

# Directional reflection of cold neutrons using nanodiamond particles for compact neutron sources

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**Abstract.** Nanodiamond Particles (NDP) are new candidates for neutron reflection. They have a large scattering and low absorption cross-sections for low-energy neutrons. Very Cold Neutrons (VCN) are reflected from NDP with large scattering angles while Cold Neutrons (CN) have a quasi-specular reflection at small incident angles. A new scattering process has been added in Geant4 in order to examine the directional reflection of CN in an extraction beam made of NDP layer. Impurities in NDP are responsible for the up-scattered neutrons, especially hydrogen which has a large cross-section. Other impurities are also considered in Geant4 in order to produce a more accurate model for NDP scattering. The new scattering process is used to model a possible configuration of target-moderator-reflector in Compact Neutron Sources (CNS). A 13 MeV proton beam striking a beryllium target is chosen. Parahydrogen is placed as a cold moderator in order to produce CN. NDP are placed around the extraction beam for scattering the CN toward the exit of the beam. The results show that CN exiting the extraction beam can be increased thanks to the implemented NDP layer.

## 1 Introduction

Nanodiamonds were firstly produced by explosive shock more than 50 years ago [1]. These particles have the size of a few nanometers. Their diamond nucleus is surrounded by an onion-like shell consisting of impurities. Recently, it has been shown that nanodiamonds are attractive materials that can be used as reflectors against low-energy neutrons [2, 3]. They have a large total cross-section (two order of magnitude more than carbon for neutrons as the energy decreases to 0.2 meV) [4]. Very Cold Neutrons (VCN) can be trapped by nanodiamonds while Cold Neutrons (CN) may have quasi-specular reflection at small angles [2, 3].

Nanodiamonds Scattering Process (NSP) has been added as a discrete process in Geant4 Monte Carlo simulation toolkit. Nanodiamonds quasi-specular reflection was experimentally measured at the Institut Laue-Langevin (ILL) in 2009 [2]. The NSP implemented in Geant4 is validated with this experiment in order to see its feasibility. Moreover, nanodiamond total cross-section was measured by transmission at J-PARC [4]. This

experiment is also validated in order to benchmark the code.

In this work we used Geant4 with the implemented nanodiamonds physics to investigate the applicability of nanodiamond reflectors for compact neutron sources. A beam of proton with the energy of 13 MeV strikes the beryllium target producing neutrons. Liquid parahydrogen is used as a moderator for CN production, while beryllium is used as reflector. Nanodiamonds are simulated as they are placed around the extraction beam in order to increase the chance of neutron reflection toward the CNS exit.

## 2 Compact Neutron Source (CNS)

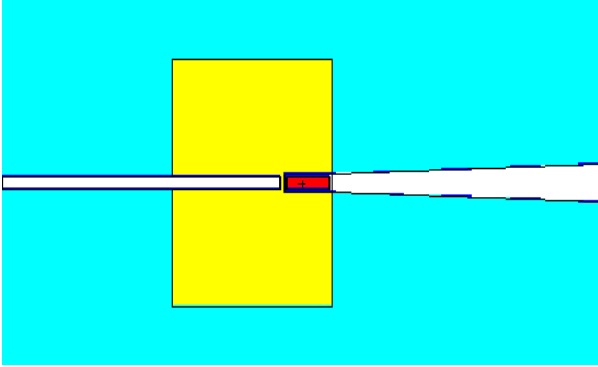
A beam of proton having the energy of 13 MeV strikes the beryllium target with the dimensions of  $1.5 \times 0.75 \times 0.2$  cm<sup>3</sup>. The neutrons produced from (p,n) reaction enter the parahydrogen cylinder with the temperature of 20 K having the radius of 3 cm and length of 14 cm. The beam extraction channel is about 1 m long starting from the center of cold moderator. Beryllium is also used as a

