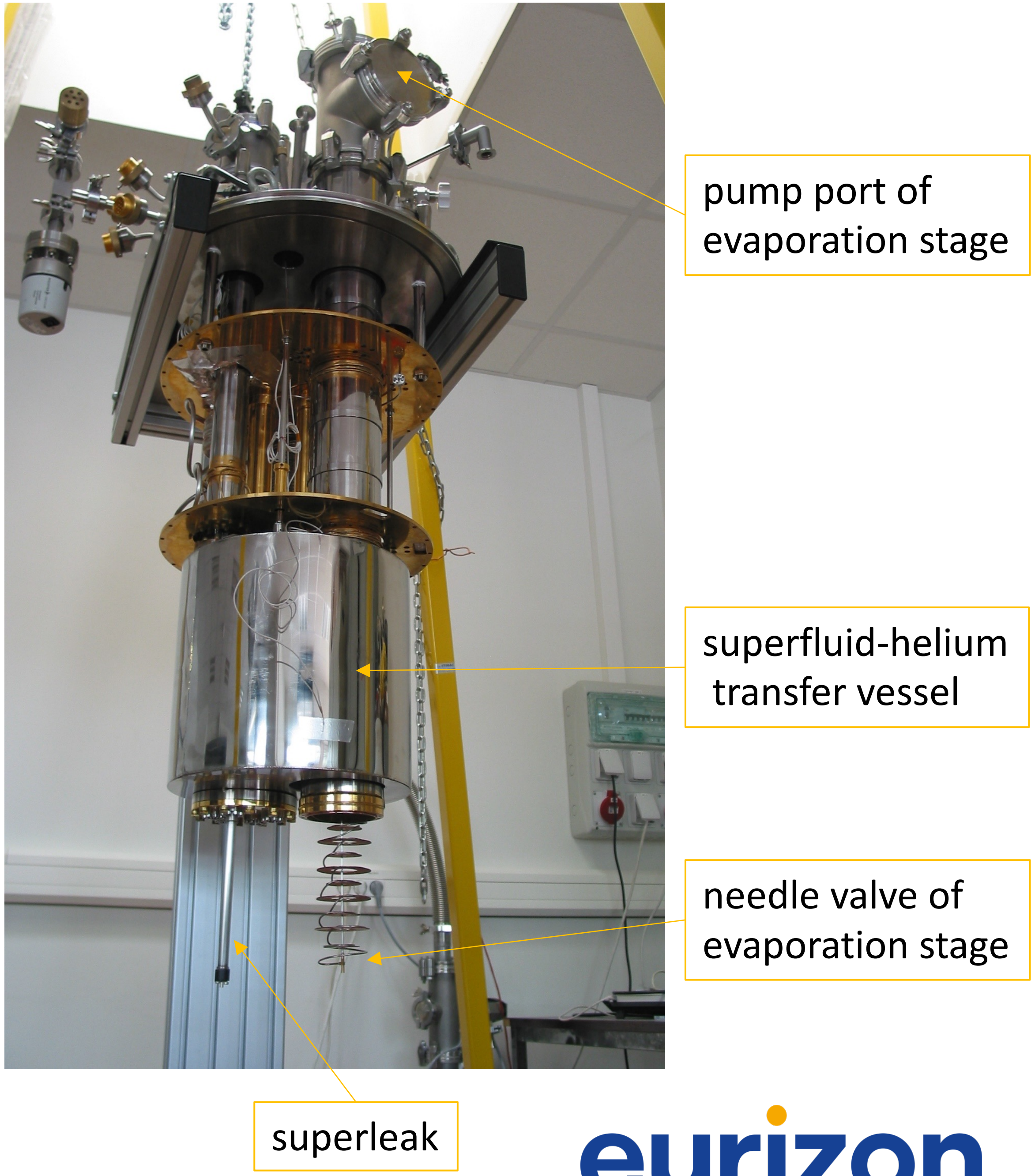
Cryostat for VCN source demonstrator

Goal: test of source prototype cryostat based on:

- Helium liquefication by GM cryo-cooler
- Purification of helium for moderator by a superleak
- Moderator material (e.g. Clathrate hydrate grains or solid-deuterium beads) immersed in superfluid-helium bath
- Helium evaporation cooling of the moderator via heat exchanger between pure and unpurified He

- Device to be tested in February 2024
- Report **D3.8** accepted as due in March 2024



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Development of reflectors based on fluorinated detonation nanodiamonds (F-DNDs) for very cold neutrons (VCNs) and cold neutrons (CNs), Valery Nesvizhevsky
Summary of the project

We performed several series of measurements with samples of designed **fluorinated detonation nanodiamonds** (F-DNDs), using small-angle neutron scattering (SANS) at D17 and PF1B, small-angle X-ray scattering (SAXS) at ID10 instrument at ESRF, neutron activation analysis (NAA) at PF1B , neutron prompt-gamma analysis (NPGA) at PF1B, neutron diffraction (ND) at PF1B, quasi-specular neutron reflection (QSNR) at D17 and PF1B, storage of very cold neutrons (VCNs) at PF2, *etc*.

For these studies, we used standard ILL instruments also developed a **new spectrometer/diffractometer option**, which can be temporarily installed at PF1B (in the framework of standard ILL user activities). It includes the following options: ND, SANS, NAA, NPGA, QSNR. In contrast to any alternative existing facility, at PF1B, ND can be measured in the full VCN and CN energy range of interest to almost all scattering angles; all mentioned methods of measurements could be applied to the same sample with the same neutron beam, thus reducing various systematics effects.

Analysis of these results has allowed us to develop the **optimum designed F-DND powders** with parameters which can be “tuned” for any particular application. All tasks of this part of the project (F-DND reflectors) are fully completed. Due to the cancellation of measurements with a solid-deuterium neutron converter, no grant budget was needed for the whole program.

We published **7 articles** including **high-impact journals**, in particular Nanomaterials (**h=5.7**), Journal of Physical Chemistry C (**h=4.2**), Materials (h=3.7), Review of Scientific Instruments (h=1.8), Journal of Neutron Research (h=0.26). These article completely describe all the performed works within the project.

This project has received funding from the European Union‘s Horizon 2020 research and innovation programme under grant agreement No. 871072.

The main results and the corresponding publications, in chronological (and logical) order

We performed a detailed characterization of standard fluorinated nanodiamonds (F-DNDs) as the first step towards the design of optimized F-DNDs [M. Herraiz, *et al*, *A multitechnique study of fluorinated nanodiamonds for low-energy neutron physics applications*, **J. Phys. Chem. C 124** (2020) 14229];

Here and further on, many non-neutron and neutron techniques are always used for every sample

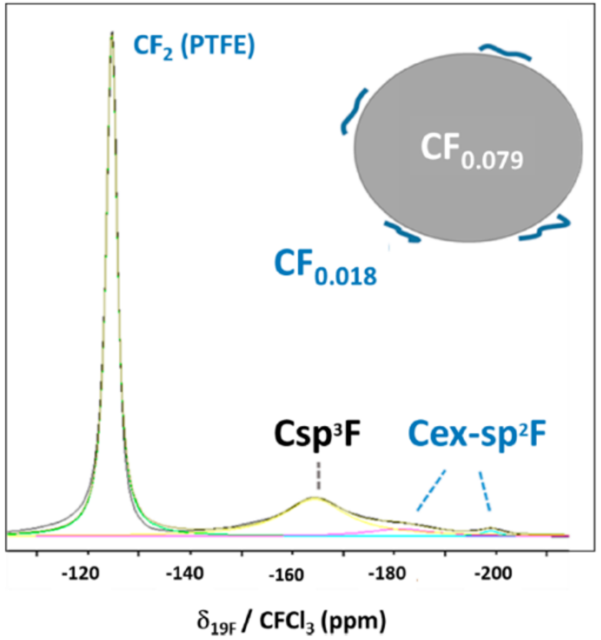


Figure 1. ^{19}F MAS NMR (30 kHz) of fluorinated NDs mixed with PTFE reference for quantification purposes.

