Verification of an Available Cross-Section Library for Neutron Interaction with Solid Deuterium Using Monte Carlo Simulation

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The calculation of neutron transport plays an important role in the development of neutron sources. The certainty of the calculation depends mainly on the choice of nuclear data library, particularly the neutron cross-sections. Nowadays, there are various types of nuclear data, and libraries already exist, such as the Japanese Evaluated Nuclear Data Library (JENDL), the Evaluated Nuclear Data Files (ENDF), the Joint Evaluated Fission and Fusion File (JEFF) organization, the TALYS Evaluation Nuclear Data Library (TENDL), the evaluated neutron data library (BROND), the ACE Application Nuclear Data Libraries, and others.

In our research, we have studied the neutron data library for solid ortho-deuterium (sD_2) at 5 K. It is one of the most effective materials that might be used in the design of very cold neutron (VCN) and ultracold neutron (UCN) sources as a converter of such neutrons. The library was developed in ACE format by the Spallation Physics Group at the European Spallation Source. It is based on the neutron scattering kernel for sD_2 proposed by Granada J.R. [1]. The main characteristics of Granada's model are contained in the mathematical formalism, including the lattice's density of states, the Young-Koppel quantum treatment of the rotations, and the internal molecular vibrations. Moreover, the elastic processes involving coherent and incoherent contributions are fully described, as are the spin-correlation effects.

To verify the library for sD_2 at 5 K, a Monte Carlo code was used to simulate the experimental cross-sections directly. Calculations were conducted, including: 1. Total cross-section for neutrons interacted with a flat layer of sD2 of a thickness of 1 cm. The initial energy range was from 10^{-2} to 10^{3} meV. The simulation results show a similarity to the measured cross-section. 2. The differential inelastic cross-section of energy transfers due to the interaction of neutrons with the initial energy of 20.4 meV. In this case, the sD2 was a sphere with a radius of 5 cm with a point isotropic neutron source at its centre. The neutron scattering data was compared with the results published by A. Frei [2], showing agreement for the range of energy loss of sub-thermal neutrons in the sD_2 converter material.

Based on the results of the calculations mentioned above, we have calculated the cross section for generating VCN with velocities from 50-200 m/s.

Moreover, for simulations relating to the production and transport of UCN, the library shows a lack of necessary data. The limitation applies to the range of neutron energies from 10^{-2} to 10^{3} meV. In the next stage of our research, we will focus on using the neutron scattering kernel for sD_2 that was proposed by Granada J.R. for the development of a data library for Geant4 extended to the UCN energy region.

1. Granada, J.R. "Neutron scattering kernel for solid deuterium." *Europhysics Letters* 86.6 (2009): 66007.
2. Frei, A., et al. "Understanding of ultra-cold–neutron production in solid euterium." *Europhysics Letters* 92.6 (2011): 62001.