

Quantitative data analysis for neutron scattering experiments using NCrystal

S. Xu, D.D. DiJulio, J.I. Marquez Damian, T. Kittelmann, R. Woracek, T. Chulapakorn,
and G. Muhrer

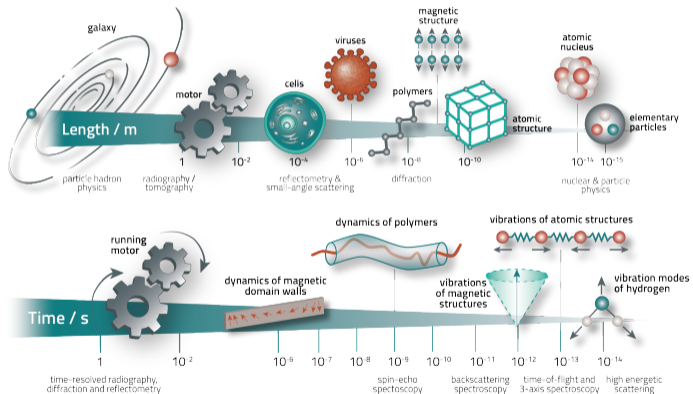
Special thanks to the KTH team (ReHEART project), the HIPPO (LANL) team, and many colleagues within the HighNESS project

Apr. 16, 2026



Neutron as a probe for exploring materials

From life-sized to atomic resolution, dynamics from seconds to a few tens of femtoseconds.



<https://ess.eu/science-using-neutrons>

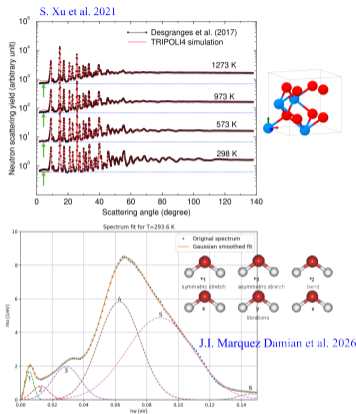
Low-energy neutron for exploring materials

◇ The **wavelengths** of low-energy neutrons are **comparable to the atomic spacing** in solids and liquids, allowing for the investigation of material structures through interference effects, e.g., **diffraction** in uranium dioxide.

◇ The **energy** of low-energy neutrons is **comparable to the excitation energies of matter**, enabling the study of atomic vibrations via **inelastic scattering**, e.g., dynamics of hydrogen in water molecule.

◇ **High penetration power** (compared to X-ray).

◇ Neutrons possess a nonzero magnetic moment, allowing for **magnetic interactions** with unpaired electrons in matter.

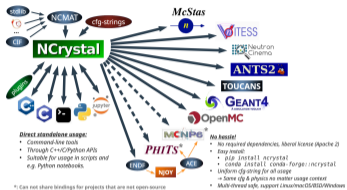


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- 1 Review of using NCrystal for analyzing neutron scattering experiments
- 2 Analysis of inelastic magnetic scattering, transmission, and imaging experiments using NCrystal
- 3 Summary

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Developed by [T. Kittelmann](#) (DMSC), supported by the Spallation Physics Group (ESS). (See also talk on Monday 13 April, *Update on NCrystal, T. Kittelmann et al.*)

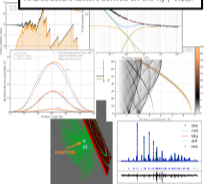
Cai et al. J. Comput. Phys. 380 (2019)

Cai and Kittelmann Comput. Phys. Commun. 246 (2020) 106851

Kittelmann and Cai Comput. Phys. Commun. 267 (2021) 108082

Elastic ($\Delta E=0$) components

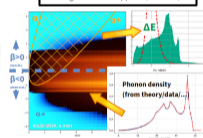
Bragg diffraction, incoherent, single crystals, isotropic materials (powders), HOPG, HKL structure factors derived on-the-fly ($\sim 0.1s$).