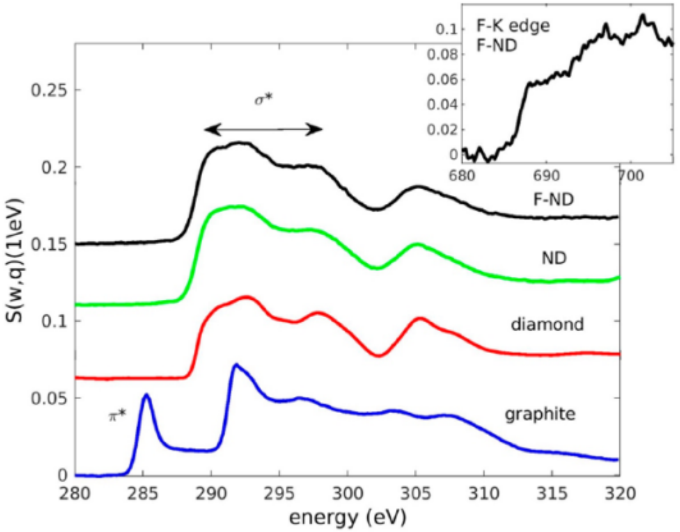


Figure 3. XRS spectra at the carbon K edge of F-NDs, NDs, graphite, and diamond powder. Graphite and diamond powders are reported as an example of pure C-sp^2 and C-sp^3 hybridization (data published in ref 29). In the inset, XRS spectra at the F−K edge for F-NDs.

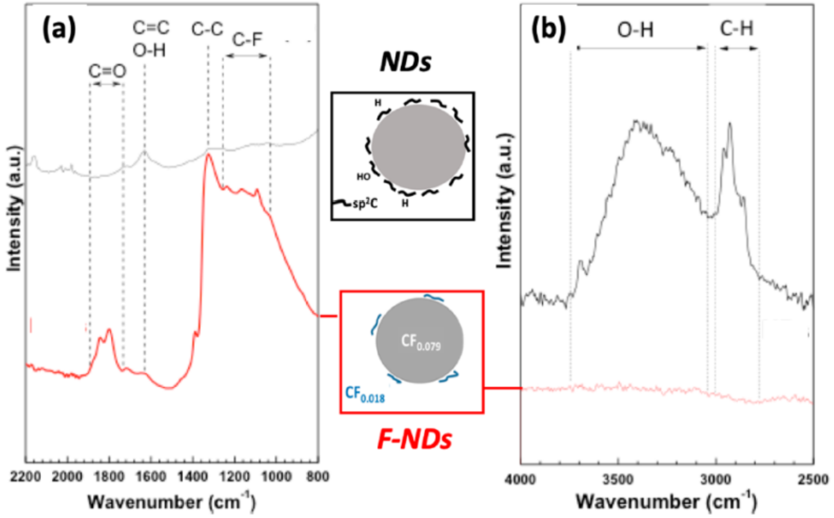


Figure 4. FTIR spectra (ATR mode) of raw and fluorinated NDs.

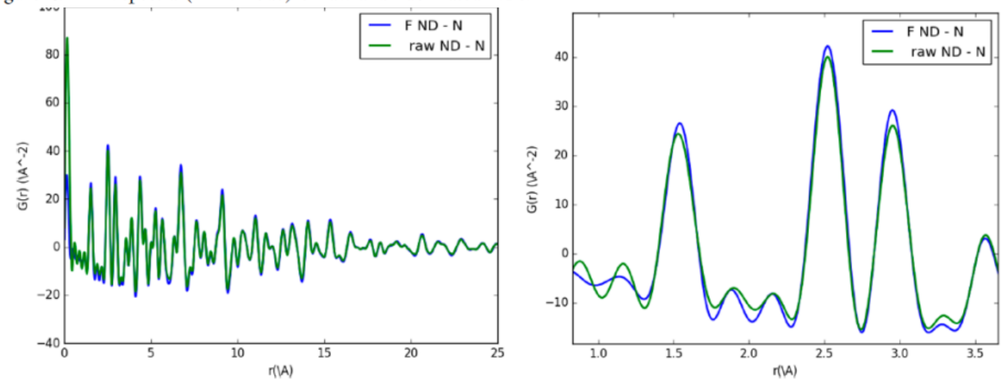


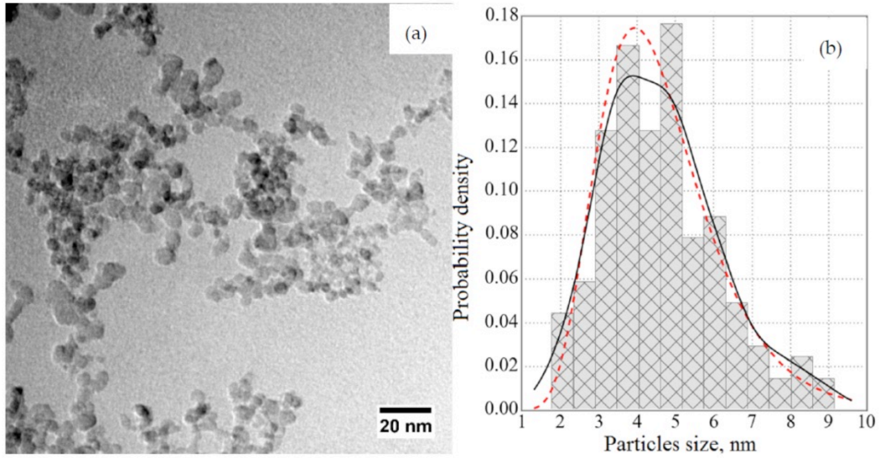
Figure 2. Experimental neutron PDFs of raw and fluorinated NDs plotted up to r = 25 Å (left panel) and magnifications, collected at the diffractometer D4C (ILL, Grenoble), using an incident neutron wavelength λ = 0.4989 Å and Q_{max} = 23.5 $Å^{-1}$.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

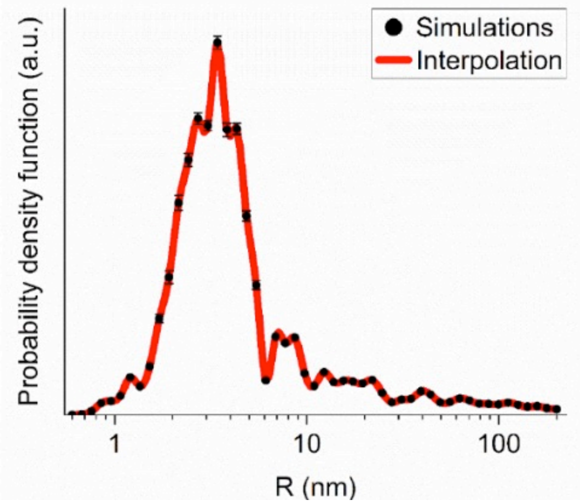
The main results and the corresponding publications, in chronological (and logical) order

