DTU

HighNESS International School on Thermal Neutron Scattering Kernel Generation

SANS plug-in for Nanodiamonds

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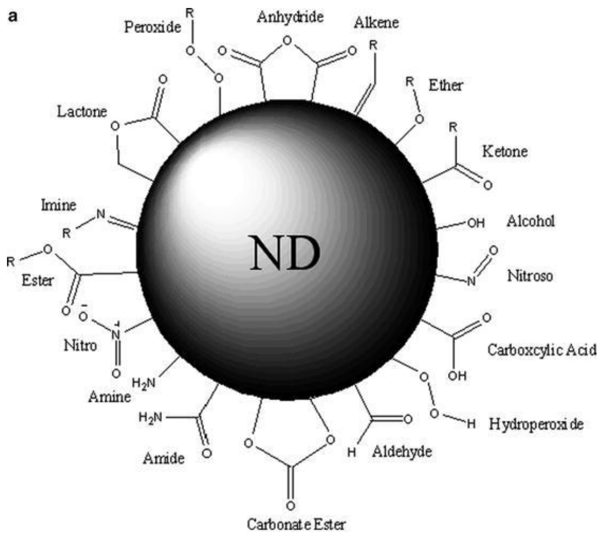
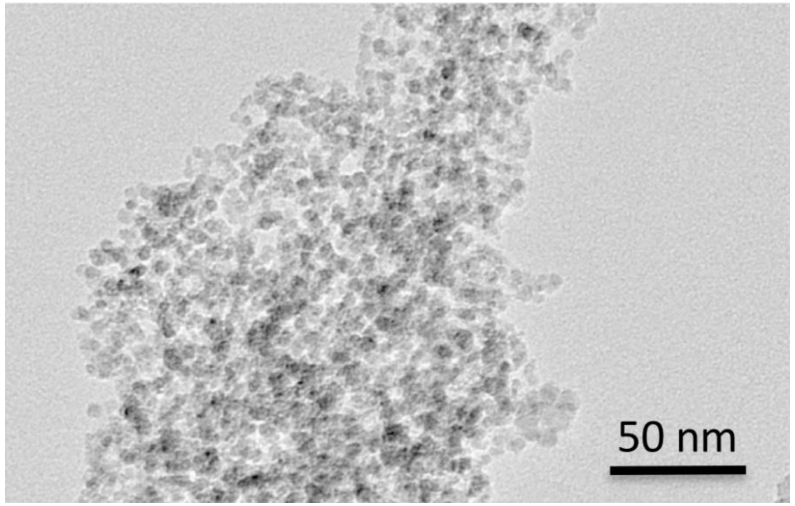
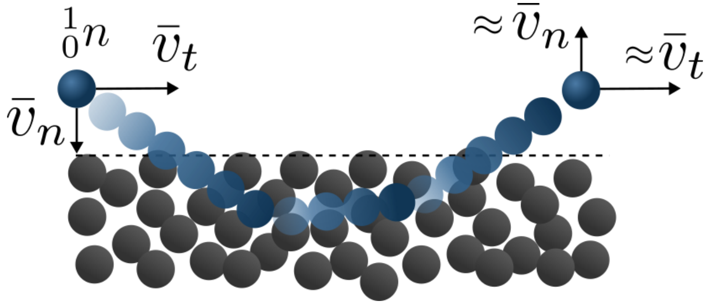
Images from [5]

What are nanodiamond particles?

- A diamond core within an onion-like shell measuring few nanometers;
- The outer surface is a shell with complex chemical composition, consisting of impurities such as carbon, oxygen, nitrogen and hydrogen;
- Nanodiamond Powder samples showed efficient reflector properties for very cold neutrons (VCN) up to 10^{-4} eV [2];
- Large cross-section for small-angle elastic scattering in the VCN wavelength, and very low absorption.







Main reference

NUCLEAR SCIENCE AND ENGINEERING
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DOI: https://doi.org/10.1080/00295639.2023.2196926

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Benchmarking of the NCrystal SANS Plugin for Nanodiamonds

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Received November 21, 2022
Accepted for Publication March 25, 2023

SCAN ME

SANSND plugin for NCrystal

SANS experimental $I(q)$ in absolute units = $\frac{d\sigma}{d\Omega}(q)$ microscopic differential per-atom cross section with units barn sr^{-1}

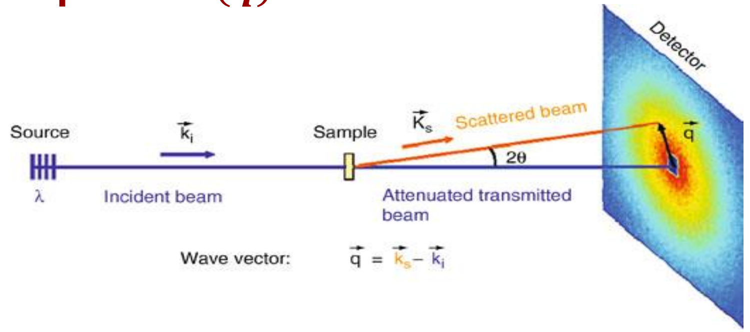
$$\sigma_{SANS}(k_0) = \int I(q)d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} I(q)d\theta$$

$$q = 2k_0 \sin\frac{\theta}{2} \longrightarrow qdq = k_0^2 \sin\theta \, d\theta$$

