

HighNESS General Meeting

Work Package 2 - Software Development

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Main Aims of Work Package

Development of software to describe low-energy neutron transport in reflectors and moderator materials.

Tasks:

- 2.1. Develop models for magnesium hydride, nanodiamonds, intercalated graphite, and clathrate hydrates. Models will be implemented in NCrystal to be used in Geant4, MCNP, PHITS, or OpenMC.
- 2.2. Develop molecular modelling techniques, such as molecular dynamics and density functional theory, in order to provide input to the models in task 2.1.

Deliverables:

- D2.1. Report and simulation software for nano-diamonds (M12)
- D2.2. Report and simulation software for MgH_2 (M12)
- D2.3. Report and simulation software for intercalated graphite (M34)
- D2.4. Report and simulation software for clathrate hydrates (M34)

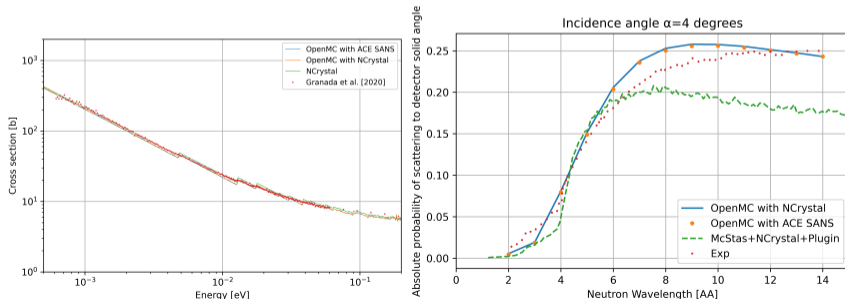


- D2.1 (nanodiamonds) and D2.2 (magnesium hydride) deliverables finished.
- Work published in NIM A (NJOY+NCrystal paper) and presented at AccApp 2021 and Nuclear Data 2022.
- Finalizing work on the nano-diamonds particles: molecular modelling.
- Work has started on the clathrate-hydrates: Molecular modelling and implementation of magnetic scattering.
- Experiment at PSI on intercalated graphites, followup proposal submitted.
- All this work is supported by NCrystal developments.

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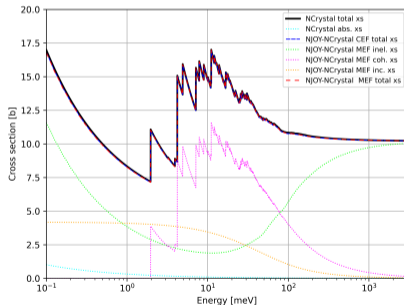
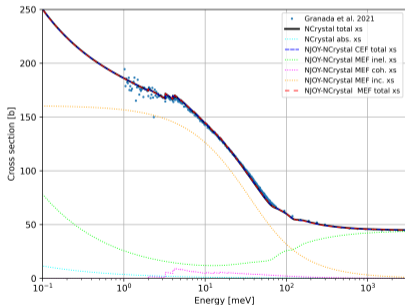
Results D2.1 (Nanodiamonds)

- Implemented as an ACE library + SANS subroutine and by direct call of NCrystal with the nanodiamond plugin.
- Based on molecular modelling including the finite-size effects of the nano-diamonds



Results D2.2 (Magnesium Hydride)

- NJOY+NCrystal mixed elastic (MEF) and current ENDF (CEF) formats.
- Phonon spectrum computed from DFT simulations by U. Milano-Bicocca.



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NJOY+NCrystal Library

- New developments led to creation of the largest TSL library to date. A total of 213 new evaluations.
- Provides extensive benchmarking for the methods developed in WP2.

The screenshot shows a GitHub repository interface. At the top, it indicates the current branch is 'master', with 1 branch and 2 tags. There are buttons for 'Go to file', 'Add file', and 'Code'. Below this is a commit history table:

| Author | Message | Time | Commits |
|-----------------------------|---|---------------------|---------------|
| Jose Ignacio Marquez Damian | Updated ZrSiO4-135 | 092046e 22 days ago | 2,102 commits |
| | endf_standard Updated ZrSiO4-135 | 22 days ago | |
| | mixed_elastic Updated ZrSiO4-135 | 22 days ago | |
| | README.md Added references to NJOY and NCrystal versions. | 4 months ago | |

Below the table is the content of the README.md file:

NJOY+NCrystal Library

This repository contains a library of thermal scattering files generated with a special version of [NJOY2016](#), modified to compute coherent scattering with [NCrystal](#). This tool, called NJOY+NCrystal, is available [here](#).

For each material, TSL files in the [ENDF-6](#) and [ACE](#) formats are included. Two versions are provided: the standard format that can either contain coherent or incoherent elastic, and one in the improved format recently [proposed](#), called "mixed elastic", which contains both. This new format is not yet supported in MCNP, but a modified version of [OpenMC](#) that supports it is provided in a [separate repository](#).

