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Monte-Carlo simulations of cold neutron transmission measurements of clathrate hydrates and graphite compounds

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The European Spallation Source (ESS), which is currently under construction in Lund, Sweden, will be the most powerful pulsed neutron source in the world. A design study project named HighNESS is dedicated to develop a second neutron source at ESS that compared to the first source, located above the spallation target and designed for high cold and thermal brightness, provides higher intensity cold neutrons, very cold neutrons (VCN) and ultra cold neutrons (UCN) [1]. This work carried out within the HighNESS project presents the Monte-Carlo simulations of cold neutron transmission measurements of clathrate hydrates as potential moderator candidates [2] and graphite compounds as reflector materials. The Monte-Carlo simulations are performed by using the neutron transport codes OpenMC [3] and McStas [4], with the neutron scattering kernels prepared by the toolkit NCrystal [5, 6, 7] developed in the project. The scattering kernels of clathrate hydrates and graphite compounds are generated thanks to the phonon density of states obtained by density functional theory (DFT) calculations. The simulated results including neutron scattering cross sections, scattering kernels and diffraction patterns are further validated by comparing with the transmission measurements performed at Institut Laue-Langevin (ILL) and Paul Scherrer Institute (PSI).

References

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