
EUROPEAN
SPALLATION
SOURCE

# Software development for moderator and reflector design at the European Spallation Source: spring 2024 update

LENS/ELENA neutron moderator workshop

**PRESENTED BY JOSE IGNACIO MARQUEZ DAMIAN, DOUGLAS DI JULIO, THOMAS KITTELMANN, SHUQI XU, AND GÜNTER MUHRER**

**17-04-2024**

# Outline

Introduction

Tools development

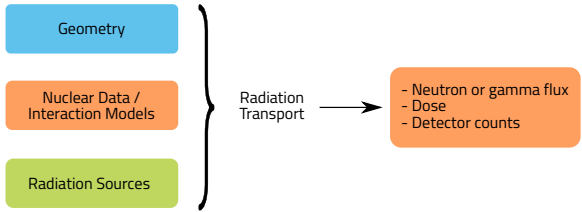
Neutron scattering models for selected materials

Other topics

Concluding remarks

# Outline

# Radiation transport



# Thermal scattering data needs at the ESS

- Nuclear data to support the moderator/reflector system under construction:
  - Liquid hydrogen moderator
  - Beryllium reflector
- Nuclear data to support future upgrades of the facility (HighNESS project):
  - Liquid deuterium moderator
  - Diamond nanoparticles
  - Clathrate hydrates with paramagnetic oxygen
  - Graphitic compounds with large d-spacing
- New tools and methods are needed for several of the materials.
- New developments can also help relax some of the limitations of previously used methods.
- Large number of developments under the HighNESS project, which are freely available online at `https://github.com/highness-eu/`

# Neutron interaction models

## PRESENT

Cross talk between neutron scattering and neutron transport
New tools: NCrystal, OClimax, Mantid, McStas, OpenMC
Free and open source software
Integrated with MD / DFT simulations

## PAST

Neutron Transport

- Driven by nuclear reactor applications.
- Closed source and export controlled.
- Difficult to incorporate condensed matter information.
- Legacy software from the 1970's (GASKET / NJOY).

Neutron Scattering

- Ecosystem of different tools, created for each instrument.
- No connection with high energy physics.

# Several approaches

- Incorporating state-of-the-art molecular modelling into the process
- Modified library format to support new physics - NJOY+NCrystal / ncmat2endf
- Extensions of NCrystal to include new physics processes - NCrystal plugins
- Modifying Monte-Carlo software to support these developments

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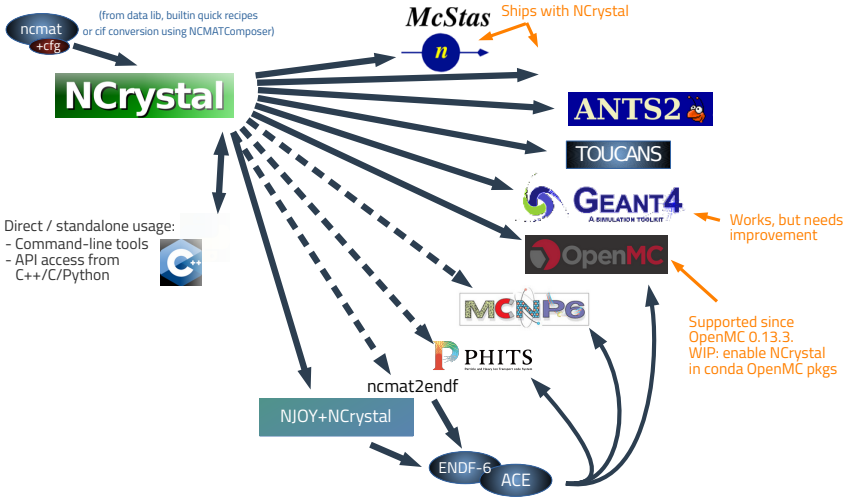
# NCrystal




Developed by Xiao Xiao Cai and Thomas Kittelmann at ESS.