Inelastic ($\Delta E \neq 0$) components

Scattering kernel based:

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



Ca0_sg225_Calciumoxide.ncmat	LiquidWater920_T293.4K.ncmat	Polycarbonate_C1603K14.ncmat	Y2O3_sg204_Yttrium_oxide.ncmat
Ca_sg225.ncmat	Lu2O3_sg206_Lutetiumoxide.ncmat	Polyester_C108804.ncmat	Y2SiO5_sg15_Y5O.ncmat
Ca_sg229_Calcium-gamma.ncmat	Lu2SiO5_sg15.ncmat	Polyethylene_C82.ncmat	Y3Al5Si2O12_sg230_YAG.ncmat
CaSiO3_sg2_Melastenite.ncmat	Mg2SiO4_sg2_MagnesiumSilicate.ncmat	Polyacilide_C9402.ncmat	Y_sg194.ncmat
CaSi2_sg25_Ceriumoxide.ncmat	MgAl2O4_sg27_MAS.ncmat	Polypyrrolone_C386.ncmat	ZnF2_sg184_ZincFluoride.ncmat
Cr_sg229.ncmat	MgCO3_sg187_MagnesiumCarbonate.ncmat	Polystyrene_C388.ncmat	ZnO_sg186_Zincoxide.ncmat
C_sg194_pyrolytic_graphite.ncmat	MgO_sg136_MagnesiumOxide.ncmat	PT_sg225.ncmat	ZnO_sg184.ncmat
C_sg227_Diamond.ncmat	MgF2_sg136_MagnesiumFluoride.ncmat	PVC_C203CL.ncmat	ZnS_sg216_Sphalerite.ncmat
Cu2O_sg226_Cuprite.ncmat	MgO_sg136_MagnesiumOxide.ncmat	Pb_sg229.ncmat	ZrF4-beta_sg04.ncmat
Cu_sg225.ncmat	MgO_sg184_MagnesiumOxide.ncmat	Rubber_C388.ncmat	ZrO2_sg127_Zirconia.ncmat
Dp201_sg206_Pyrrusiumoxide.ncmat	MgO_sg125_Periclase.ncmat	SiC_sg184.ncmat	ZrO2_sg14_Zirconia.ncmat
Epoxy_Araldite696_C1882803.ncmat	Ni_sg184.ncmat	SiC-beta_sg214_BetaSiliconCarbide.ncmat	Zr_sg184.ncmat

134 materials (v4.3.0):
Crystals (110), amorphous solids (16), liquids, gasses, ...

Small (few kB) file sizes:
- Entire collection normally embedded in NCrystal shared library.

Easy universal cfg:
"Al_sg225.ncmat;temp=250K"
"Rubber_C388.ncmat;comp=inelas"
- Same physics in all applications!

NCrystal for neutron experiment analysis

NCrystal has been employed to solve problems by many of our colleagues.

Total cross section or attenuation coefficient:

- ◇ lithiation phases of graphite Strobl et al. Adv. Energy Mater. 2025, 15, 2405238
- ◇ CuCrZr Sumarli et al. Virtual Phys. Prototyping 2024, 19(1)
- ◇ boron nitride and polylactic acid Sebold et al. Sci Rep 14, 19348 (2024)
- ◇ CuCrZr and tungsten Minniti et al. Nucl. Fusion 65 (2025) 026041
- ◇ CaH₂ and H₂O Simoni et al. Phys. Chem. Chem. Phys., 2023, 25, 30821

Bragg edge analysis:

- ◇ steel and uranium Hirsh et al. Sci Rep 15, 12901 (2025)

Modeling neutron interaction:

- ◇ sapphire filter in the Dingo imaging beamline Jakubowski et al. Sci Rep 15, 11233 (2025)
- ◇ neutron detection for imaging Povoli et al. 2023 JINST 18 C01056

Small-angle neutron scattering:

- ◇ porous nuclear-grade graphite K. Ramić et al. Carbon 244 (2025) 120619

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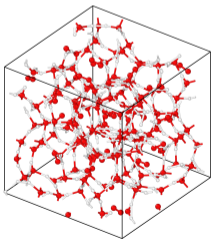
Magnetic neutron scattering

IOP Publishing
J. Phys.: Condens. Matter 36 (2024) 385504 (15pp)
Journal of Physics: Condensed Matter
https://doi.org/10.1088/1361-648X/ac9947

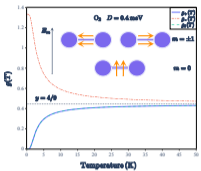
Physical model of neutron scattering by clathrate hydrate and C₆₀ hosting paramagnetic oxygen molecules

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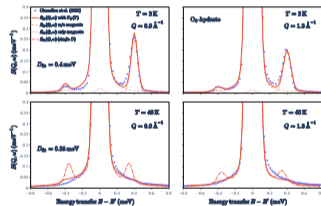
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O₂-hydrate is considered as a potential neutron moderator material for producing very cold neutrons (investigated in the HighNESS project led by V. Santoro).