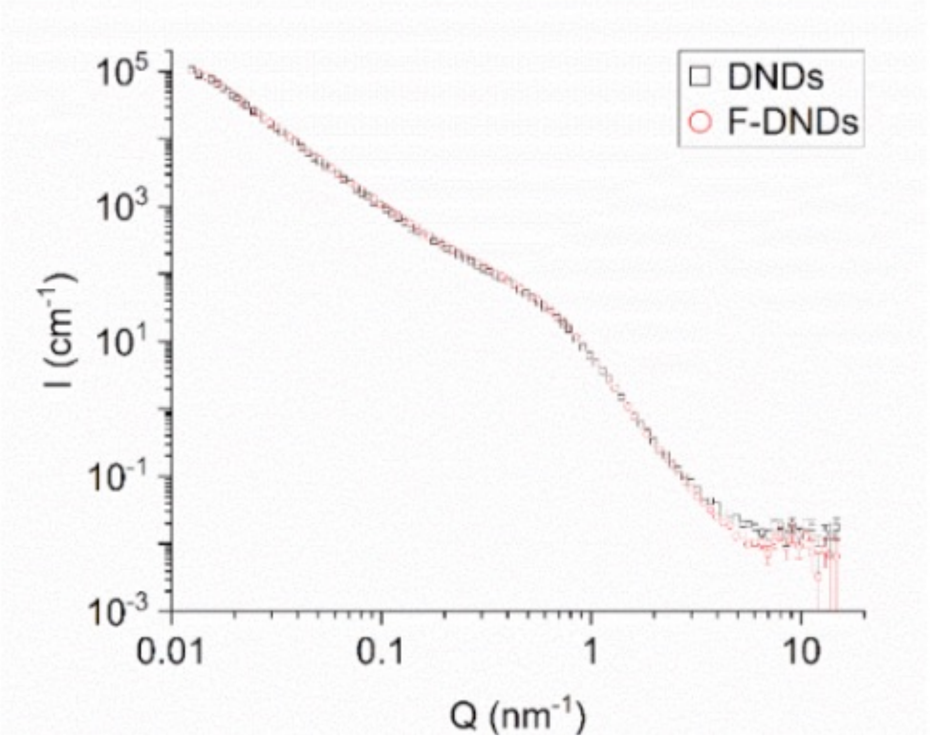
We confirmed that fluorination does not affect the scattering properties of F-DNDs while largely reduces neutron losses [A. Bosak, *et al*, *Fluorination of Diamond Nanoparticles in Slow Neutron Reflectors Does Not Destroy Their Crystalline Cores and Clustering While Decreasing Neutron Losses*, **Materials 13** (2020) 3337];

Samples characterization with TEM



DND and F-DND size distribution extracted from SANS measurements at D11





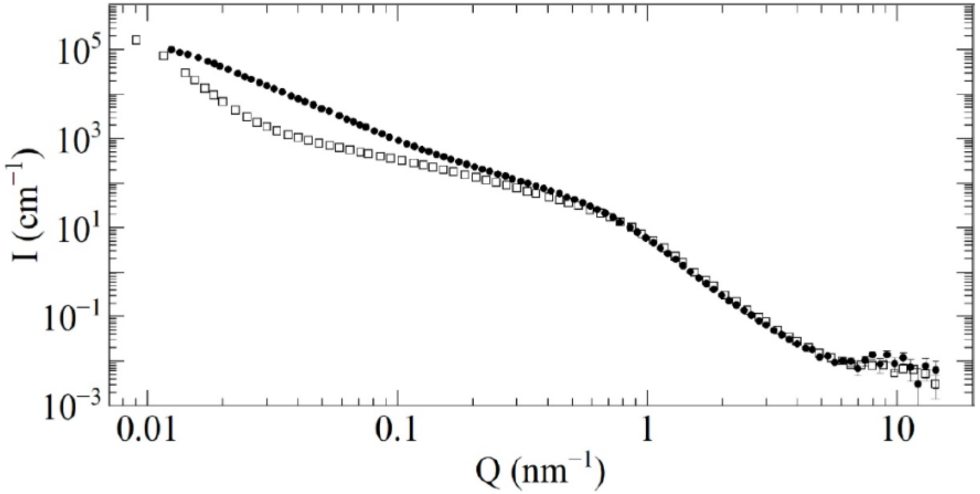
The result: fluorination hugely reduces neutron losses but it does not affect neutron scattering

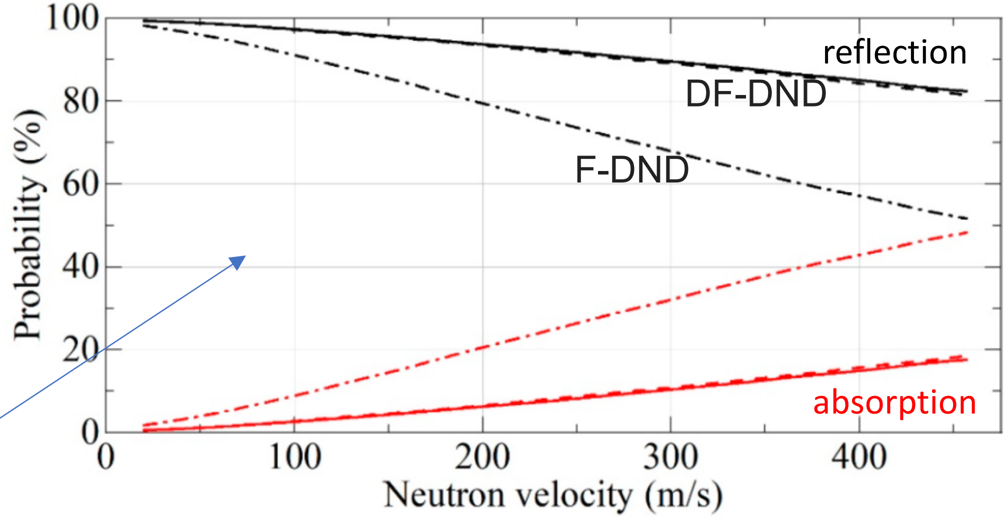
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

The main results and the corresponding publications, in chronological (and logical) order

De-agglomeration of F-DNDs improves the efficiency of F-DND reflectors [A. Aleksenskii, *et al*, *Clustering of Diamond Nanoparticles, Fluorination and Efficiency of Slow Neutron Reflectors*, **Nanomaterials 11** (2021) 1945];

D11, SANS sample characterization shows the effect of F-DND deagglomeration at small Q values; as expected, no effect at large Q values

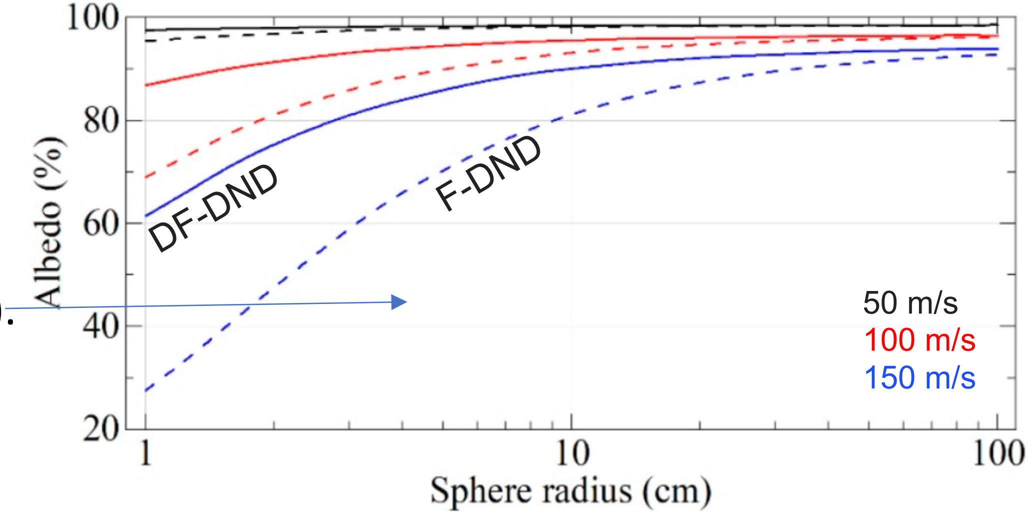




The reflectivity from an infinite flat reflector with standard F-DND and deagglomerated DF-DND powders (on top).