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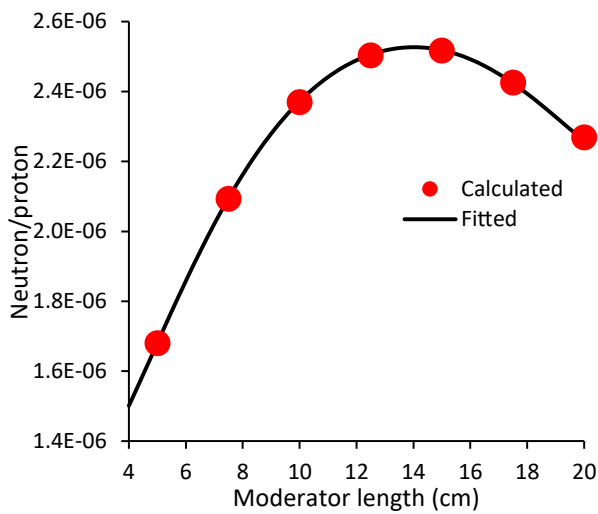
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reflector while steel is modeled as a shield. **Fig. 1** shows the proposed CNS for simulation study. The length of cold moderator has been optimized by testing different dimensions in order to have the highest possible cold flux after the moderation. However, the dimensions of the reflector, and overall geometry setup, was not optimized. Additionally, the target should be considered as ideal, as in a realistic configuration the target would probably have to have a larger area. The chosen geometry is apt to study the effect of nanodiamond reflector on the outgoing flux. **Fig. 2** shows the variation of CN production as a function of the moderator length for the wavelengths longer than 2.6 Å. **Table 1** illustrates the material and the dimensions of proposed CNS.

### 3 Nanodiamond Scattering Process (NSP) in Geant4



**Fig. 1.** Proposed CNS for simulation study.



**Fig. 2.** CN production versus moderator length in CNS.

**Table 1.** CNS structure specifications.

Component	Material	Dimension
Target	beryllium	1.5×0.75×0.2 cm <sup>3</sup>
Moderator	liquid parahydrogen	r = 3cm h = 14 cm
Reflector	beryllium	66×66×66 cm <sup>3</sup>
Shield	steel	50×50×102 cm <sup>3</sup>
Clad	aluminum	-

A discrete process has been added in Geant4, a Monte Carlo simulation toolkit in order to implement the scattering of neutron in nano-dispersed media [5]. **Fig. 3** shows this implementation procedure. The particle size is selected, from which the cross-sections are calculated. Neutron position and momentum are updated based on the new scattering angle and cross-sections. This procedure is used as long as neutron is in the nano-dispersed media. Shell impurities are also added as a normal material in order to consider the up-scattered neutrons. Carbon, oxygen, nitrogen, and hydrogen are the most common impurities available in the nanodiamond shell. The scattering cross-section of neutron in nanodiamonds was calculated in [6, 7] using the first Born approximation. Considering the center-of-mass system (c.m.s), the scattering amplitude can be defined as:

$$f(\theta) = -\frac{2m}{\hbar^2} V_0 R^3 \left( \frac{\sin(qR)}{(qR)^3} - \frac{\cos(qR)}{(qR)^2} \right) \quad (1)$$

where  $V_0$  is the real part of NDP Fermi potential,  $R$  is the particle size and  $q$  is the momentum transfer. The total elastic scattering cross-section is provided by the following formula:

$$\sigma_s = \int |f|^2 d\Omega = 2\pi \left| \frac{2m}{\hbar^2} V \right|^2 R^6 \frac{1}{(kR)^2} I(kR) \quad (2)$$