# NCrystal

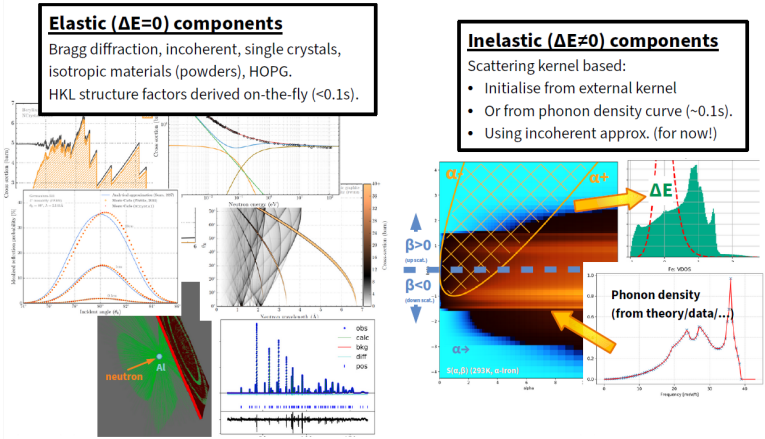
**Elastic (ΔE=0) components**

Bragg diffraction, incoherent, single crystals, isotropic materials (powders), HOPG.
HKL structure factors derived on-the-fly (<0.1s).

**Inelastic (ΔE≠0) components**

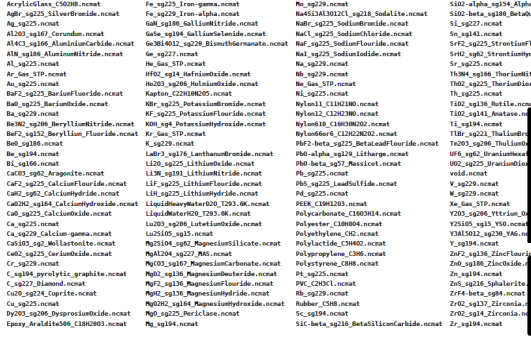
Scattering kernel based:

- Initialise from external kernel
- Or from phonon density curve (~0.1s).
- Using incoherent approx. (for now!)




Physics can be extended through development of plugins. We created plugins for small-angle neutron scattering, magnetic scattering and texture effects.

# NCrystal




**132 materials (v3.0.0):**
Crystals (108), amorphous solids (16), liquids, gasses, …

**Easy universal cfg:**
"Al_sg225.ncmat;temp=250K"
"Rubber_C5H8.ncmat;comp=inelas"
- Same physics in all applications!
- Cfg variables documented at:
github.com/mctools/ncrystal/wiki/CfgRefDoc

**Small (few kB) file sizes:**
- Optionally embed in binary and avoid need for actual files.

**Easy to create more:**
- Hand-write NCMAT file (human readable ASCII, format well-defined & versioned) or use new NCMATComposer.
- Convert from ENDF, CIF, online crystal DB carbohydrate chemical formula, Quantum Espresso output, …
- Request help on GitHub/ncrystal.

**Can be converted to other formats:**
- To .laz/.lau for McStas
- To ENDF via the NJOY-NCrystal project
- But limited by target format physics capabilities!

NCrystal supports many materials out of the box. Easy to create more.

# NCrystal

[1]:
```
import numpy as np
import NCrystal as NC
import NCrystal.cifutils as nccif
```

Step 1: Create base `ncmat` model from `cif` information.

[2]:
```
cifsrc = nccif.CIFSource('ni.cif')
c_ni = NC.NCMATComposer.from_cif(cifsrc)
```

```
Loading data from file ni.cif
Attempting to load CIF data with gemmi
Self-consistency of structure was verified by spglib
```

Step 2: Replace dynamic information with VDOS.

[3]:
```
vdos_data = np.loadtxt('ni.dat')
c_ni.set_dyninfo_vdos(c_ni.find_label('Ni'), vdos_egrid=vdos_data[:,0], vdos=vdos_data[:,1])
```

Step 3: Export `ncmat` file and convert to `ENDF-6` format.

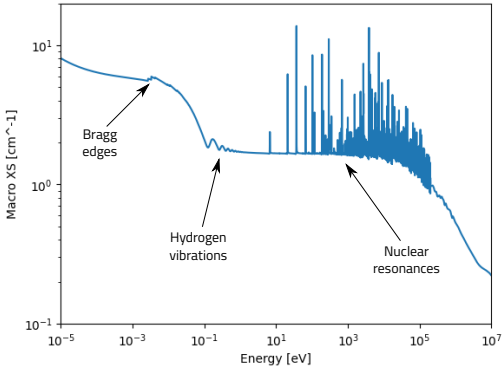
[4]:
```
a = c_ni.write('ni.ncmat')
!../ncrystal_ncmat2endf.py --name Ni ni.ncmat
```

```
Get nuclear data...
Prepare ENDF file tsl_Ni.endf...
Renumber lines...
Write ENDF file tsl_Ni.endf...
Files created:
  tsl_Ni.endf
```

NCrystal supports many materials out of the box. Easy to create more.