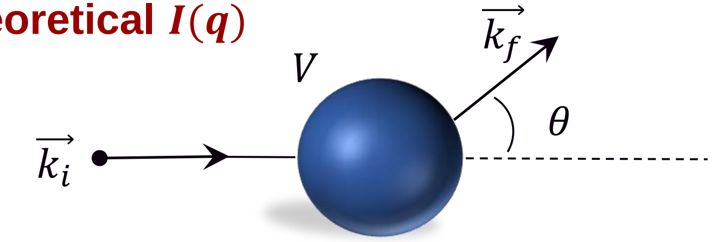
$$\sigma_{SANS}(k_0) = \frac{2\pi}{k_0^2}\int_0^{2k_0} I(q)qdq$$

total microscopic per-atom cross section

Empirical $I(q)$



Theoretical $I(q)$



Empirical models

- *Piece-wise power law*

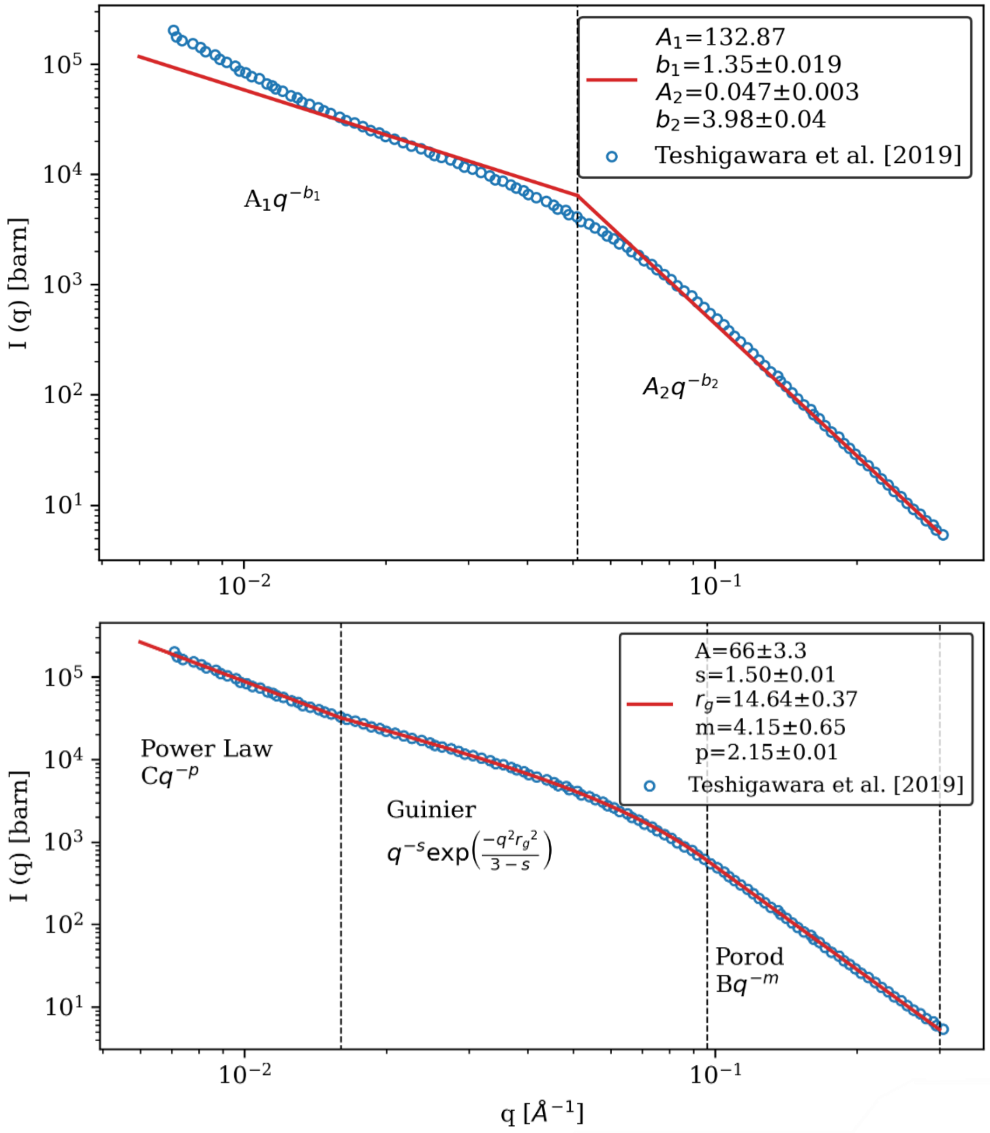
$$I(q) = \begin{cases} A_1 q^{b_1} & q < Q_0 \\ A_2 q^{b_2} & q > Q_0 \end{cases}$$

- *Guinier-Porod + power law*

$$I(q) = \begin{cases} Cq^{-p}, & Q_{min} \leq q \leq Q_1 \\ q^{-s} e^{\frac{-q^2 r_g^2}{3-s}}, & Q_1 < q < Q_2 \\ Bq^{-m} & q \geq Q_2 \end{cases}$$

- *Data file*

Data from [1]



Theoretical model

Scattering amplitude per nanoparticle for hard sphere model using first Born approximation [8]:

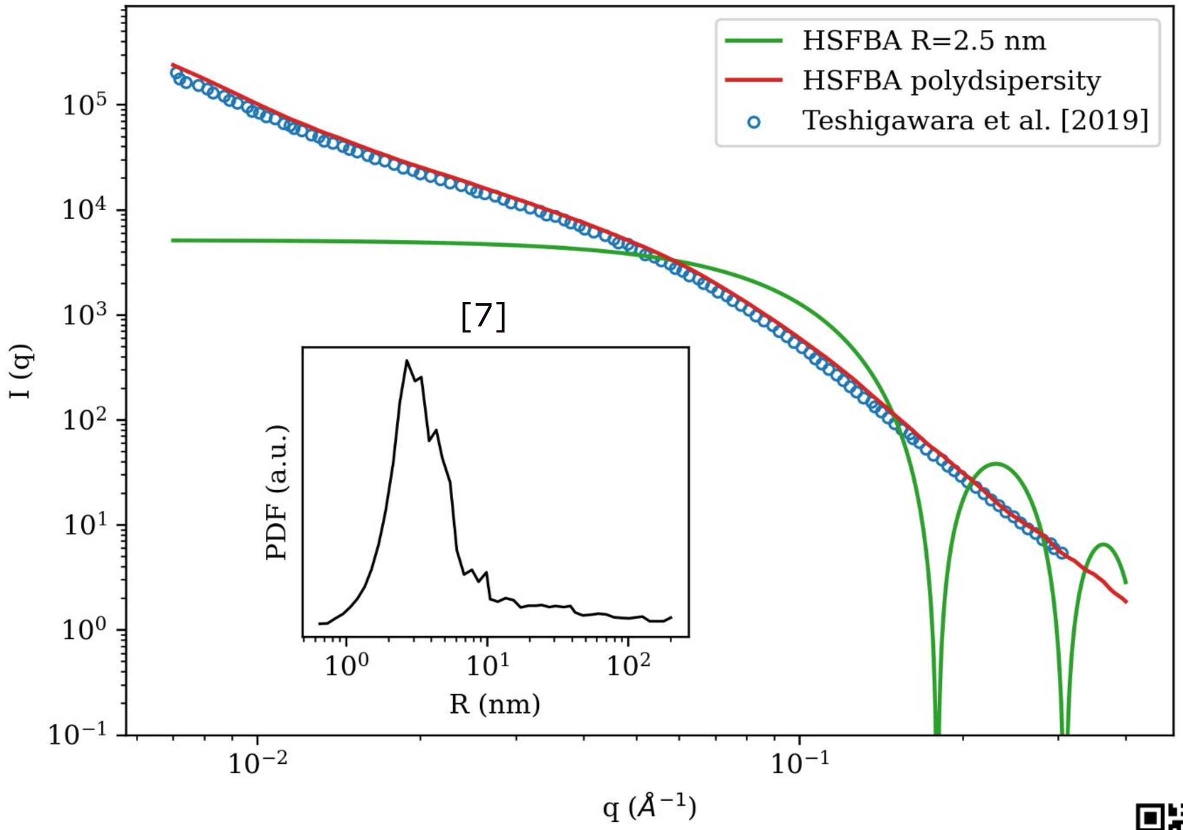
$$f(\theta) = -\frac{2m}{\hbar^2} V R^3 \frac{1}{(qR)} \left(\frac{\sin(qR)}{(qR)^2} - \frac{\cos(qR)}{qR} \right)$$