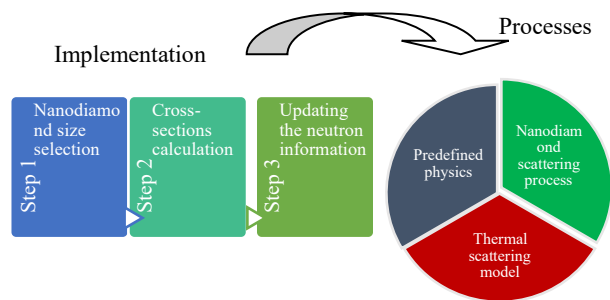
where,

$$I(kR) = \frac{1}{4} \left( 1 - \frac{1}{(2kR)^2} + \frac{\sin(4kR)}{(2kR)^3} - \frac{\sin^2(2kR)}{(2kR)^4} \right) \quad (3)$$

where  $k$  is the incident neutron wave vector. Finally, with the help of optical theorem, the total absorption cross-section in the nanodiamond particle can be calculated as:

$$\sigma_a = \frac{4\pi}{3} \frac{2m}{\hbar^2} V_1 R^4 \frac{1}{kR} \quad (4)$$

Where  $V_1$  is the imaginary part of the NDP Fermi potential.

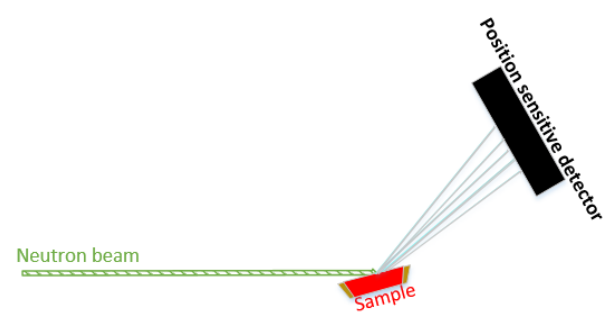


**Fig. 3.** Nanodiamond scattering process in Geant4.

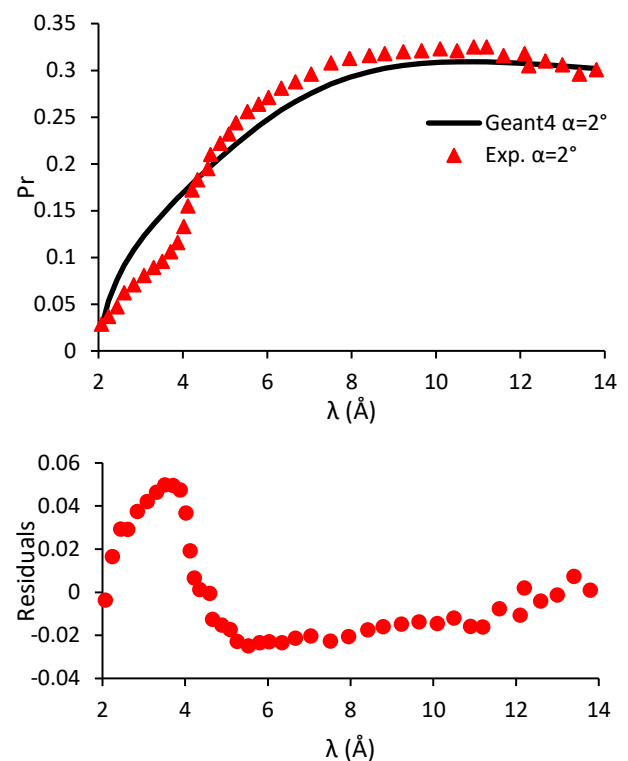
#### 4 Quasi-specular reflection of Cold Neutrons (CN) in nanodiamonds

The quasi-specular albedo of CN in NDP at small incident angles was tested for the first time at Institut Laue-Langevin (ILL) in 2009. This quasi-specular reflection is due to the multiple-scattering of CN in nano-dispersed media. CN with short wavelengths compared with the particles' size have small scattering angles in NDP. Therefore, they are going to penetrate deep into NDP and do not come back to the surface until they are absorbed if they have large incident angles. In the ILL experiment, a beam of CN with the wavelength in the range of 2-14 Å stroke a sample of NDP having the size of 2 nm with small incident angles. The reflected neutrons were detected by position sensitive detectors placed 110 cm far from the center of the sample with the height of 5 cm. Different small incident angles were tested to observe the quasi-specular reflection of CN from NDP. **Fig. 4** shows the scheme of the first experiment for benchmark. For more information related to this experiment refer to Ref. [2].