# OpenMC + NCrystal integration

- OpenMC supports NCrystal materials from version 0.13.3.
- In these materials, NCrystal physics replaces nuclear elastic scattering below 5 eV. Above that energy and for other reactions, ACE files derived from evaluated nuclear data libraries are used.
- This allows to integrate NCrystal with Monte Carlo simulations of neutron moderators and nuclear reactors, giving OpenMC the ability of on-the-fly thermal scattering.



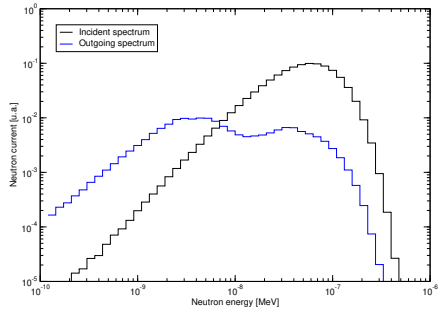

Macroscopic total neutron cross section of ZrH2 computed with OpenMC + NCrystal.

# Modifications to PHITS

- Support for continuous energy thermal scattering ACE files (`ifeng = 2` files).
- Support for mixed elastic ACE files.
- Support for small angle scattering from nanoparticles.
- Support for detector contributions for all three cases.

$\rightarrow$ Now PHITS supports all new ACE TSL files.

- The next step: direct NCrystal integration.




Spectrum from a cylindrical, 30 cm-diameter, 30 cm-high solid deuterium converter with a thermal source. Results for $10^6$ particles.

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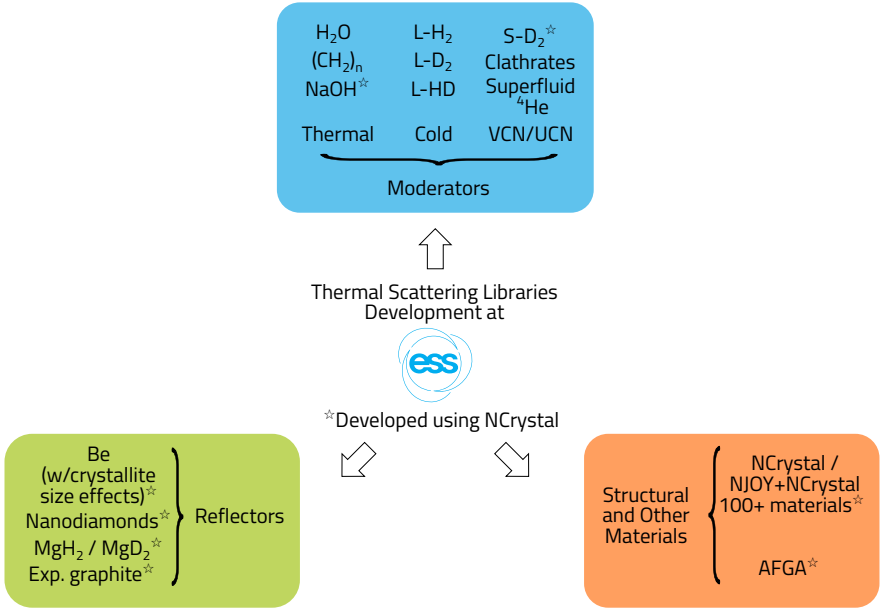
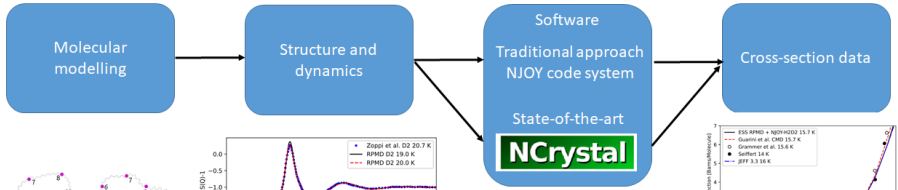

$H_2O$
$(CH_2)_n$
NaOH☆
L-$H_2$
L-$D_2$
L-HD
S-$D_2$☆
Clathrates
Superfluid $^4$He
Thermal
Cold
VCN/UCN
Moderators
Thermal Scattering Libraries Development at
ess
☆Developed using NCrystal
Be (w/crystallite size effects)☆
Nanodiamonds☆
$MgH_2$ / $MgD_2$☆
Exp. graphite☆
Reflectors
Structural and Other Materials
NCrystal / NJOY+NCrystal 100+ materials☆
AFGA☆