Fermi Potential **ND radius**

Then $I(q)$ is just:

$$I(q) = \frac{|f(\theta)|^2}{N_C}$$

No. of C in ND



How to enable it?

https://github.com/highness-eu/ncplugin-SANSND

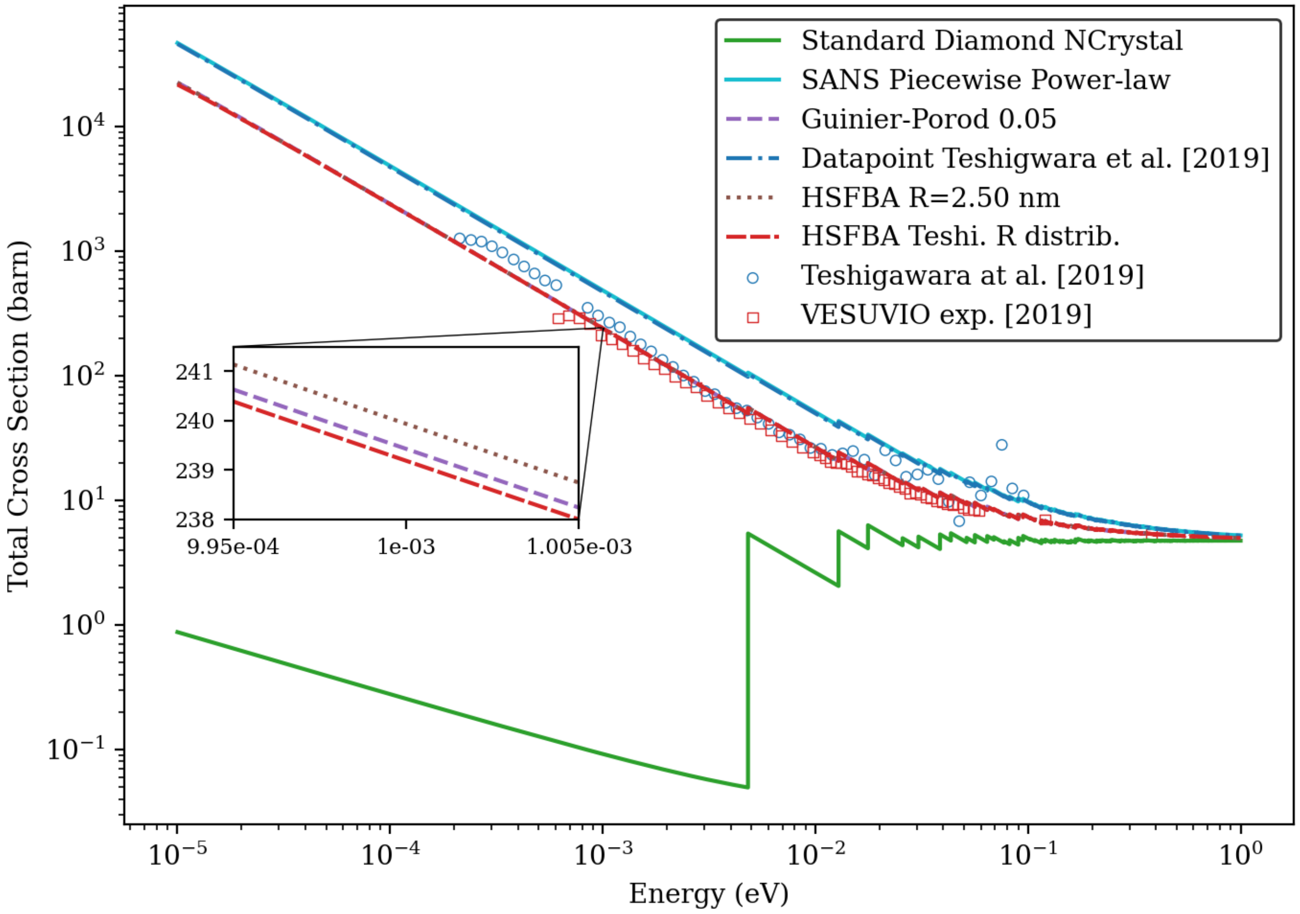
The plugin comes with a SANSND_nanodiamond.ncmat file:

- set the right density;
- choose the model;
- pass the right parameters

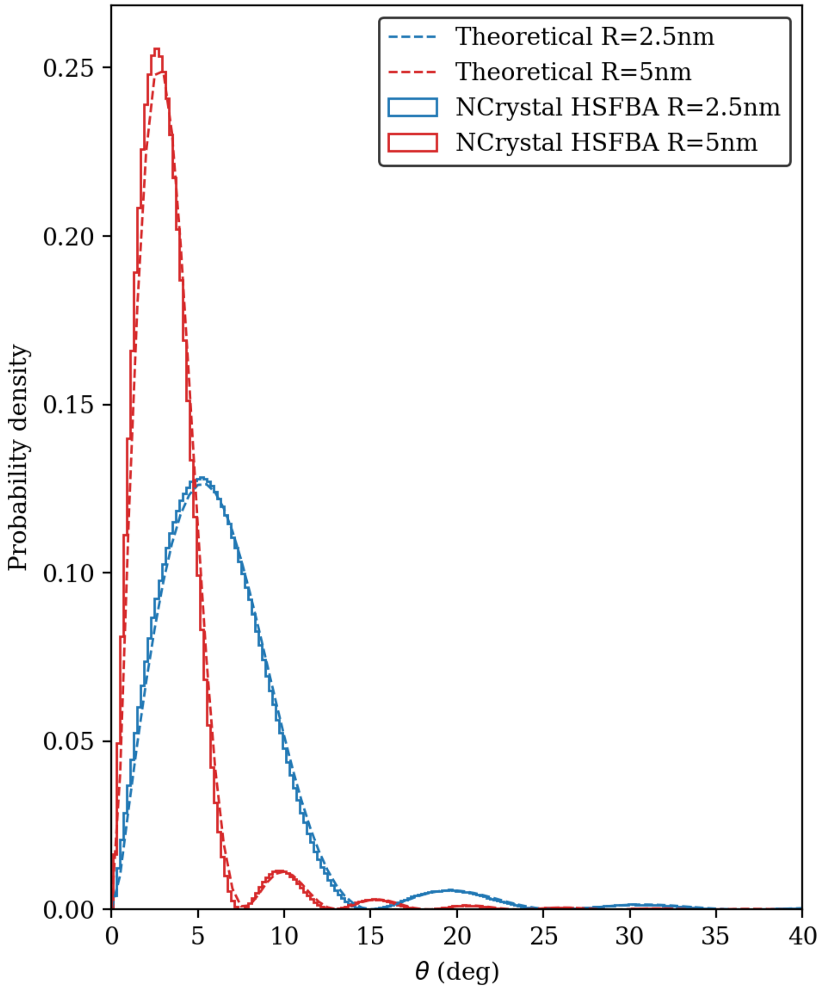
```
@CUSTOM_SANSND
# custom physics that enables SANS for Nanodiamond particles
2.0                              # plugin version
model                            # model string input (see Plugin Readme)
parameters                       # relevant parameters (see Plugin Readme)
```

Model	Inupt name	Input parameters
Piece-wise power law	PPF	$A_1\ b_1\ A_2\ b_2\ Q_0$
Guinier-Porod + power law	GPF	$A\ s\ r_g\ m\ p\ Q_{min}$
Input data file	FILE	filename
Hard Sphere First Born Approximation	HSFBA	R in nm or R distribution filename

Benchmark



Standard Diamond NCrystal
SANS Piecewise Power-law
Guinier-Porod 0.05
Datapoint Teshigwara et al. [2019]
HSFBA R=2.50 nm
HSFBA Teshi. R distrib.
Teshigawara at al. [2019]
VESUVIO exp. [2019]
Total Cross Section (barn)
Energy (eV)
241
240
239
238
9.95e-04
1e-03
1.005e-03



Theoretical R=2.5nm
Theoretical R=5nm
NCrystal HSFBA R=2.5nm
NCrystal HSFBA R=5nm
Probability density
θ (deg)

Nesvizhevsky backward reflection experiment [2]

- Nanodiamond powder sample of 4×4 cm^2
- 0.4mm and 6mm thickness
- Monochromatic VCN-CN source
- Simple counting monitors
- Cadmium Beamstop

$$R = \frac{\text{Backward counts}}{\text{Forward counts} + \text{Backward counts}}$$