An analogous analysis for a cavity with infinitely thick walls (on bottom).

Result: large improvement due to deagglomeration

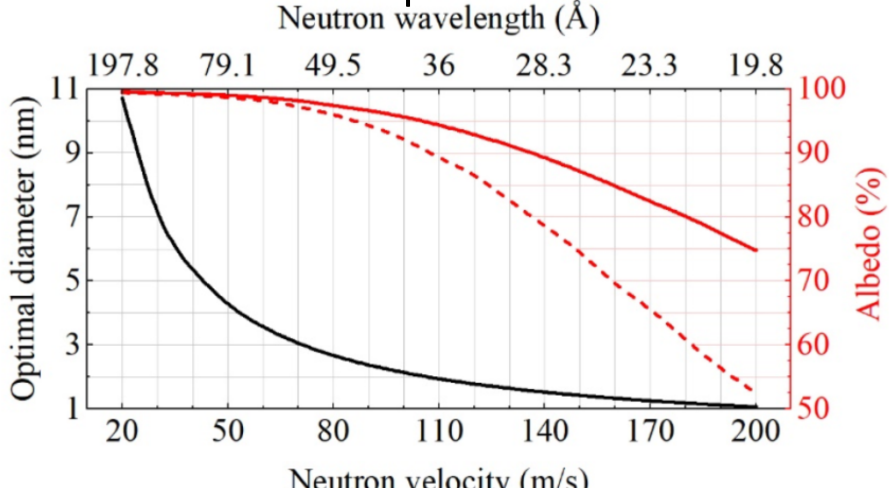


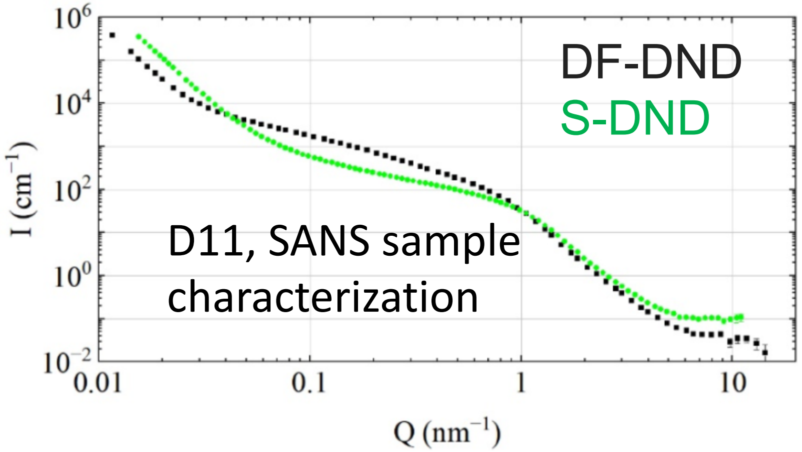
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

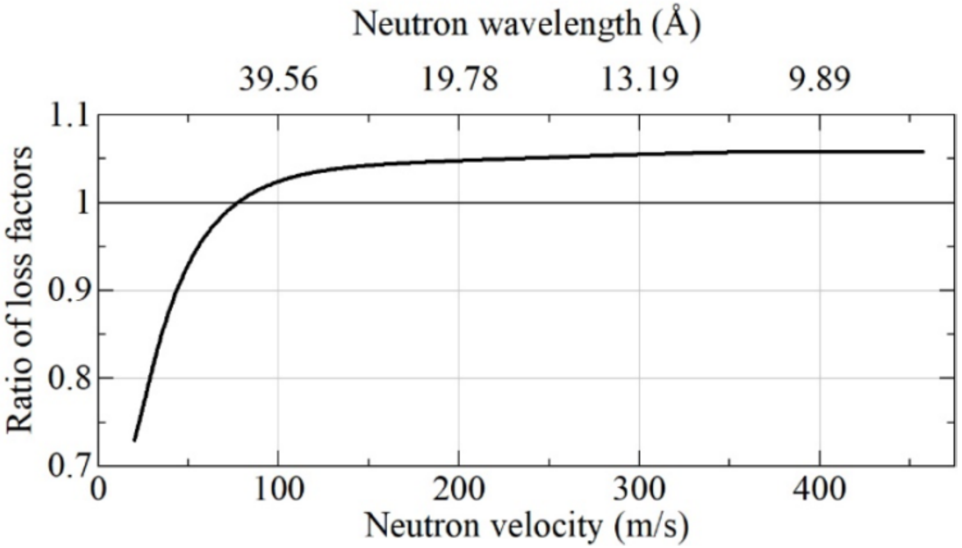
The main results and the corresponding publications, in chronological (and logical) order

Optimal sizes of F-DNDs (~5 nm) are found for diffusive reflection of very cold neutrons (VCNs) [A. Aleksenskii, *et al*, *Effect of Particle Sizes on the Efficiency of Fluorinated Nanodiamond Neutron Reflectors*, **Nanomaterials 11** (2021) 3067];

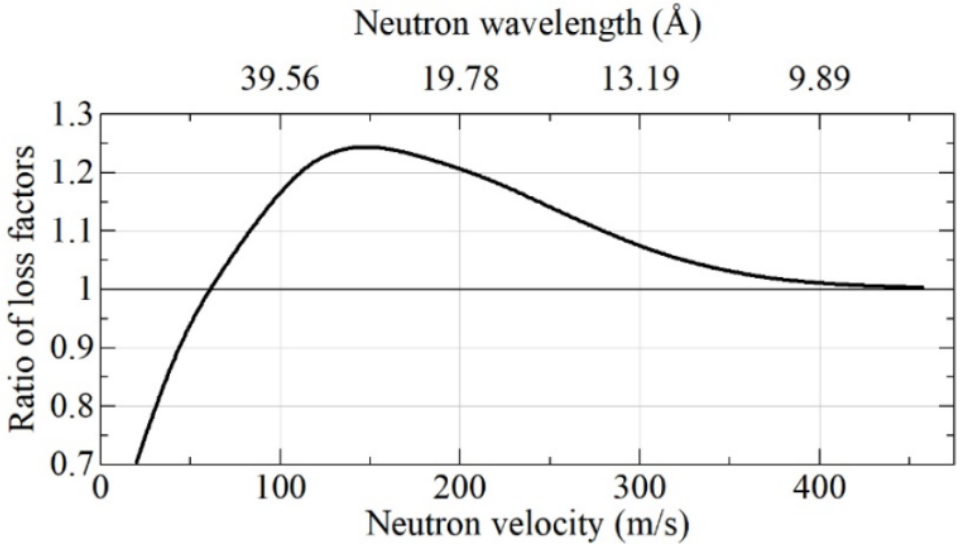
Calculated reflectivity from the DND medium with optimum DND diameters







The ratio of reflectivity from an infinite flat reflector with 4.3 nm F-DND and 3.4 nm F-DND powders (smaller F-DND are better for smaller neutron wavelengths; larger F-DND are better for larger neutron wavelengths)