# New Libraries for Hydrogen and Deuterium




Liquid hydrogen and deuterium

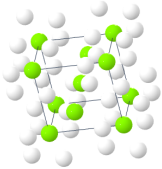
EPJ Web of Conferences **284**, 17006 (2023) https://doi.org/10.1051/epjconf/202328417006
*ND2022*

**Generation of thermal neutron scattering libraries for liquid para-hydrogen and ortho-deuterium using ring-polymer molecular dynamics**

*Douglas D.* DiJulio[1,*], *Jose Ignacio* Marquez Damian[1], *Gunter* Muhrer[1]

Submitted for consideration to be included in ENDF/B-VIII.1, alternative to the Bariloche evaluation in JEFF-3.3.

# Magnesium Hydride



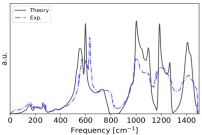




**Figure 12:** Neutron-weighted theoretical phonon DOS compared with an experimental spectrum from inelastic neutron scattering [36]. The theoretical density of states has been computed using the tetrahedron method using a $20 \times 20 \times 30$ **q**-grid for interpolation and then convoluted with a Gaussian function with standard deviation of 5 $cm^{-1}$ to better match the experimental resolution.

NCrystal

NJOY + NCrystal

MCNP6

PHITS

Particle and Heavy Ion Transport code System

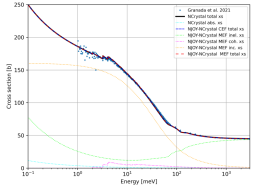
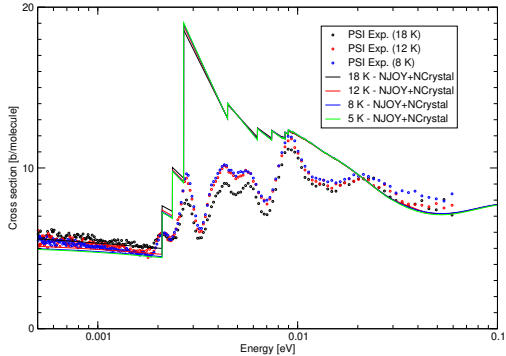



**Figure 13:** Total scattering cross section comparison for $MgH_2$.

NJOY+NCrystal: Ramić, Kemal, et al., Nucl. Instrum. and Meth. in Phys. Res. A: 1027 (2022): 166227.

# Solid deuterium

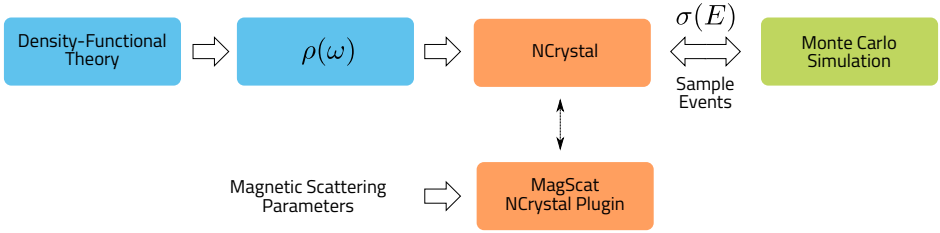
- Based on the model by Granada from 2009.
- Spin correlation is treated as a correction factor to the incoherent elastic component.
- Coherent elastic is included with an hcp basis for the molecular centers, plus an analytical molecular form factor.
- Both elastic components are included using the mixed elastic format.
- Corrects magnitude of elastic component in the IKE and old CAB models.
- TODO: include static structure factor for amorphous solid.



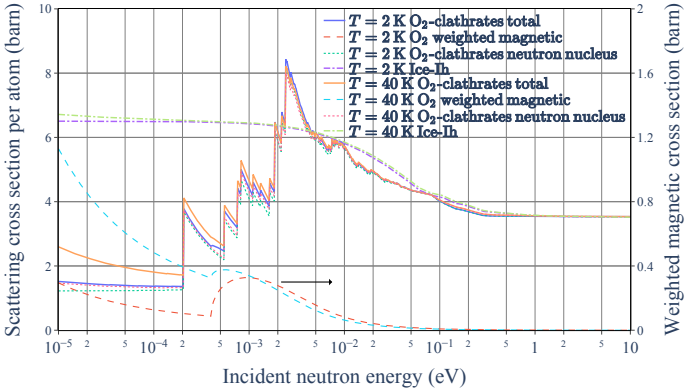
# Magnetic Scattering in $O_2$-Clathrate hydrates

Clathrate hydrates are ice-like compounds having a cage structure. Small molecules such as methane can be enclathrated in the cage, stabilising the structure.