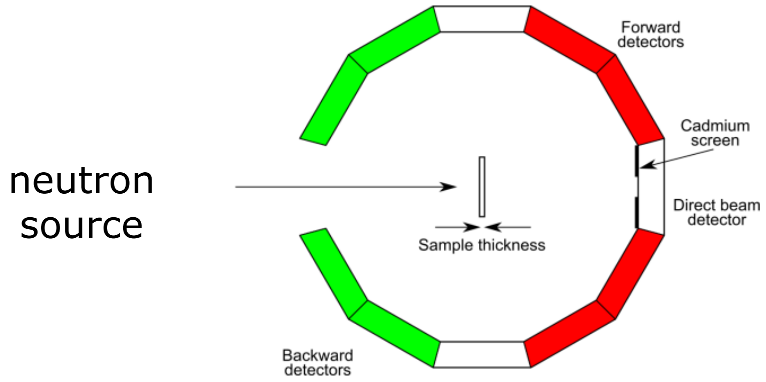
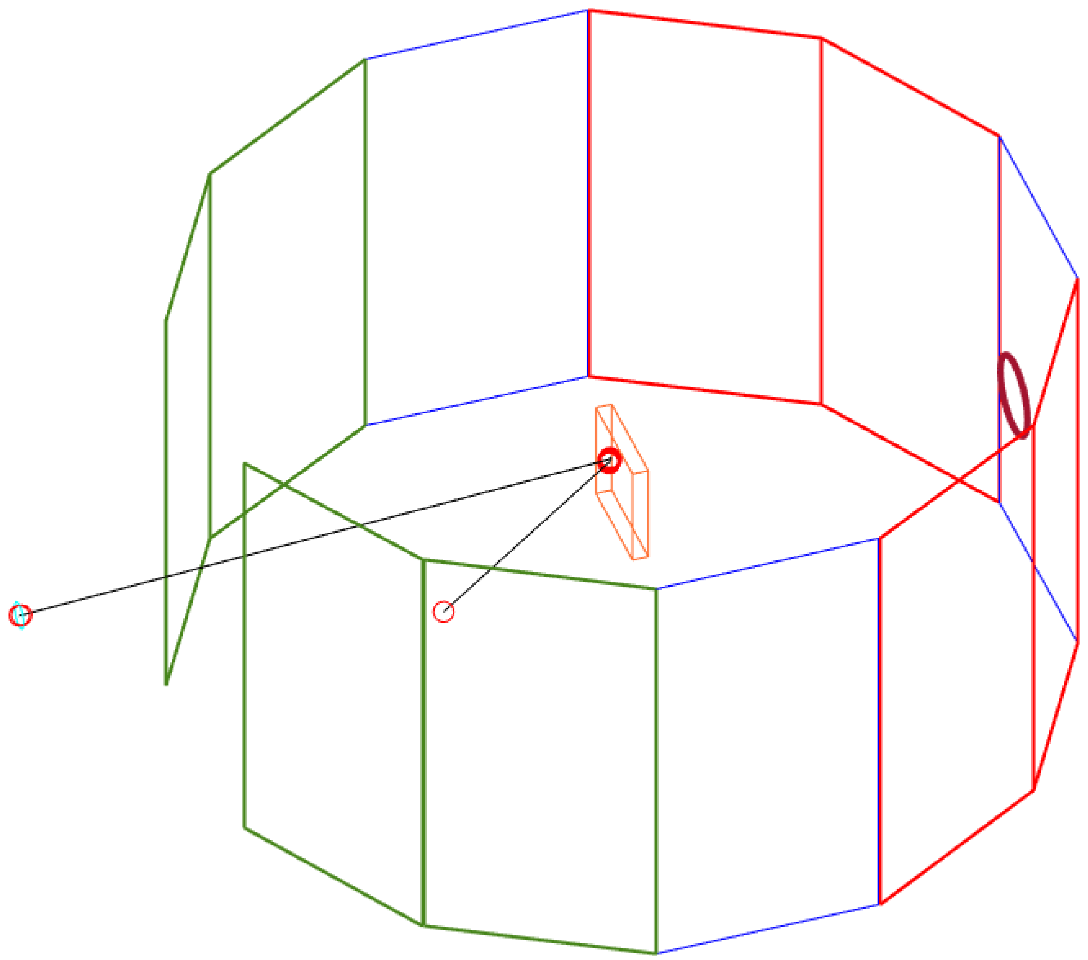
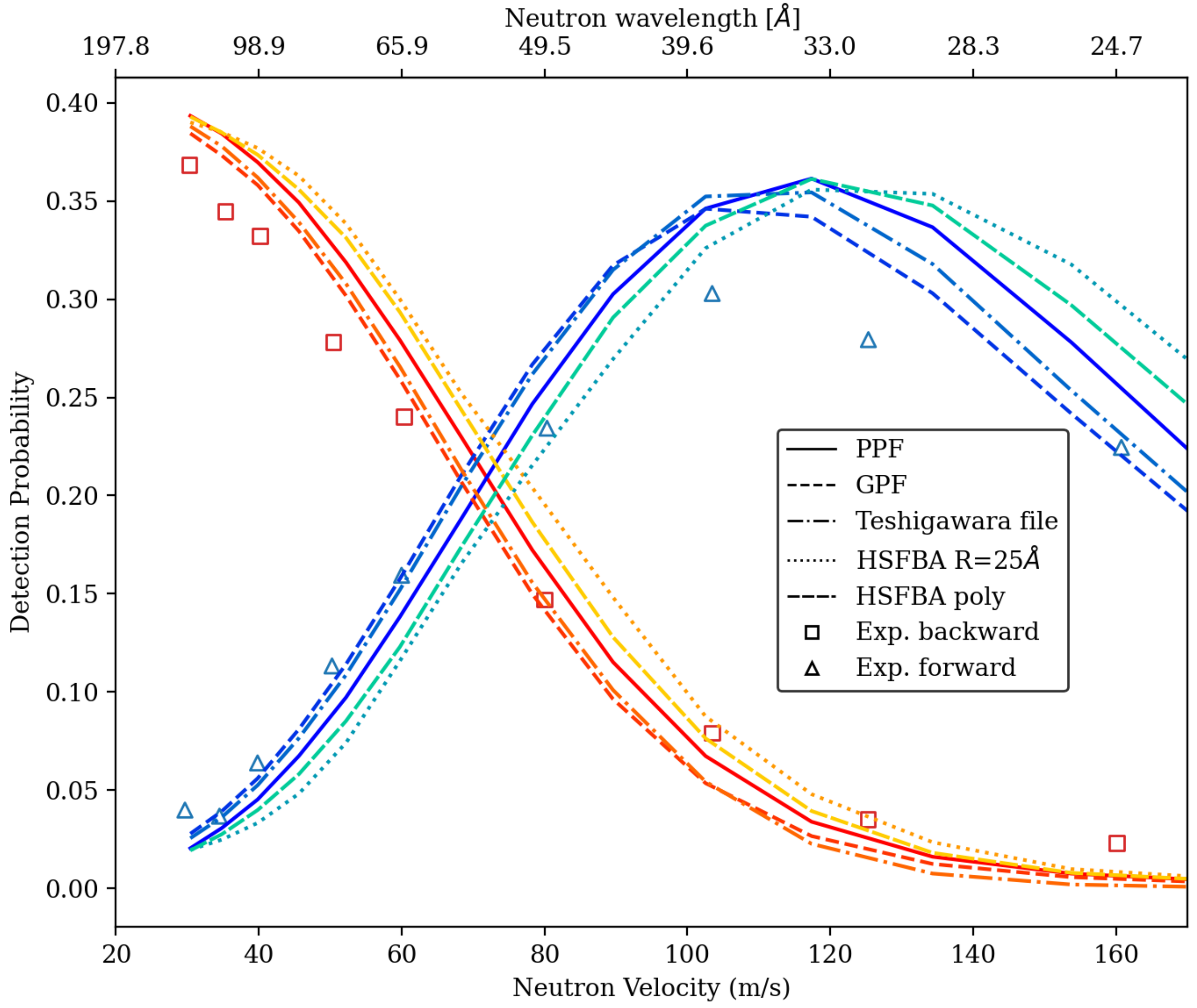


