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Converters of very cold and ultracold neutrons: Monte Carlo simulation of their properties and specifics of available data libraries and software

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The calculation of neutron transport is crucial for the development of neutron sources. The accuracy of these calculations depends on the quality of the nuclear data libraries used, which provide information on neutron cross-sections. There are several nuclear data libraries widely used in the world such as the Evaluated Nuclear Data Files (ENDF), the Japanese Evaluated Nuclear Data Library (JENDL), and the TALYS-based Evaluated Nuclear Data Library TENDL, among others.

In our research, we focused on the neutron cross-section library for solid ortho-deuterium (sD2) at 5 K, which is a promising material for the development of the intense sources of very cold (VCN) and ultracold neutrons (UCN). The library was developed in ACE format by the Spallation Physics Group at the European Spallation Source, based on a model developed by J.R. Granada [1]. The model includes details of the lattice density of states, molecular rotations, and internal molecular vibrations, as well as elastic and inelastic processes involving spin-correlation effects.

We have used a Monte Carlo code and this data library for sD2 at 5 K to calculate the cross-sections and found that the results are similar to the measured cross-sections. We also simulated the differential inelastic cross-section of energy transfers when neutrons interact with sD2, comparing our results with those published by A. Frei [2]. Our results showed agreement with Frei's results for sub-thermal neutrons in the sD2 converter material.

In addition, we have also calculated the cross-section of the conversion of VCN with velocities from 50 to 200 m/s using sD2 at 5 K, liquid deuterium at 20 K, water ice at 115 K, and solid mesitylene (C9H12) at 20 K. The wavelength range of incident neutrons for these calculations is from 1 to 20 Å.

In particular, our investigation has shown that the existing libraries are insufficient to provide the necessary data for simulations involving the production and transport of ultracold neutrons (UCNs). Specifically, the data gap is evident in the energy range from 10^{-2} to 10^{3} meV. In the next phase of our research, we plan to use J.R. Granada's neutron scattering kernel for sD2 to develop a new cross-section library for Geant4, with a focus on extending its coverage to the energy range relevant for UCNs.

References

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