The newly implemented process in Geant4 was used in order to benchmark the CN quasi-specular reflection from NDP. In this simulation, CN were irradiated on the surface of the sample containing NDP with the angles of 2° and 3°. **Fig. 5** and **6** show the simulation results of neutron Probability (Pr) detection in position sensitive detectors. Due to the incomplete modelling of interplanar distance in the nanodiamond lattice, the simulation results are different from the experiment for the neutrons with wavelength in the range of 2-4 Å. It has already been shown that this distance is equal to 3.57 Å [8]. However, the residuals drop dramatically for neutrons having wavelength larger than 4 Å indicating a good agreement between data and simulations.



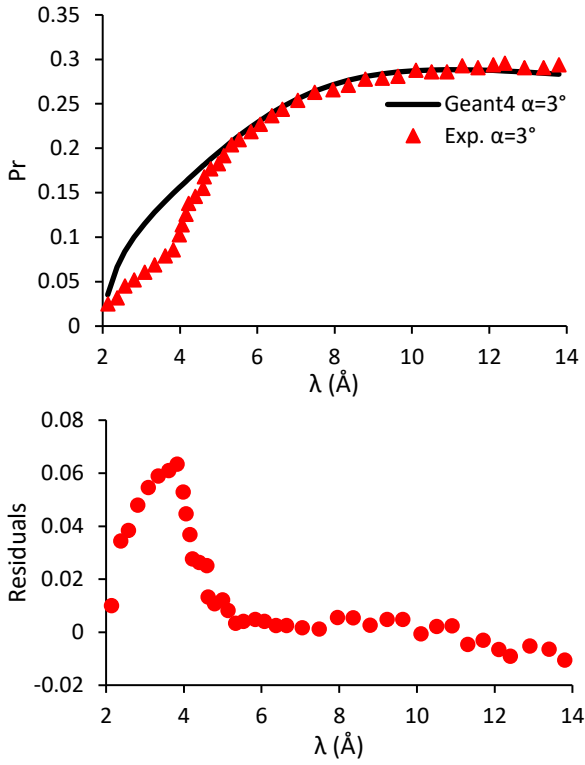
**Fig. 4.** Scheme of CN quasi-specular reflection experimental setup.



**Fig. 5.** Quasi-specular reflection of CN with incident angle of 2°.

#### 5 Nanodiamonds total cross-section measurement

Total cross-section of NDP produced using detonation explosives was calculated using the transmission measurement in the energy range of 0.1 – 100 meV at J-PARC [4]. Moreover, it was shown that the inelastic scattering contribution compared to the elastic scattering cross-section is negligible. Having removed the NDP



**Fig. 6.** Quasi-specular reflection of CN with incident angle of 3°.

moisture by means of vacuum heat treatment, a plate of NDP was prepared using a pressing jig in a glovebox filled with helium gas at atmospheric pressure. The average size of nanoparticles was 5.1 nm. The plate was placed in experimental setup, after its homogeneities were examined.

Neutron transmission  $R(E)$  was obtained as the ratio of neutron detection with or without the sample as:

$$R(E) = \frac{\phi_{WND}(E)}{\phi_{WOND}(E)} \quad (5)$$

Where the  $\phi_{WND}(E)$  and  $\phi_{WOND}(E)$  are the neutrons measured by detector with NDP and without NDP plate.