All temperatures are provided in ENDF-6 format, but only the first one is provided in ACE format because of space requirements. Nevertheless, pdf plots created with ACER are provided for all the temperatures.

Evaluations in this release were generated with [NJOY2016 2016.61_njoyncrystal](#) and [NCrystal v2.6.1_njoyncrystal](#).

More details can be found in the following papers:

- K. Ramic, J.I. Marquez Damian, T. Kittelmann, D.D DiJulio, D. Campi, M. Bernasconi and V. Santoro. "NJOY+NCrystal: an open-source tool for creating thermal neutron scattering libraries" (to be submitted)
- X.-X. Cai and T. Kittelmann, NCrystal: A library for thermal neutron transport, Computer Physics Communications 246 (2020) 106851, <https://doi.org/10.1016/j.cpc.2019.07.015>

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All developments are freely available online

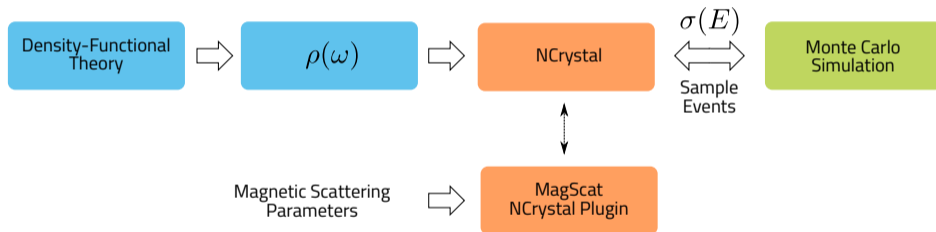
They are hosted on Github, following the Data Management Plan:

- OpenMC+Ncrystal:
https://github.com/highness-eu/openmc/tree/mixed_ncrystal
- NCrystal nanodiamonds plugin:
<https://github.com/highness-eu/ncplugin-SANSND>
- NJOY+Ncrystal:
https://github.com/highness-eu/NJOY2016/tree/njoy_ncrystal,
https://github.com/highness-eu/ncrystal/tree/njoy_ncrystal
- NJOY+Ncrystal Library:
<https://github.com/highness-eu/NJOY-NCrystal-Library>



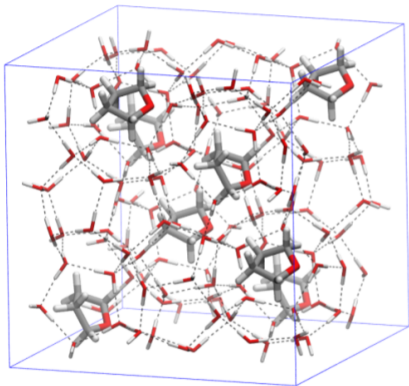
Deliverable D2.3 (Intercalated graphite)

- Creating scattering models and testing: Using NJOY+NCrystal.
- Measurements at PSI and follow-up proposal submitted with WP3.
- Survey of possible materials. Carbon / fluorine / oxygen intercalated compounds; C_{60} ; Other compounds.
- Microscopic modelling by UNIMIB.



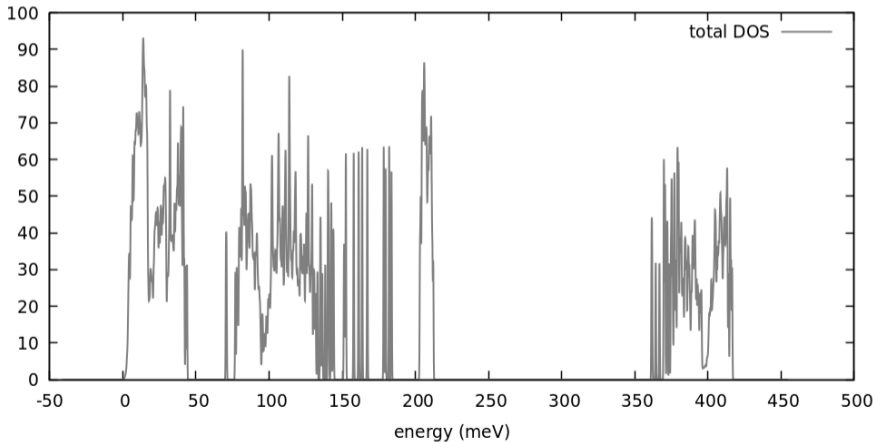
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DFT Simulations