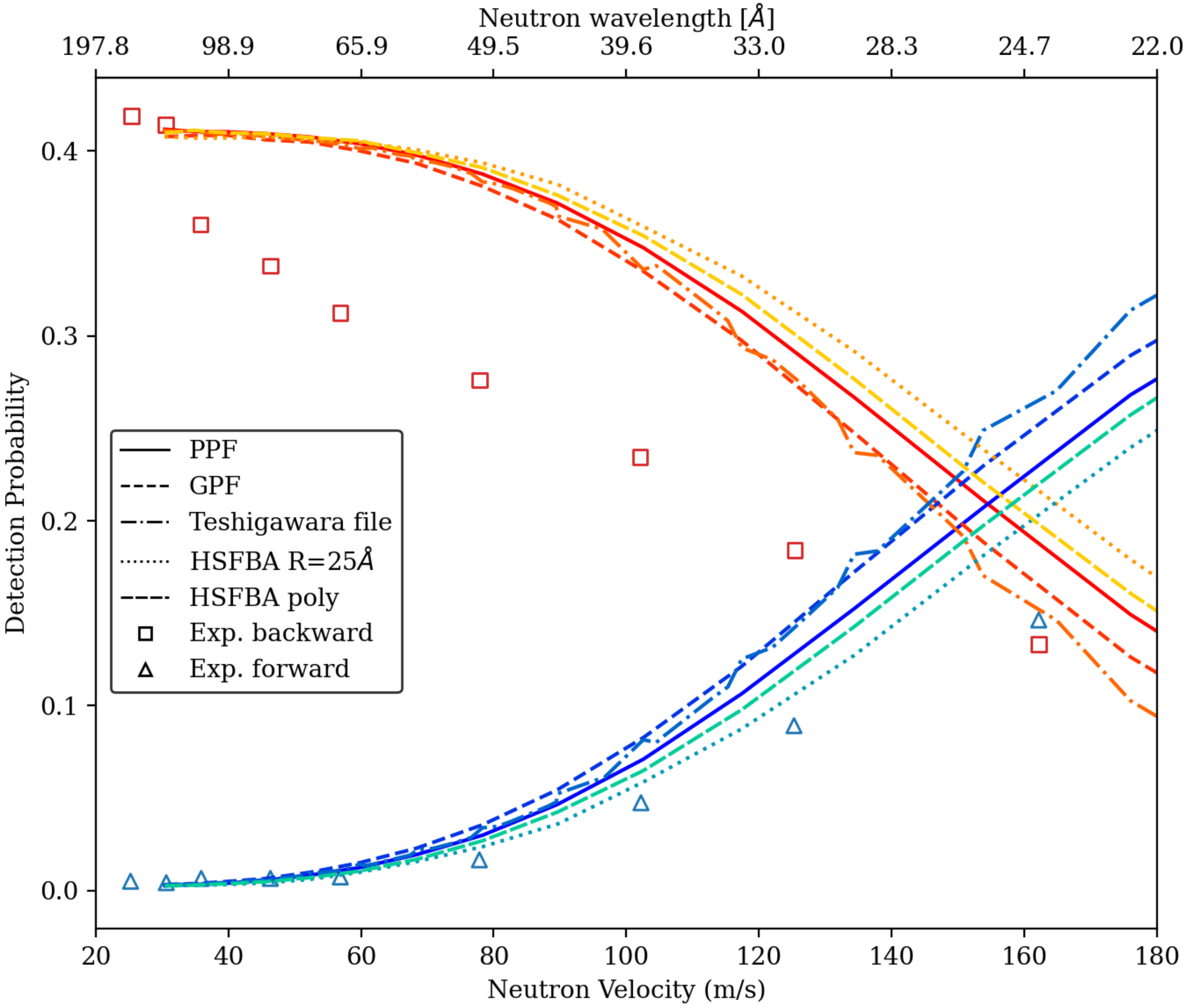
Image from [3]



Benchmark on 0.4 mm sample



Benchmark on 6 mm sample



Low-angle reflectometry benchmark

- Comparison with study about Nanodiamond quasispecular reflection of cold neutrons: Nesvizhevsky et al. (2018) [4]

- Goal: test the plugin in more complex configurations where angular distribution of reflected neutrons is essential.

