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Implementation of a small-angle scattering model in MCNPX for very cold neutron reflector studies

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Abstract. Current neutron moderator media do not sufficiently moderate neutrons below the cold neutron regime into the very cold neutron (VCN) regime that is desirable for some physics applications. Nesvizhevsky et al [1] have demonstrated that nanodiamond powder efficiently reflect VCN via small angle scattering. He suggests that these effects could be exploited to boost the neutron output of a VCN moderator. Simulation studies of nanoparticle reflectors are being investigated as part of the development of a VCN source option for the SNS second target station. We are pursuing an expansion of the MCNPX code by implementation of an analytical small-angle scattering function [2], which is adaptable by scattering particle sizes, distributions, and packing fractions in order to supplement currently existing scattering kernels. The analytical model and preliminary studies using MCNPX will be discussed.

1. Introduction

Cold neutron (CN) beams with energies of $10^{-4} - 10^{-2}$ eV (2.86 – 0.286 nm), for which there are broad scientific applications in fundamental neutron physics and for studying materials, are typically produced through scattering from a cryogenic hydrogenous moderator typically operated at temperatures in the 10-20 K range and with effective cold neutron thermal distributions somewhat warmer. Technologies also exist for producing ultracold neutrons (UCN) with energies below 10^{-7} eV. At present, very cold neutrons (VCN) in the intermediate energy range between UCN and CN is desirable for some physics applications and efficient VCN moderators have not yet been developed.

An intriguing potential material for VCN production taking advantage of small angle neutron scattering from a low absorption, high optical potential material has been proposed [1]. The characteristic diameter of nanoscale materials is on the order of 5.0 nm and is similar in magnitude to VCN wavelengths. A material with a low absorption cross section allows the material to behave as a reflector via multiple small angle scattering events analogous to beryllium and graphite reflectors used in nuclear reactors. In particular, carbon has a small absorption cross section of 0.0035 barns and detonation nanodiamonds can be produced in large quantities

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through an explosive process [3]. Detonation nanodiamonds form large agglutinates with sizes on the order of microns, and can be purified through sonication followed a milling procedure to isolate primary particles $4.5 \text{ nm} \pm 0.5$ in size [4], producing nanoparticles composed of a diamond-like core and a graphite-like shell [5]. Quasi-specular reflection of cold neutrons from diamond nanoparticles has been observed experimentally [6].

Current scattering kernels do not include small angle neutron scattering, which is required to perform transport calculations of powder filter materials. As part of the design effort for the Spallation Neutron Source second target station, an analytical small angle neutron scattering model has been incorporated into MCNPX in order to perform transport calculations and to investigate potential VCN reflector materials. The analytical model describes a Percus-Yevick hard-sphere fluid [2] with the ability to vary the polydispersity, packing fraction, and contrast.

2. Model

The scattering intensity for a medium containing a distribution of particles with diameters σ_i is given by

$$I(k) = \rho \int_0^\infty P_i^2(k) f(\sigma_i) d\sigma_i + \rho \int_0^\infty \int_0^\infty P_i(k) P_j(k) H_{ij}(k) f(\sigma_i) f(\sigma_j) d\sigma_i d\sigma_j, \quad (1)$$

where ρ is the particle number density, k is the momentum transfer, $H_{ij}(k)$ is the pair structure function as derived by Blum and Stell [7]. The particle size distribution function, $f(\sigma)$, is given by the Schulz Γ function,

$$f(\sigma) = \frac{\sigma^z e^{-\frac{\sigma}{b}}}{b^{z+1} \Gamma(z+1)} d\sigma, \quad (2)$$

where z is the Schulz width factor representing the polydispersity and $b = \sigma_\mu / (z+1)$. This distribution has mean particle diameter σ_μ and variance of $\sigma_\mu^2 / (1+z)$. The normalized k th moment of the Schulz distribution is