An analogous analysis for a cavity with infinitely thick walls

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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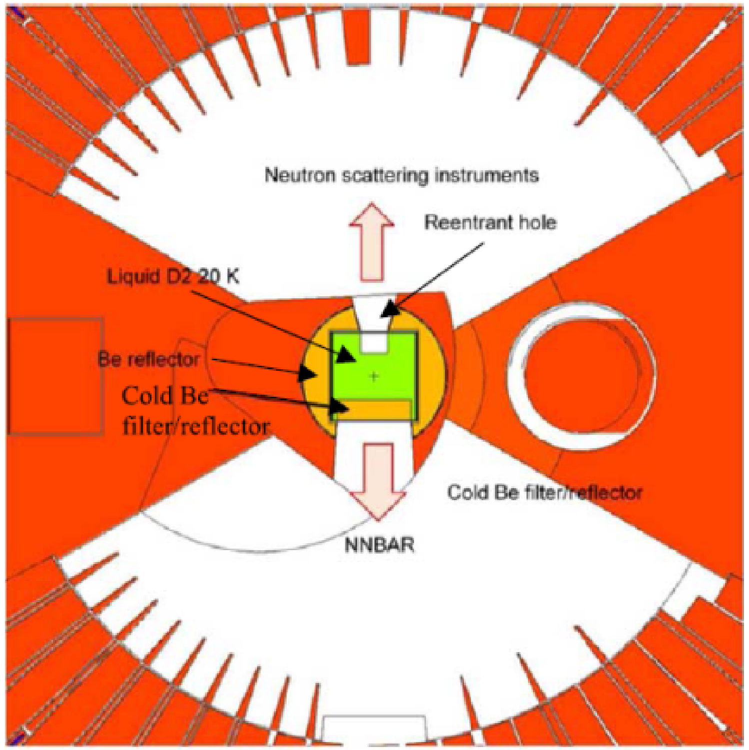
The main results and the corresponding publications, in chronological (and logical) order

A concrete scheme for using DND reflectors at ESS for the enhancement of VCN fluxes (a factor of ~10) is proposed [V.V. Nesvizhevsky, *Why very cold neutrons could be useful for neutron-antineutron oscillation searches*, **J. Neutron Res. 24** (2022) 223];

One motivation for using VCN is the factor of >10 improvement in the sensitivity of the experiment searching for neutron-antineutron oscillations over the best current design



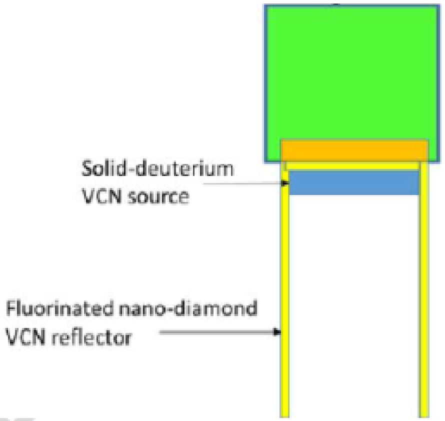


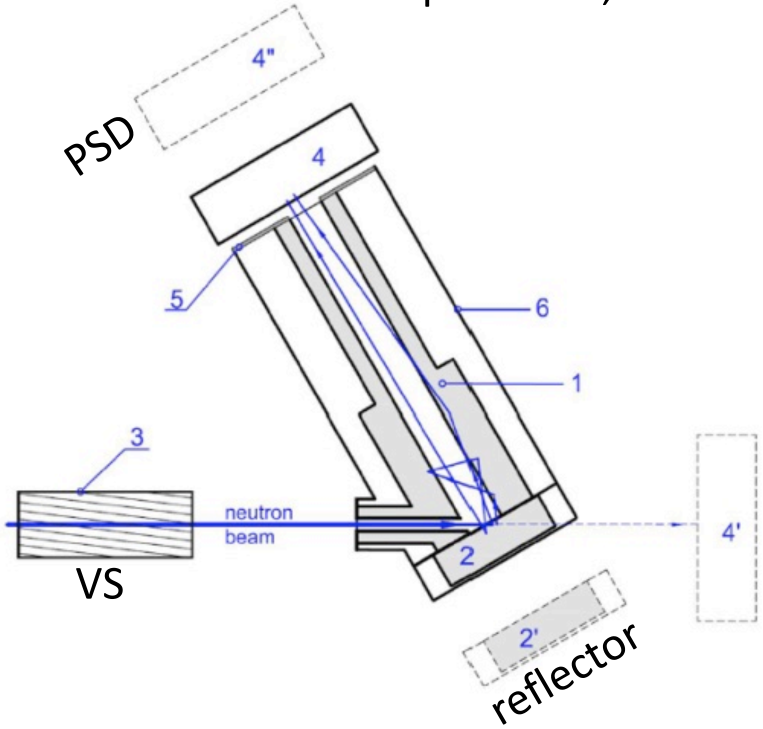
Fig. 1. Figure is taken from "L. Zanini et al., Very Cold and Ultra Cold Neutron Sources for ESS, these proceedings". At left, the current design for the implementation of a large-volume liquid-deuterium source of CN. The green coloring indicates regions of 20 K. The downward facing arrow at bottom illustrates CN passing through a Be filter (orange) and feeding a $n-\overline{n}$ experiment. A dedicated solid-deuterium VCN converter with an F-DND reflector could be added to this design, as is shown below.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

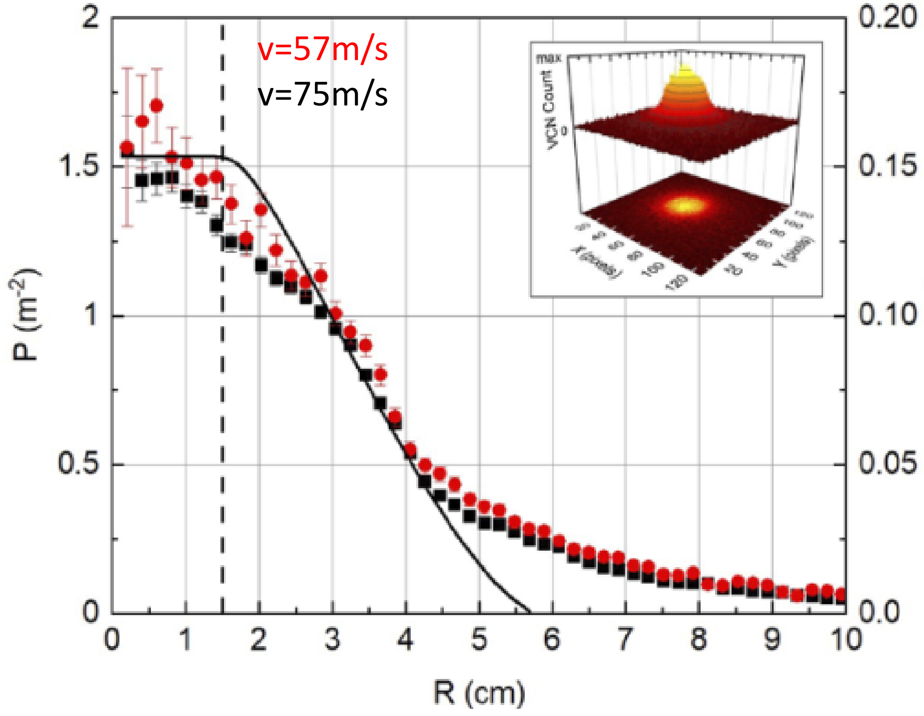
The main results and the corresponding publications, in chronological (and logical) order

A major gain (a factor of ~10) in the directed flux of VCNs due the use of DND reflectors is demonstrated experimentally [Chernyavsky, S.M., *et al*, *Enhanced directional extraction of very cold neutrons using a diamond nanoparticle powder reflector*, **Rev. Sci. Instr. 93** (2022) 123302];