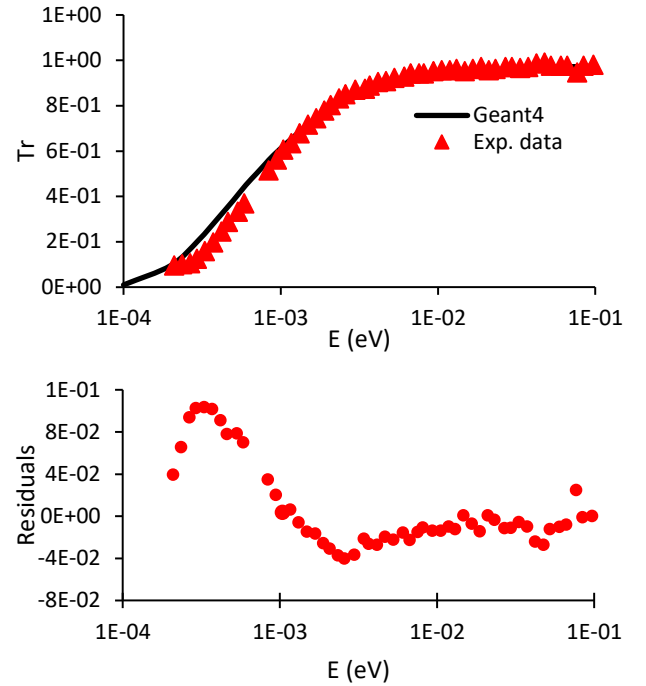
The total cross-section was determined using the attenuation equation as follows.

$$\sigma(E)_{total} = -\frac{1}{N_{ND} d_{ND}} \ln \left( \frac{\phi_{WND}(E)}{\phi_{WOND}(E)} \right) \quad (6)$$

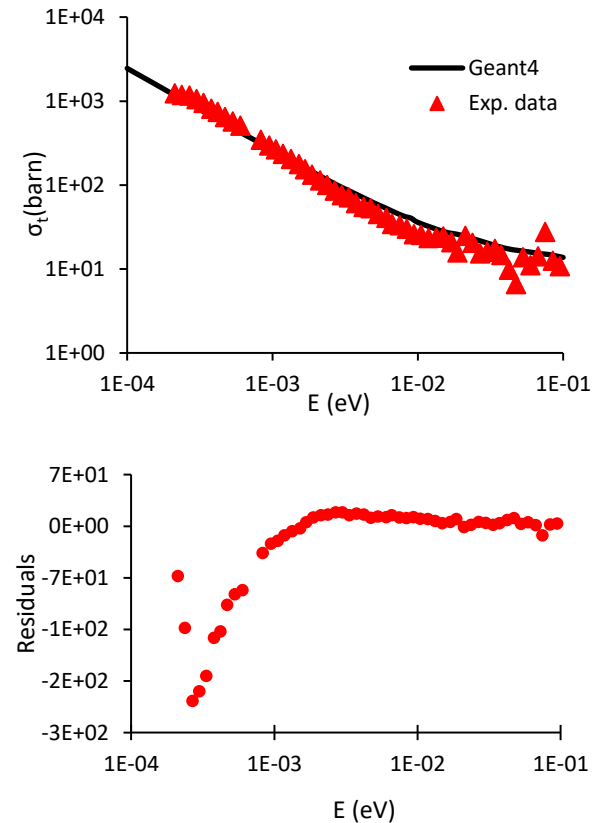
Where  $N_{ND}$  and  $d_{ND}$  are the number density and thickness of the sample respectively.

**Fig. 7 and 8** show the neutron transmission and total cross-section respectively. The simulation shows that

there is a good agreement between the prepared model in Geant4 and the experimental data.



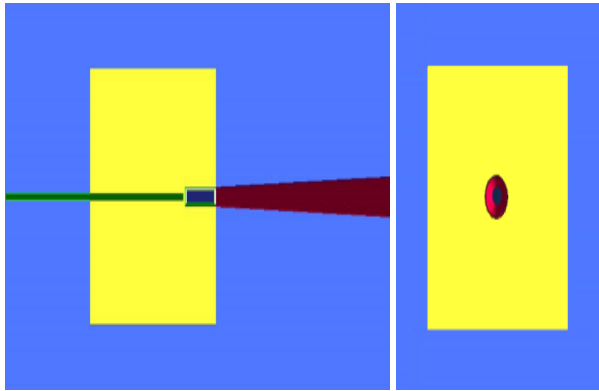
**Fig. 7.** Simulation of neutron transmission of nanodiamonds in Geant4.