$$\langle \sigma^k \rangle = \int_0^\infty \sigma^k f(\sigma) d\sigma = \frac{(z+k)!}{z!(z+1)^n} \sigma_\mu^k, \quad (3)$$

which gives an expression for the particle number density, ρ ,

$$\rho = \frac{6\eta(1+z)^2}{\pi\sigma_\mu^3(2+z)(3+z)}, \quad (4)$$

where η is the volume packing fraction. The scattering amplitude for hard spheres with uniform scattering length density is given by

$$P_i(k) = 4\pi p k^{-3} [\sin(k\sigma_i/2) - \frac{1}{2}k\sigma_i \cos(k\sigma_i/2)], \quad (5)$$

where $p^2 = (p_0 - p_{\text{med}})^2$ is the contrast between the medium and the particles. Note that two errors in the equations of the original publication [2] were found while verifying the results before implementing the analytical model in MCNPX. There is a factor of k^{-3} that is missing from equation 3 and equation 20 is missing an overall multiplicative factor of 9 and also contains an extra factor of ρ .

The analytical model is invoked via a material modification card, **ms**, on which the model parameters are specified. The macroscopic scattering cross section for the small angle neutron scattering mode is then calculated as a function of $k\sigma_\mu$ using the analytical function in logarithmic bins over 10 decades with 1000 bins per decade in order to provide sufficient

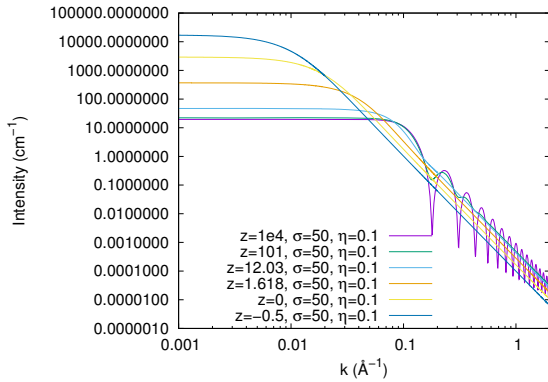


Figure 1. Scattering intensity for $p = 8.09422 \times 10^{-6} \text{Å}^2$, $\eta = 0.1$.

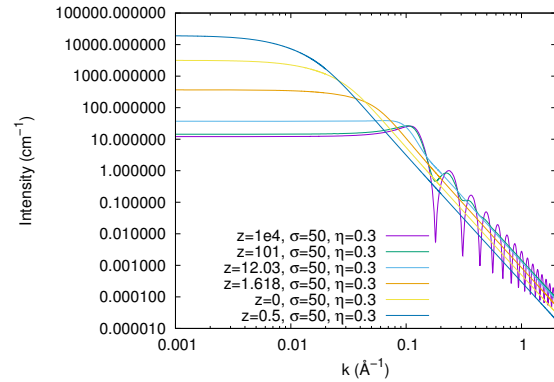


Figure 2. Scattering intensity for $p = 8.09422 \times 10^{-6} \text{Å}^2$, $\eta = 0.3$.

resolution of features in the cross section. Numerical precision becomes an issue for $k\sigma_\mu < 0.1$ and the analytical function and a series expansion in k is used below this region. The calculation transitions from using the analytical function to the series expansion in a region where each agrees at the 10^{-6} level. Figures 1 and 2 depict the calculated scattering cross section as a function of momentum transfer for 5.0 nm detonation nanodiamonds in 100% water at two different packing fractions and varying degrees of polydispersity with $z = 10^4$ corresponding to an essentially monodisperse sample. The calculated cross section is integrated as a function of $k\sigma_\mu$ in order to produce a total macroscopic cross section which is then converted to a microscopic cross section in units of barns through the particle number density, ρ .

3. Results

Simulations of simple representations of a SANS instrument and a reflectometer instrument were done in order to demonstrate the behavior of the SANS mode in MCNPX.