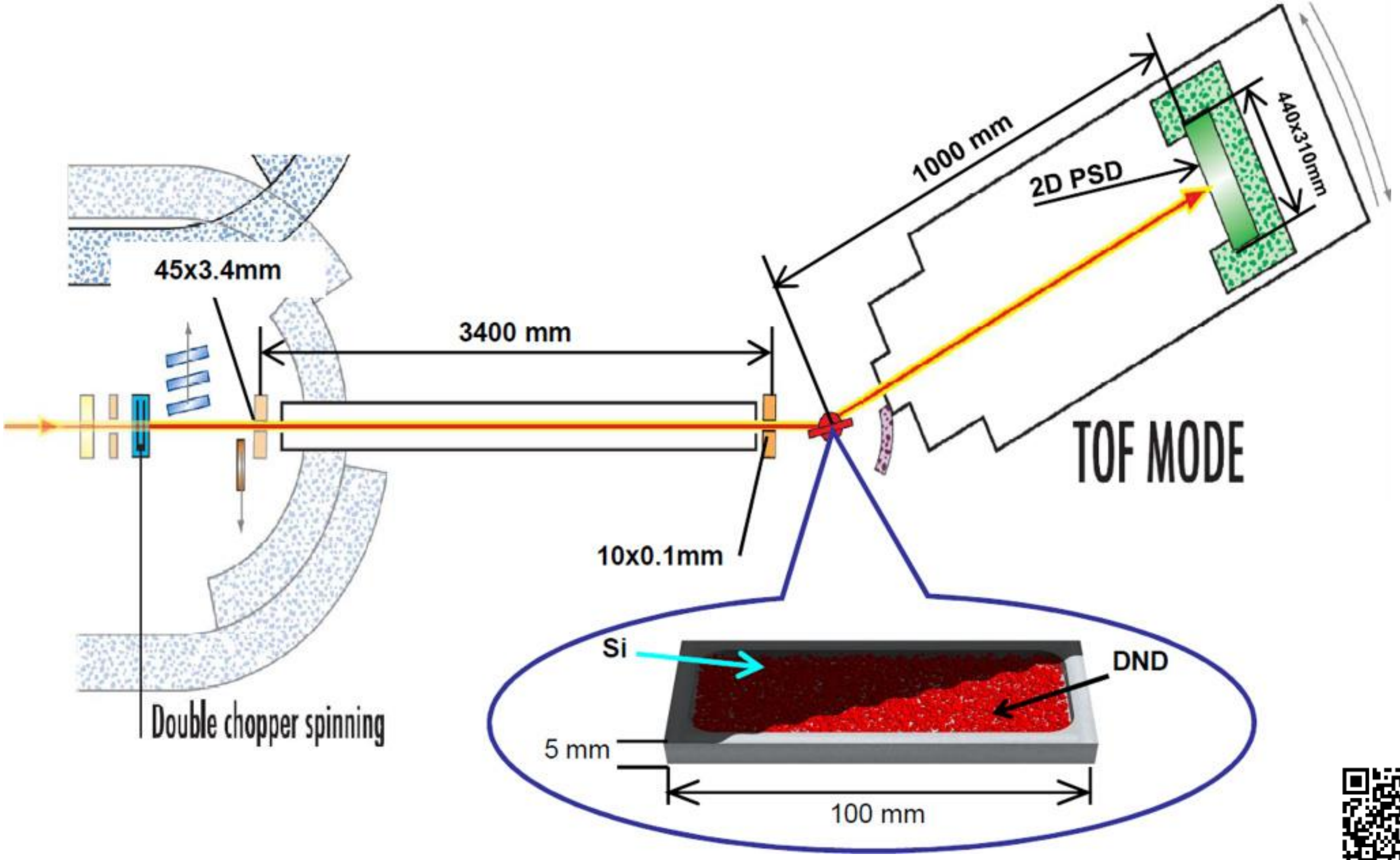
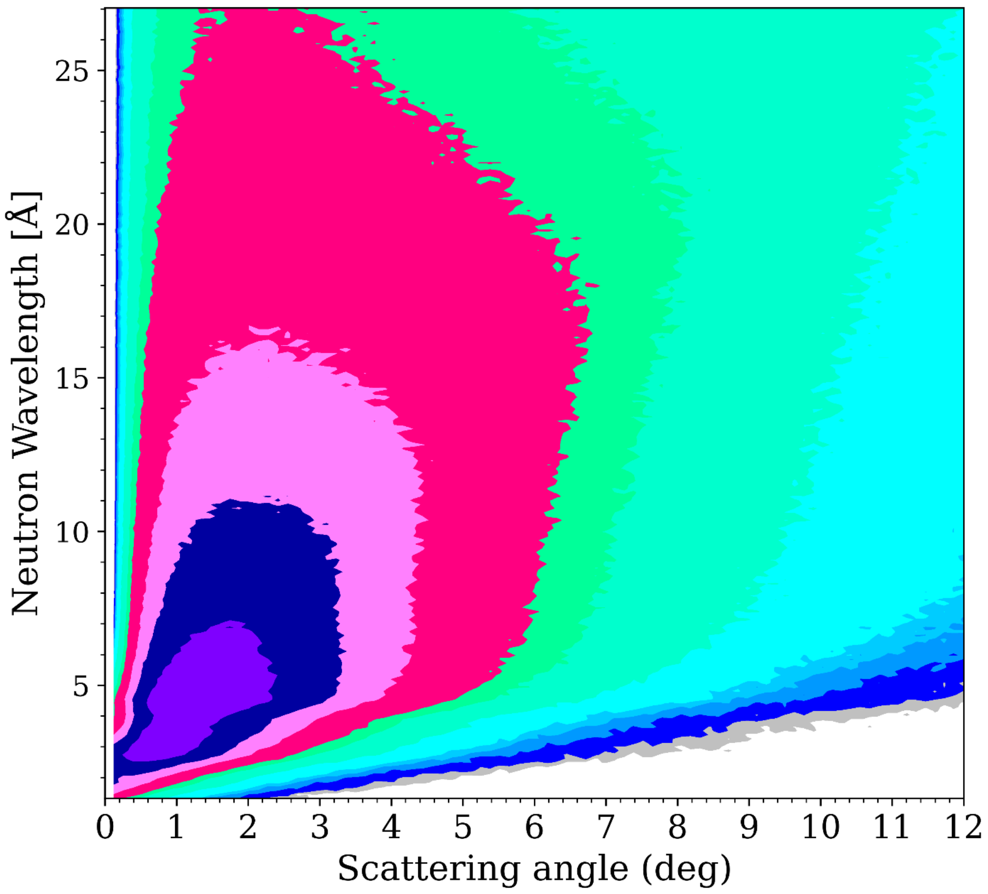
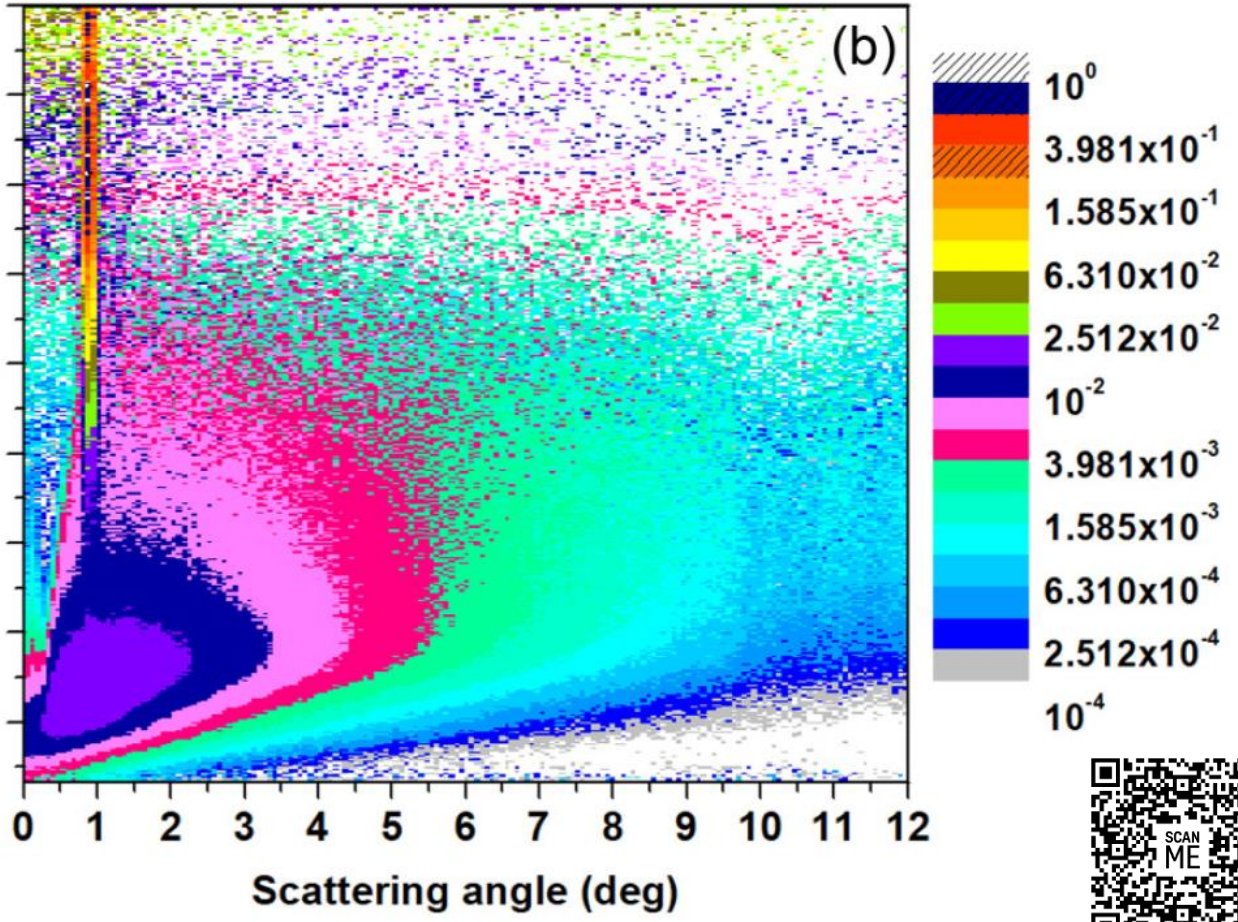