Magnetic neutron scattering model of paramagnetic O₂ developed by O. Zimmer (ILL).



Particular interests in neutron-nucleus and magnetic scattering physical model study and implementation.

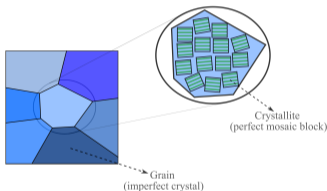
Extinction in beryllium metal (1/2)




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Impact of extinction effects on neutron transmission in solid beryllium metal

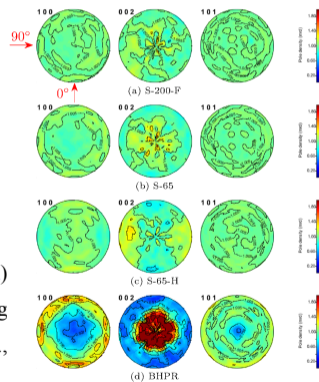
S. Xu,^{a*} D. D. DiJulio,^{a*} J. I. Marquez Damian,^a S. C. Vogel,^b A. M. Long,^b T. Y. Hirsh,^c T. Kittelmann,^a V. Kuksenko^d and G. Muhrer^a



The extinction effects in beryllium (**neutron reflector material**) have been studied by **D.D. DiJulio** for years, and are gaining attention in the imaging and nuclear data communities (e.g., Armco Iron led by T. Chulapakorn & R. Woracek).

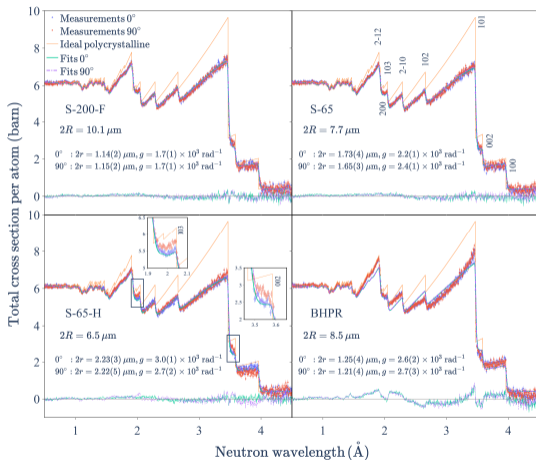
research papers

Time-of-flight neutron **transmission and diffraction** measurements were conducted on four solid beryllium grades by S.C. Vogel at the HIPPO instrument (LANL).



The pole figures show that except for the BHPR sample, the others exhibit only **mild texture**.

Extinction in beryllium metal (2/2)



Lower cross section (or higher transmission) is observed compared to the ideal polycrystalline assumption, which can be interpreted using the [Becker & Coppens extinction model](#) (improved by [Kittelmann et al. 2026](#)). This study highlights [neutron time-of-flight transmission](#) as a [sensitive method](#) for investigating [extinction phenomena](#). It underscores the importance of accounting for extinction in quantitative imaging data analysis.

Detecting hydrogen by neutron imaging

Trace amounts of hydrogen can lead to significant degradation of mechanical properties in high-strength steels and Ni-based alloys.

Devi et al. 2024

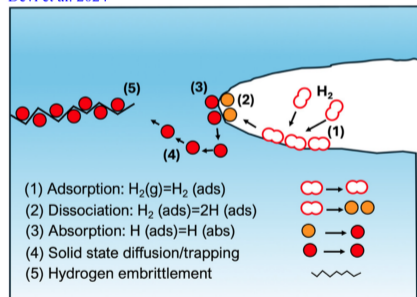


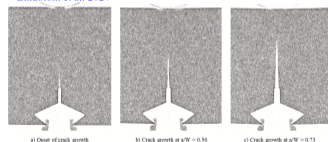
Fig. 1 Introduction of hydrogen to materials, and the steps leading to hydrogen embrittlement.