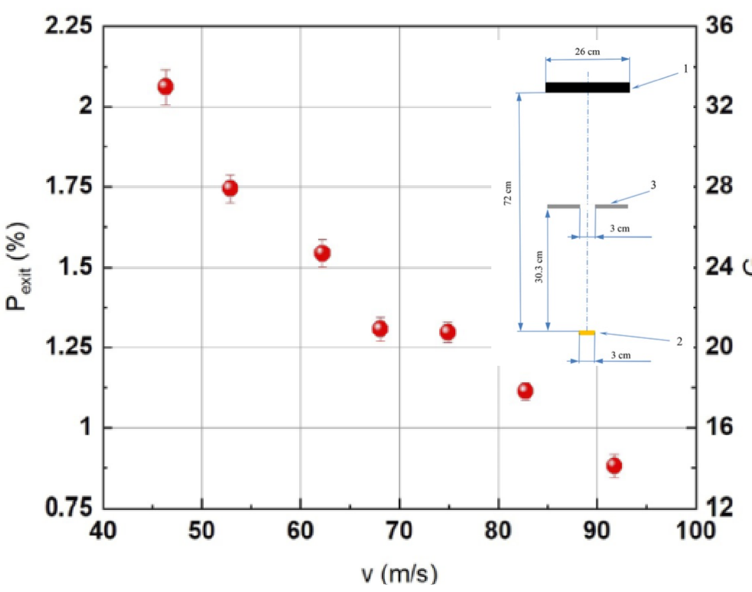
Scheme of the experiment, PF2



Directional extraction of VCN from the F-DND tube



Total gain factor (right vertical scale)



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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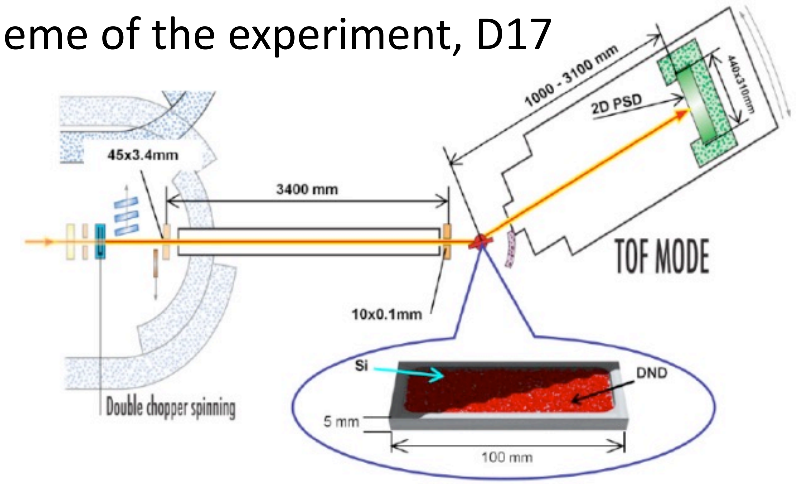
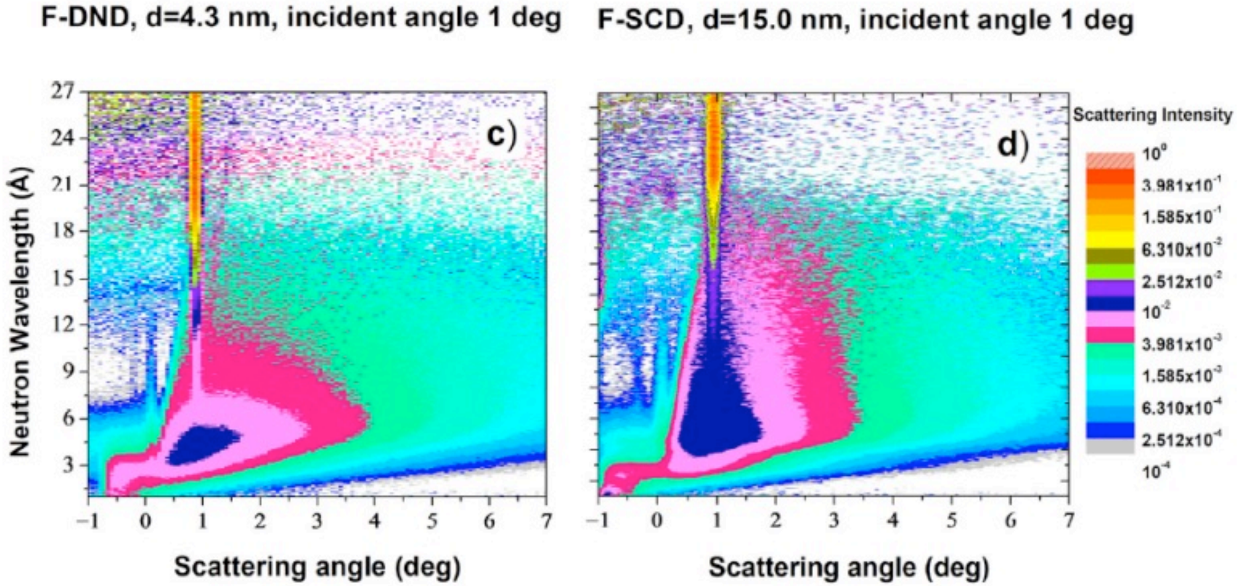
The main results and the corresponding publications, in chronological (and logical) order

Optimal sizes of DNDs (~10 nm) are found for quasi-specular reflection of cold neutrons (CNs). [A. Bosak, *et al*, *Effect of Nanodiamond Sizes on the Efficiency of the Quasi-Specular Reflection of Cold Neutrons*, **Materials 16** (2023) 703];

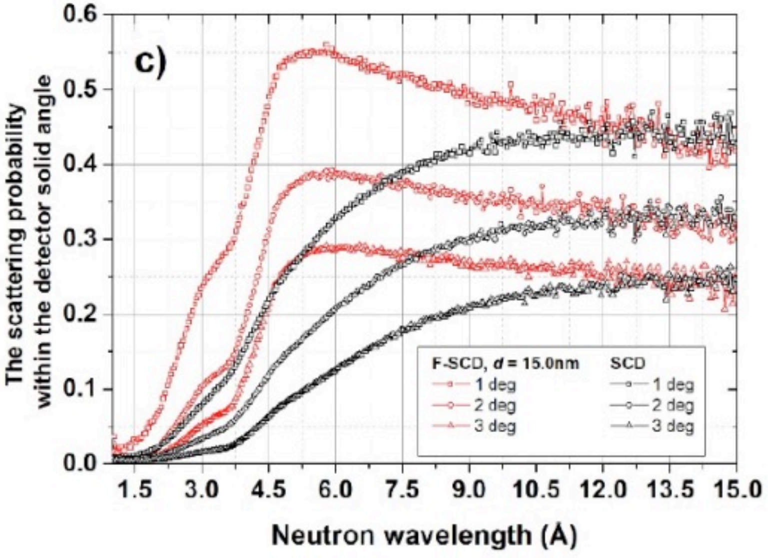
Scheme of the experiment, D17

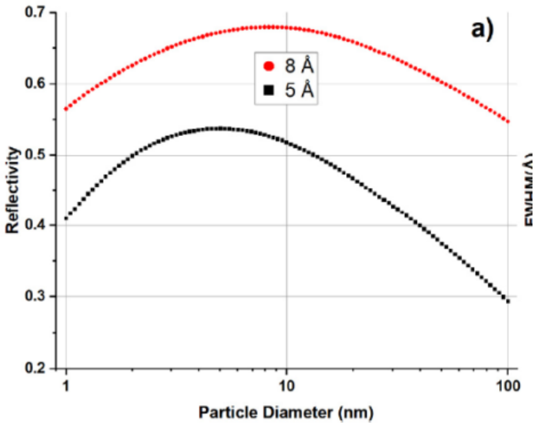


Scattering maps (as a function of neutron wavelength and scattering angle)



Effect of fluorination on the 15 nm ND sample for the incident angles of 1°, 2° and 3° (“red curves” are systematically higher than “black curves”)





Optimum F-DND sizes are around 10 nm for all neutron wavelengths

This project has received funding from
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Task 3.5: Prototype of advanced polarized neutron diffractometer; **A. Goukassov -** CEA/LLB, ESS, ILL, FZJ

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Original Task;
WP3. Task 3.5: Prototype of advanced polarized neutron diffractometer for PIK reactor

Milestone MS17
Simulations and performance of advanced polarized neutron diffractometer
31 July 2021 Partners CEA-LLB and PNPI
(Goukassov and Zobkalo)

Planning
- Modelling of polarized neutron diffractometer DiPol at PIK reactor
- Monochromator optimization
- Polarizer optimization

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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Original Task;
WP3. Task 3.5: Prototype of advanced polarized neutron diffractometer for PIK reactor

Monochromator optimization

HOPG is chosen as a mandatory choice for the monochromator, with possible add on of a Cu(220) one.