Fig. 1 from [4]

Probability of scattering

Fig. 2b from [4]





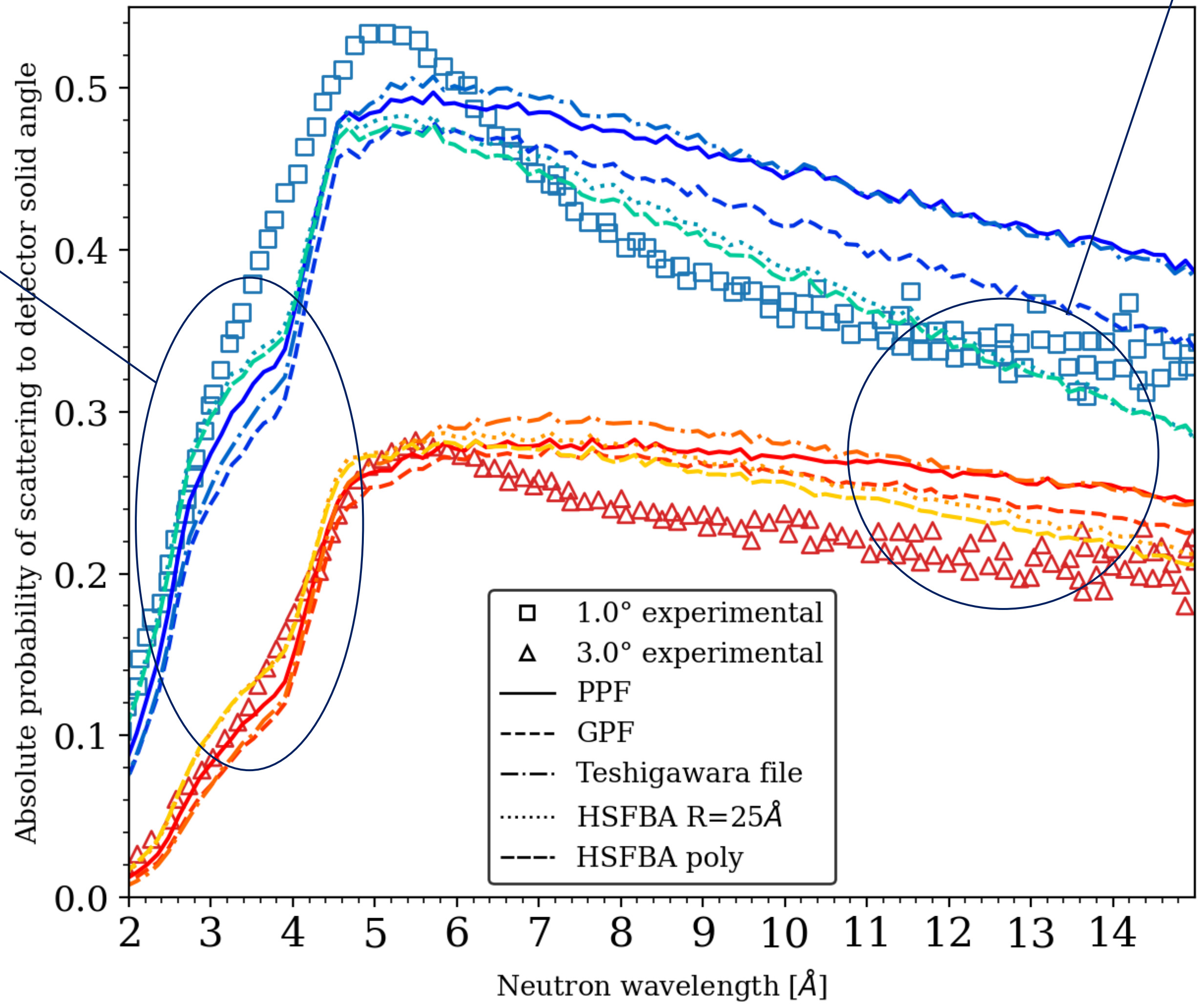
Reflection probability in λ

Decrease due to finite vertical size of the detector

Quasi-specular reflection suppressed due to:

- Diffraction on the crystal lattice of the diamond core at 3.57Å;
- Too small scattering angles at individual ND at wavelengths of ~3Å and below;

Cutoffs are not sharp due to the finite size of nanoparticles



Conclusions

- We added nanodiamond SANS scattering process to NCrystal
- Both empirical and theoretical models available
- Several ND properties in reflection of VCN well captured by our approach
- Impurities not taken into account, so just ideal ND
- We are working on further benchmarking the plugin for the enhancement of neutron extraction from Compact Accelerator-based Neutron Source and general directional extraction

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