Available H Mapping Techniques (Yu et al. 2024):

- ◇ Thermal desorption spectroscopy (TDS): no spatial resolution
- ◇ Secondary ion mass spectrometry (SIMS) or atom probe tomography (APT): limited by small sample volumes (or destructive)

Neutron imaging is a promising techniques due to its high penetration depth and intrinsic sensitivity to hydrogen, while quantitative analysis remains challenging.

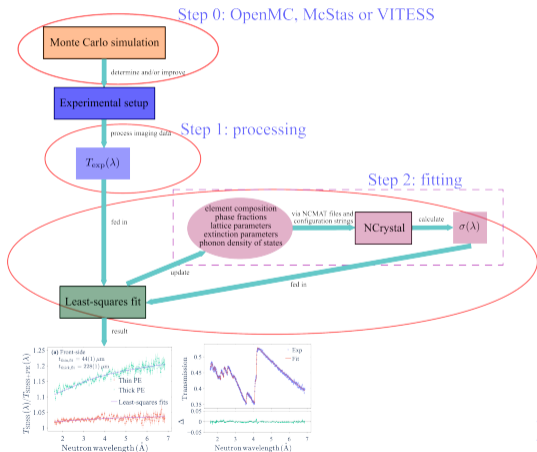
Lindblom et al. 2024



ReHEART project (led by J. Pan (KTH) & R. Woracek). Neutron white beam measurements achieved. Operando wavelength-resolved neutron imaging data to be analyzed.

Quantitative neutron imaging analysis

Workflow for quantitative imaging analysis:



1 Quantification in wavelength-resolved neutron imaging: 2 exemplified using stainless steel and polyethylene for 3 mimicking hydrogen

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5 Liu ^c, D.D. DiJulio ^a, T. Kittelmann ^e, A. Losko ^f, S. Athanasopoulos ^a, J.
6 Pan ^c, A. Larsson ^b, G. Muhrer ^a, W. Kockelmann ^g, R.S. Ramadhan ^g, A.
7 Wolfertz ^f, and R. Woracek ^{a,f}

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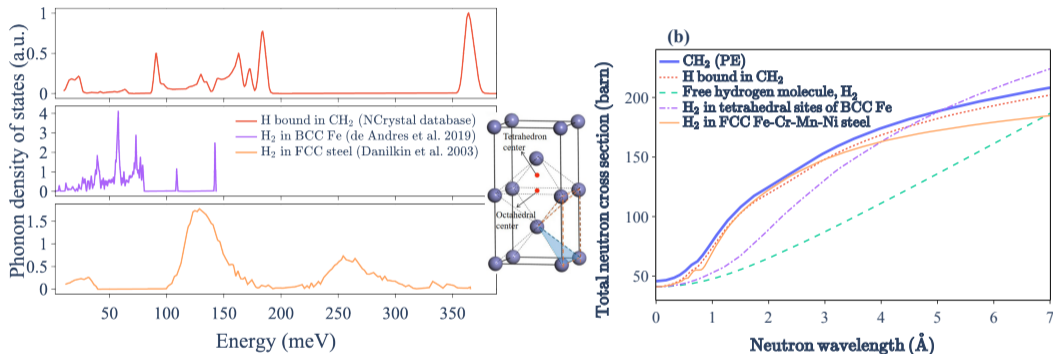
^fForschungs-Neutronenquelle Heinz Maier-Leibnitz, 85748, Garching, Germany

^gISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, UK

Paper in preparation.

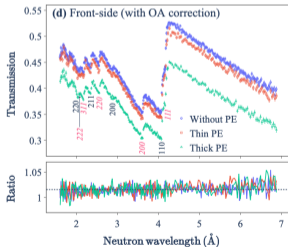
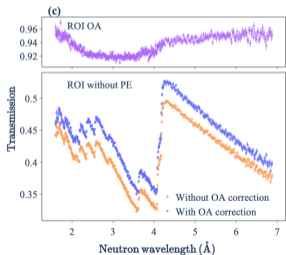
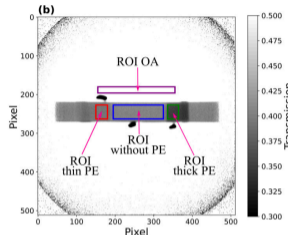
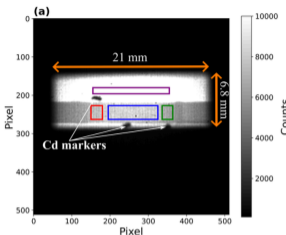
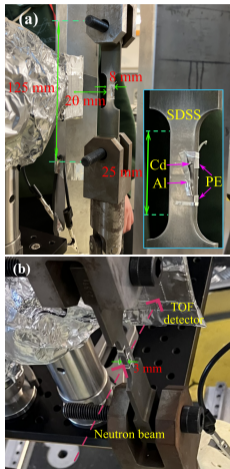
Is it reasonable to mimic hydrogen using polyethylene (PE)?