- Oxygen-containing clathrate hydrates: neutron inelastic magnetic scattering.
- A plugin was developed based on the model from Oliver Zimmer.



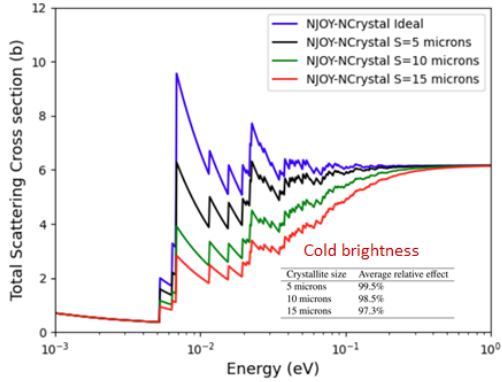
# Cross-sections for $O_2$-Clathrate hydrates



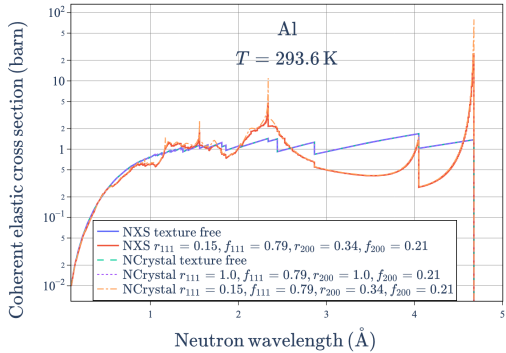

Cross sections calculated for 136 D2O + 24 O2

# Crystallite and texture effects in materials

- Standard tools assume idealized polycrystalline materials.
- Real materials exhibit effects due to crystallite size and texture.




NJOY+NCrystal with crystallite effects




Texture plugin

D.D. DiJulio et al., EPJ Web of Conferences 284, 17013 (2023) ND2022

# Small-angle scattering for nanodiamonds

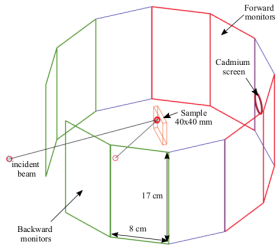



Fig. 3. Scheme of the simulated Nesvizhevsky at al. measurements of backward reflection.[9]

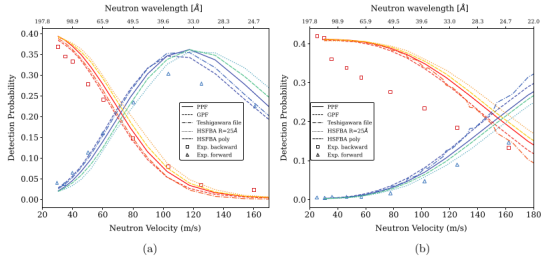



Fig. 4. Detection probability for backward scatter on a (a) 0.4-mm and (b) 6-mm ND sample. The squares are the measured points for the backward reflection, while the triangles are for forward reflection. Different models are represented with lines.

NUCLEAR SCIENCE AND ENGINEERING

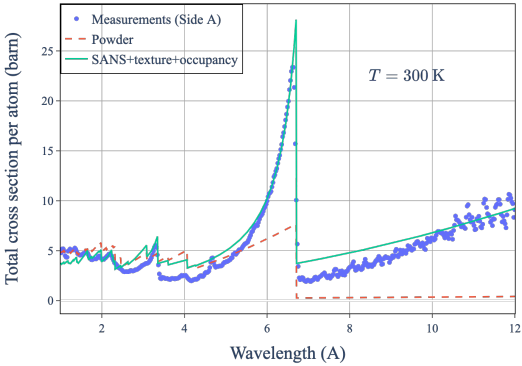
DOI: https://doi.org/10.1080/00295639.2023.2196926



## Benchmarking of the NCrystal SANS Plugin for Nanodiamonds

Nicola Rizzi,[a]* Jose I. Marquez Damian,[b] Thomas Kittelmann,[b] Bent Lauritzen,[a] Esben Klinkby,[a,b] Quentin Estiez,[c] and Valentina Santoro[b]