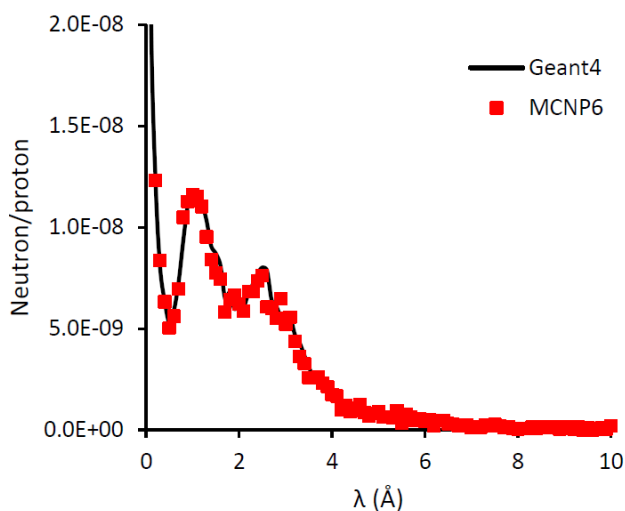
**Fig. 8.** Simulation of nanodiamonds total cross-section in Geant4.

## 6 Nanodiamonds application in CNS

The proposed CNS was modeled in Geant4 Monte Carlo simulation toolkit as shown in **Fig. 9**. The neutron spectrum exiting from the extraction beam is shown in **Fig. 10**. A MCNP6 model of the same geometry was built and the Geant4 simulations were compared with MCNP6.



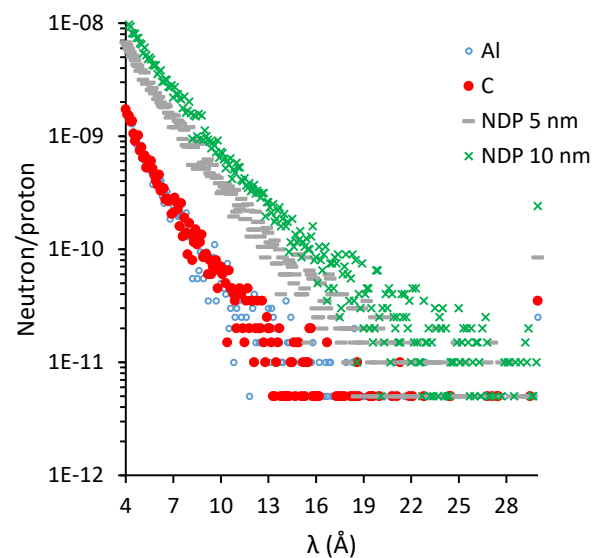
**Fig. 9.** CNS model prepared in Geant4.



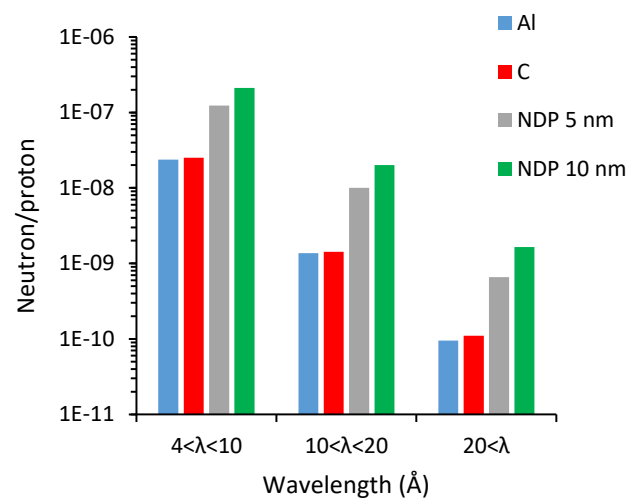
**Fig. 10.** CNS neutron spectrum at exit.