The SANS configuration consists of a white beam of cold neutrons collimated to a radius of 0.5 mm incident on a 1 mm thick volume containing a mixture of water and carbon representing nanodiamonds with diameter of 50 nm. The neutron flux is tallied 50 cm away from the scattering volume using a segmented surface tally with 1600 cylindrical segments with radii varying in increments of 0.625 mm to a maximum radius of 100 cm. The neutron flux in each annulus is binned by neutron energy. Figure 3 shows the scattered profile for neutrons of two different wavelengths and two different packing fractions.

The reflectometer configuration includes 0.5 mm beam with divergence of 0.4 mrad incident on the 5 cm thick sample volume composed of pure nanodiamonds with a density of 0.4 g cm^{-3} , meant to simulate a configuration similar to that of Cubitt [6]. The angle of incidence, θ , is varied from 1 to 10 degrees with the detector at an angle of $2\theta + 10$ degrees. The neutron spectrum is tallied at the detector position in order to determine the reflectivity of the sample. The sample is composed of monodisperse nanodiamonds with a diameter of 50 nm. The calculated reflectivity is shown in figure 4.

4. Discussion

First simulation results agree qualitatively with expectations. Experimental verification of the model in order to provide a quantitative benchmark is in the early planning stages.

The reflectivity simulations suggest that a thick nanodiamond powder could serve as a reflector of CN, with a reflection probability approaching 50% for grazing incidence. A nanodiamond reflector could increase CN fluxes provided that it could withstand the high

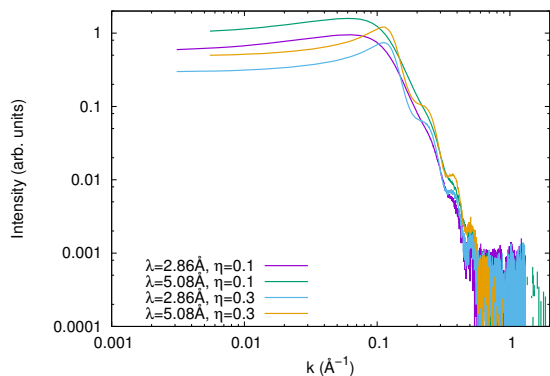


Figure 3. Calculated scattering profile for $p = 8.09422 \times 10^{-6} \text{ Å}^2$, $\sigma_\mu = 50 \text{ nm}$, and $z = 10^4$.

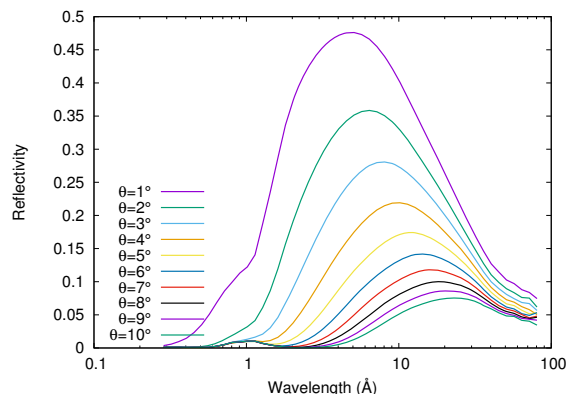


Figure 4. Calculated reflectivity for varying angle of incidence.

radiation environment close to a reactor core where traditional supermirror neutron guides cannot reach.

The seams between individual neutron guide elements give rise to artifacts in the beam profile and beam divergence at the exit of the neutron guide and nanoscale powders are often used to smear these artifacts. The implementation of SANS represents a powerful tool for conducting transport simulations involving nanoscale powders within MCNPX, for which conventional scattering kernels do not presently exist.

This model will be used in a design and optimization campaign for a VCN source, in which the nanoscale material acts as a VCN reflector. The neutronics performance of a moderator with a VCN reflector will be investigated as a function of polydispersity, packing fraction, and particle size.

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