Polarizer optimization

Polarizing bender was considered as polarizer and analyzer units. The McStas simulations were performed to optimize the dimensions vs transmission and high polarization level.

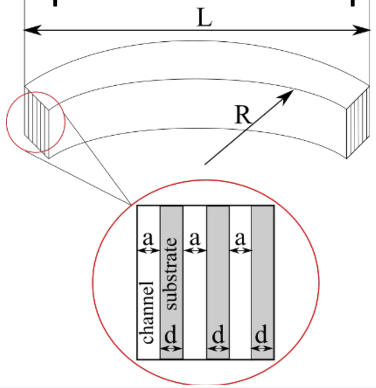
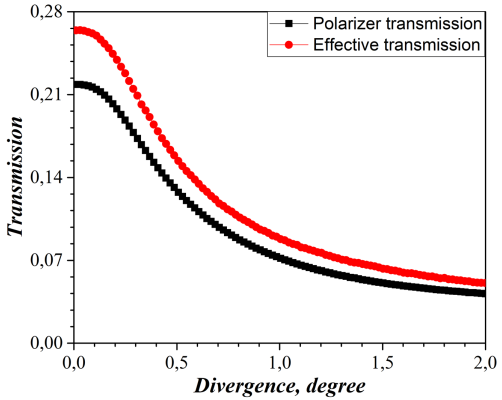


Fig. 1. Schematic drawing of polarizing bender.



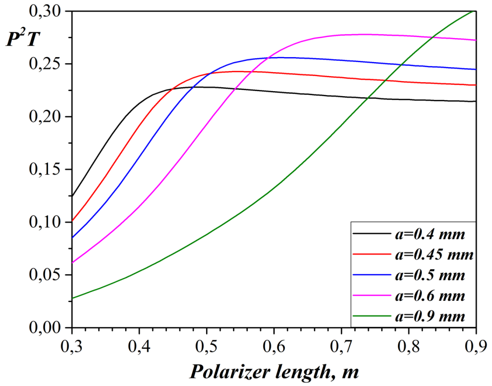


Fig. 1. Polarizer transmission and quality parameter P^2T

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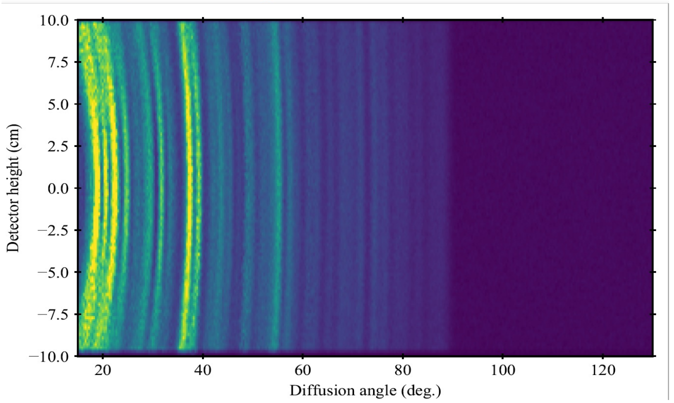
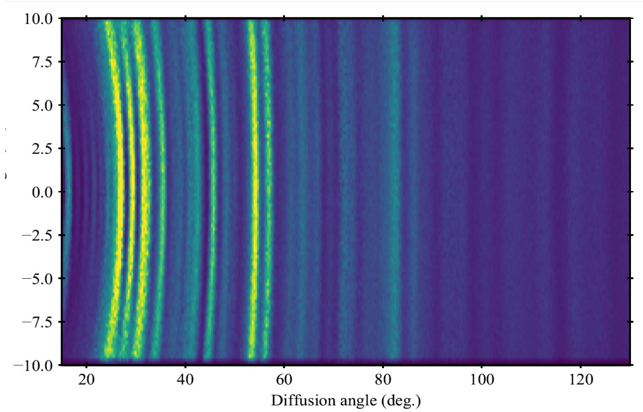
Original Task;
WP3. Task 3.5: Prototype of advanced polarized neutron diffractometer for PIK reactor

Expected diffractometer performance

Examples of simulated 2D diffraction patterns from standard sample NaCAlF for two different wavelength 0.7 Å (left) and 1 Å (right) are shown in figure





MS17 Report delivered in July 2021

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

EURIZON: WP3 Neutrons (since 2023)

- **ST 3.5**: Prototype of advanced polarized neutron diffractometer
  A. Goukassov (CEA/LLB, ESS, ILL, JCNS)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Task 3.5: Prototype of advanced polarized neutron diffractometer

Task Leader: Arsen Goukassov, CEA-LLB
Partners involved: ESS,JCNC, ILL
Description of work:

The aim of this task is prototyping of new elements improving the performance of polarized neutron diffraction experiments on advanced neutron sources. Software will be developed and implemented at polarized neutron diffractometer POLI of JCNS@MLZ (Jülich Centre for Neutron Science) and will be accommodated for further using at diffraction instruments at the ESS.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Cryspy- Deliverables N2 Task 3.5 (m 48)

Current state (September 2022)

Milestone/ deliverable	Name	Partner in charge of task	Start month	End month	Type of deliverab le
D3.5.2	CrysPy software for the data analysis adapted for area detectors	LLB	18	48 01/01/24	Report

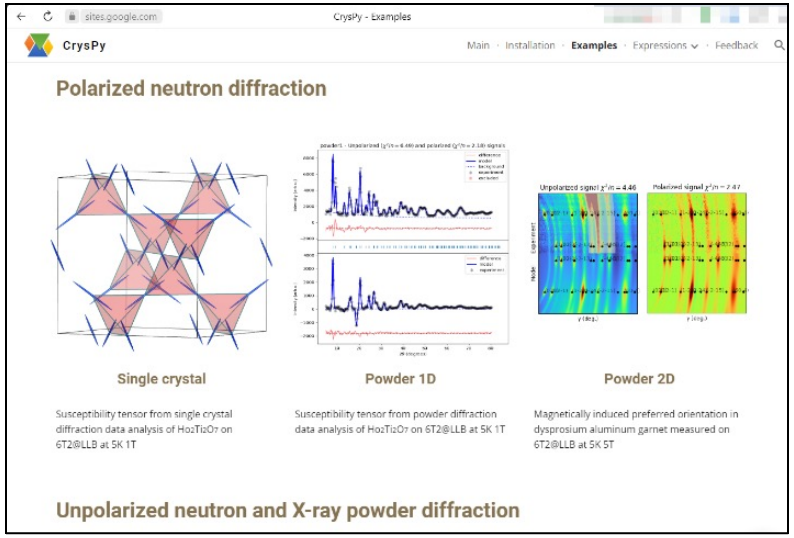
CrysPy is the only one library in the world that allows analyzing polarized neutron diffraction experiments both on single crystals and powders. Developed by LLB the latest release of CrysPy includes the following new features:

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CrysPy: a crystallographic library for neutron data analysis

- *Local magnetic anisotropy* by PND in *powders* and *single crystals*;
- *Nuclear structure* refinement
- *Spin density* reconstruction by MEM