In order to see the effect of using NDP for directional neutron reflection, a NDP layer was placed instead of aluminum layer in the beam extraction cone. The thickness of this layer was 3 mm. Two sizes of NDP were tested in the simulation. The density of NDP in the simulation was considered  $0.6 \text{ g/cm}^3$ . **Fig. 10** shows the neutron spectrum at the exit of CNS. Since the Bragg scattering has not been implemented yet, the simulation is not reliable for the neutrons in the range of 2-4 Å. Therefore, in **Fig. 11**, the difference of using diverse materials, namely, Aluminum (Al), Carbon (C), NDP with the size of 5 nm and 10 nm is shown only above 4 Å. The integral number of neutrons in different wavelength ranges is shown in **Fig. 12**, while the ratio of flux increase

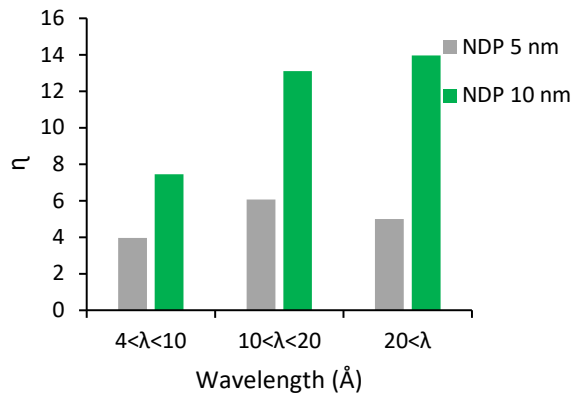
using NDP with respect to carbon is shown in **Fig. 13**. NDP help increase the flux more than 5 times for the neutrons in the range of 4-10 Å while this value reaches ten times more for neutrons having the wavelength longer than 10 Å. **Fig. 14** shows the angular distribution of neutrons exiting the beam. We observe that the CN flux at low divergence, i.e., of interest in neutron scattering, is increased by about the factor of two. For larger divergence, the flux increase is much larger. Such an increase could be used in applications where the neutron divergence is not of interest (e.g. irradiation experiments), or, for instance, to transport CN to a second moderator placed at a distance from the target, such as a UCN convertor.



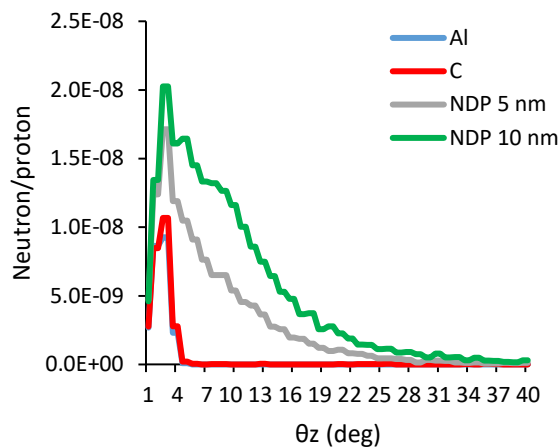
**Fig. 11.** CNS neutron spectrum with the wavelength more than 4 Å at exit.



**Fig. 12.** Integral number of neutrons for different wavelengths at exit.



**Fig. 13.** Ratio of neutron increase using NDP in CNS.



**Fig. 14.** CN angular distribution in CNS ( $4 \text{ Å} < \lambda < 10 \text{ Å}$ ).

## 7 Conclusions

Nanodiamond particles (NDP) were used in a case study of Compact Neutron Source (CNS) in order to increase the number of Cold Neutrons (CN) at exit. CN have a quasi-specular reflection from NDP if the incident angles are small. The scattering process of CN from NDP was implemented in Geant4 Monte Carlo simulation code as a discrete process. The new implemented model was benchmarked with two experiments previously performed in order to observe the quasi-specular reflection of CN and to measure the total cross-section of NDP by transmission. NDP were placed as a layer in the beam extraction cone of the CNS to increase the CN directional

reflection toward the exit. The simulation results showed that the number of CN were increased significantly when the NDP layer was used. However, the model lacked the Bragg scattering process for the neutrons in the range of 2-4 Å. Moreover, it was observed that the NDP with a larger size are more efficient in terms of CN increase at exit. The implementation of NDP in extraction beam helps optimizing the CNS while providing the possibility of carrying out experiments where the neutron divergence is not of primary importance.

## References

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