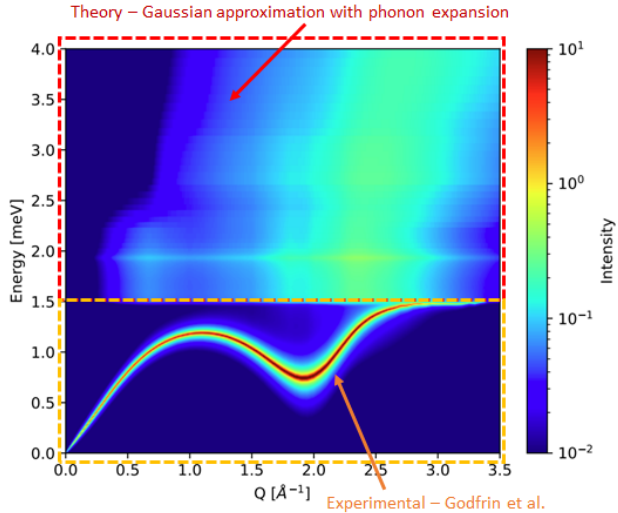
# Texture and SANS in graphitic compounds




Application of both the texture and SANS plugins in NCrystal.

# Superfluid Helium

- We created scattering kernels to be used with Monte-Carlo simulations in Superfluid Helium.
- Constructed from combination of experimental and theoretical data.




J.R. Granada, et al., Nucl. Instr. and Methods in Physics Research A 1053 (2023) 168284

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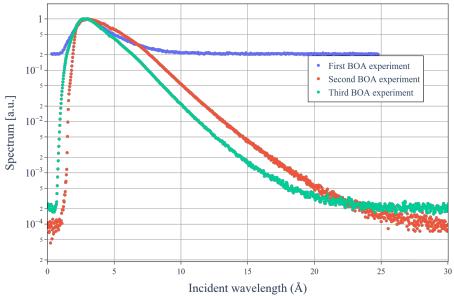
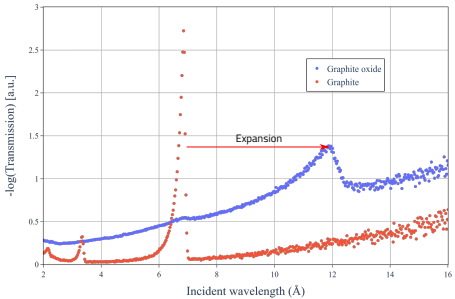
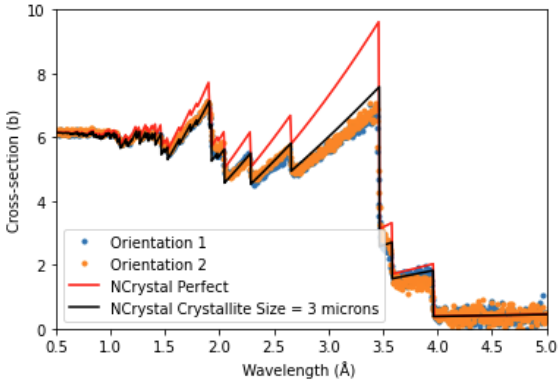
# Benchmark experiments: graphitic compounds

- Benchmark experiments are critical for development of new models, especially very-cold and ulra-cold materials.
- Carried out measurements at the BOA beamline at PSI for graphitic compounds together with support of ESS Chemistry and Life Science Support Group.



# Benchmark experiments: beryllium




- Transmission and texture measurement of beryllium in the diffractometer HIPPO at LANSCE.
- Preliminary transmission results show reduction of cross section, compatible with extinction models.
- Although, further analysis is needed to discard possible texture effects.

# HighNESS School on Thermal Scattering

- First school of its kind. Held in May at the ESS.
- Included 40 participants registered from around the world.
- School material available online:
  `https://github.com/highness-eu/TSL_School`

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# Concluding Remarks

- The ESS Spallation Physics group develops new methods for treating nuclear data in Monte-Carlo simulations through various approaches.
- Modified library format to support new physics: NJOY+NCrystal / ncmat2endf
- Extensions of NCrystal to include new physics processes: NCrystal plugins
- Modifying Monte-Carlo software to support these developments: OpenMC, PHITS.
- Work is motivated by applications of the current facility and future upgrades, but also has applications to other nuclear systems.
- We work on release and maintain the codes, models and data libraries: feedback is much appreciated. If new features or materials are needed, we are open to collaboration.