Transmission dependant on H dynamics



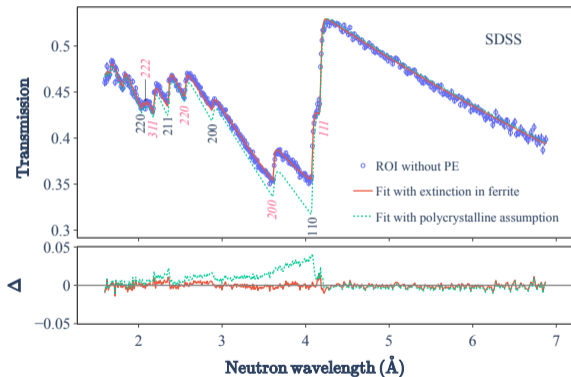
These results demonstrate the sensitivity of the neutron signal to hydrogen dynamics. Our workflow can be readily applied to quantify hydrogen concentrations in Fe-based alloys.

Step 1: Data processing



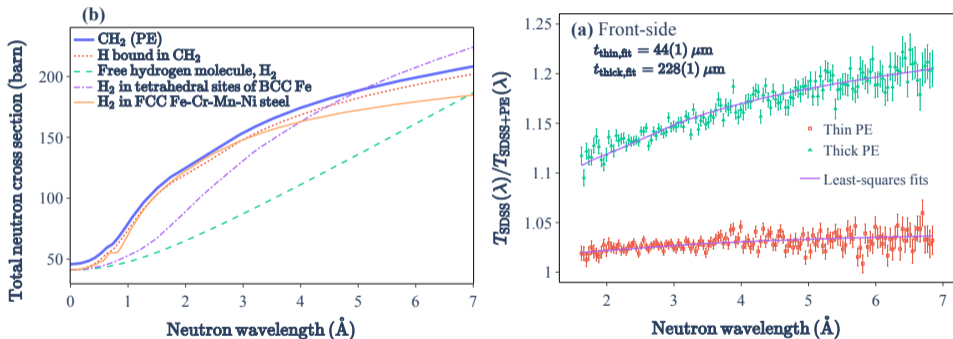
Step 2: NCrystal-based Bragg edge analysis

The NCrystal-based least-squares fitting routine simultaneously resolves multiple microstructural parameters, lattice parameters, phase fractions, and element composition.



Hydrogen concentration analysis

If we focus primarily on the hydrogen concentrations, we can fit the ratio of transmission signals using the cross section calculated by NCrystal.



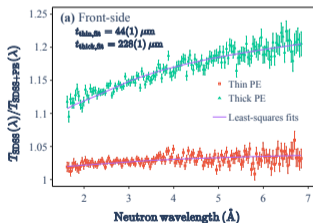
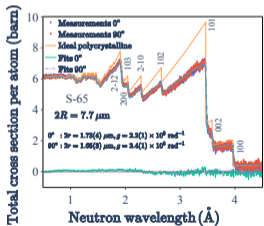
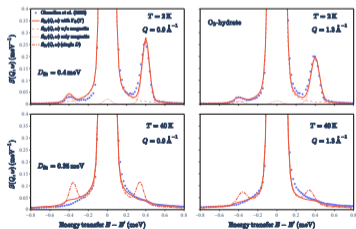
We have obtained promising results in quantifying hydrogen signals (both electrochemical and gas-charging) from measurements performed at RADEN (J-PARC).

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Summary

- Implementation and validation of physical model of magnetic neutron scattering of O_2 -hydrate.
- Highlight of sensitivity of neutron transmission measurement to extinction phenomenon.
- Quantification of hydrogen signals in neutron radiography experiments.



Thank you for your attention!