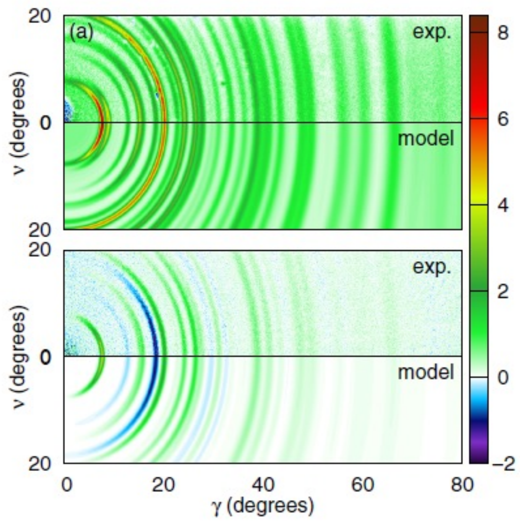
- https://cryspy.fr
- https://ikibalin.github.io/cryspy/
- Python 3.7-3.10, Crystal and data in CIF format



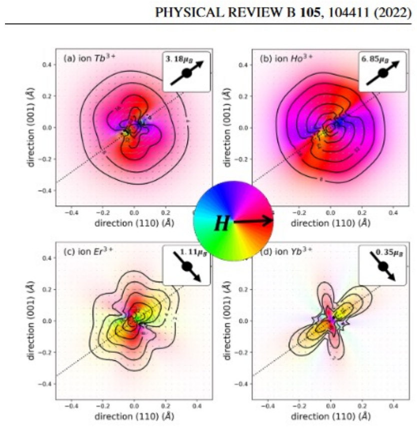
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Cryspy- Deliverables N2 Task 3.5 (m 48)

Two-dimensional Rietveld refinement procedure is implemented. Two-dimensional area detectors increase the efficiency of the instrument by an order of magnitude.



Magnetization density reconstruction. Newly developed maximum entropy reconstruction procedure in CrysPy taking into account the local anisotropy goes beyond the dipole approximation.



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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Cryspy- Deliverables N2 Task 3.5 (m 48)

Software dissemination.

The source code of the CrysPy library has been published on the GitHub server: github.com/ikibalin/cryspy. The educational materials and 'training' experimental data are presented on the internet page: https://www.cryspy.fr

the CrysPy library has been presented at the International conferences ICDM9 2022,(Aarhus, Denmark), PNCMI2021, (Washington), Robert-Stewart school (Nancy, France), Polarized neutron workshop 2022 in ORNL (USA), ILL 2022 (Grenoble, France), ESS-ILL 2022 user meeting (Lund, Sweden), ICSM2023 (Fethie), AOCNS2023 and was a subject of other workshops.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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Publications in international journals 2019-2023

CrysPy developments

I.A. Kibalin, A. Gukasov, *Local magnetic anisotropy by polarized neutron powder diffraction: Application of magnetically induced preferred crystallite orientation.* Physical Review Research, **1** (2019) 033100

I.A. Kibalin, F. Damay, X. Fabreges, A. Goukassov, and S. Petit, *Competing Interactions in Dysprosium Garnets and Generalized Magnetic Phase Diagram of S = 1 spins on a Hyperkagome Network*, Physical Review Research, **2** (2020) 033509

I.A. Kibalin and A. Gukasov, *Asphericity of magnetisation density and anisotropy in rare-earth pyrochlores via polarized neutron diffraction and iterative entropy maximization*, submitted Phys. Rev. B, **105** (2022) 104411

CrysPy   using

I. V. Golosovsky; **I. A. Kibalin; A. Gukasov**; A. G. Roca; A. López-Ortega; M. Estrader; M. Vasilakaki; K. N. Trohidou; T. C. Hansen; I. Puente-Orench et al. Elucidating Individual Magnetic Contributions in Bi-Magnetic Fe3O4/Mn3O4 Core/Shell Nanoparticles by Polarized Powder Neutron Diffraction. Small Methods, 2023-10 DOI: 10.1002/smtd.202201725

Sandeep K. Gupta, Hannah H. Nielsen, Andreas M. Thiel, Emil A. Klahn, Erxi Feng, Huibo B. Cao, Thomas C. Hansen, Eddy Lelièvre-Berna, **Arsen Gukasov, Iurii Kibalin**, Sebastian Dechert, Serhiy Demeshko, Jacob Overgaard*, and Franc Meyer. Multi-Technique Experimental Benchmarking of the Local Magnetic Anisotropy of a Cobalt(II) Single-Ion Magnet. JACS Au 2023, 3, 2, 429–440

W.J.A. Blackmore, S.P.M. Curley, R.C. Williams, S. Vaidya, J. Singleton, S. Birnbaum, A. Ozarowski, J.A. Schlueter, Y.-S. Chen, B. Gillon, A. Goukassov, **I. Kibalin**, D.Y. Villa, J.A. Villa, J.L. Manson, P.A. Goddard, *Magneto-structural Correlations in Ni2+–Halide···Halide–Ni2+ Chains*, Inorganic Chemistry, **61** (2022) 141

I. Kibalin, A. Gukasov, *Quantifying Magnetic Anisotropy Using Polarized Neutron Powder Diffraction,* Neutron News, (2021) 1

E.A. Klahn, A.M. Thiel, R.B. Degn, **I. Kibalin**, A. Gukassov, C. Wilson, A.B. Canaj, M. Murrie and J. Overgaard, *Magnetic anisotropies of Ho(III) and Dy(III) single-molecule magnets experimentally determined via polarized neutron diffraction*, Dalton Transactions, **50** (2021) 14207

E.A. Klahn, E. Damgaard-Møller, L. Krause, **I. Kibalin**, A. Gukasov, S. Tripathi, A. Swain, M. Shanmugam, J. Overgaard, *Quantifying magnetic anisotropy using X-ray and neutron diffraction*, IUCrJ, **8** (2021) 833

M. Souhassou, **I. Kibalin**, M. Deutsch, A.B. Voufack, C. Lecomte and N. Claiser, *Spin-resolved charge density and wavefunction refinements using MOLLYNX: a review*, Acta Cryst., **B77** (2021) 706

E.K. Nigmatullina, **I.A. Kibalin**, V.P. Sedov, A.A. Borisenkova, A.A. Bykov, I.V. Golosovsky, *'Phantom' atoms and thermal motion in fullerene C60 revealed by x-ray and neutron diffraction*, Journal of Physics: Condensed Matter, **33** (2021) 455401

L. Ding, C. Hu, E. Feng, C. Jiang, **I.A. Kibalin**, A. Gukasov, MF. Chi, N. Ni and H. Cao, *Neutron diffraction study of magnetism in van der Waals layered $MnBi_{2n}Te_{3n+1}$*, Journal of Physics D: Applied Physics, **54** (2021) 174003

I. Kibalin, A.B. Voufack, M. Souhassou, B. Gillon, J.-M. Gillet, N. Claiser, A. Gukasov, F. Porcher and C. Lecomte, *Spin-resolved atomic orbital model refinement for combined charge and spin density analysis: application to the YTiO3 perovskite*, Acta Crystallographica Section A, **77** (2021) 96

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To summarize the results of WP3

- Task 1:
  - Increase of cold neutron flux of a reactor by a factor of up to 3 is possible by using flat moderators! (ILL x 3)
  - Cold Moderator Test Facility (CMTF) at the Budapest Research Reactor is set up
  - Bi-spectral (thermal and cold) extraction works!

- Task 3:
  - Increase of very cold neutron flux by a factor of 10 possible by using Nano Diamonds as moderator !

- Task 5:
  - CrysPy is the only one library in the world that allows analyzing polarized neutron diffraction experiments both on single crystals and powders.

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