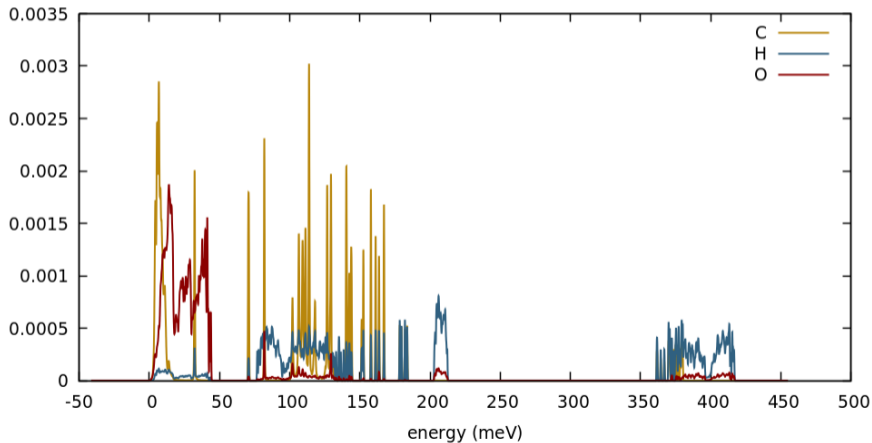


- Tetrahydrofuran (THF) SII hydrate model optimised with DFT
- THF occupies the large cages, unit cell has 136 water molecules and 8 THF molecules
- Phonon DOS computed using CP2K and phonopy





DFT Simulations - projected density of states



Neutron slowdown by paramagnetic materials

It is theoretically verified the production of VCN by paramagnetic materials encaged in clathrate hydrates, and deuterated O2-clathrate hydrates appear particularly promising (Zimmer 2016). The double differential magnetic scattering cross section for unpolarized neutrons is given by:

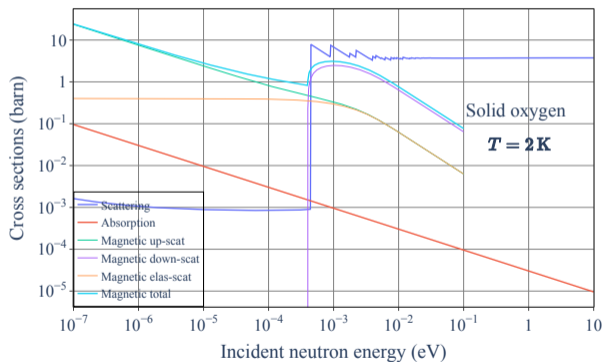
$$\frac{d^2\sigma}{d\Omega dE'} = b_m^2 \frac{k'}{k} \exp(-2W) |F(\kappa)|^2 \quad \text{Magnetic form factor}$$
$$\times \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \left(\frac{1}{3} \langle S^+ S^-(t) + S^- S^+(t) \rangle + \frac{2}{3} \langle S_z^2 \rangle \right) \exp(-i(E - E')t/\hbar) dt.$$

Inelastic (down & up-scattering) Elastic

Oliver Zimmer. Phys. Rev. C, 93:035503, Mar 2016.

Magnetic cross sections of solid oxygen

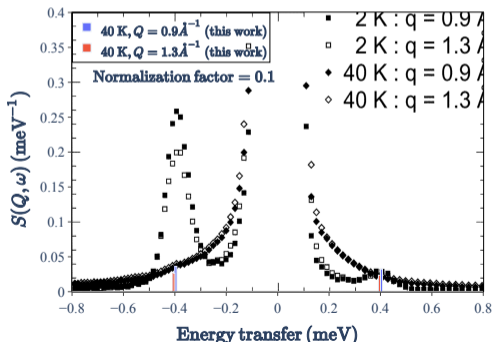
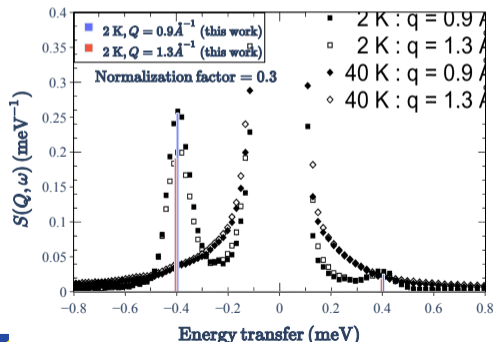
Solid oxygen ($\text{Pm}\bar{3}n$) is investigated. The cross sections are calculated by using NCrystal-3.0.0+MagScat plugin.



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Investigation of Chazallon's experiments

Though the peaks at around 0.4 meV are tentatively attributed to crystal field effects by the authors, we reproduce correctly with the magnetic formulae derived by Zimmer. Monte-Carlo simulations by using OpenMC+NCrystal are ongoing.



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NCrystal 3.0

- Improved data library: 131 materials
- Framework support for multiphase materials.
- Framework for SANS physics, including utilities for easier handling of SANS plugins.
- Improved integration with McStas, supporting McStas 2.x and 3.x and supporting NCrystal materials in McStas Union. Thanks to collaboration with Mads Bertelsen.
- Going forward: improving sampling and biasing for UCN and VCN production.



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Summary

- Deliverables D2.1 and D2.2 have been finalized.
- Software and data were released according to the data management plan and results were presented in a NIM A paper and the AccApp conference.
- Implementation of magnetic scattering model is ongoing in parallel to the molecular modelling simulations of clathrates with DFT
- Work on graphitic compounds has started. First experiment carried out with a followup proposal submitted for later this year.

