Evaluation of thermal neutron scattering law of nuclear-grade isotropic graphite

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Abstract: We have started a project entitled "Development of Nuclear Data Evaluation Framework for Innovative Reactor" in 2021. The objective of this project is to establish a scheme to improve the accuracy of nuclear data required in the development of innovative nuclear reactors within a short time period through collaboration between experiments and evaluations. Graphite is a candidate of moderator in innovative nuclear reactors such as molten salt reactors. Scattering of thermal neutrons by the moderator material has a significant impact on the reactor core design. Currently, ENDF/B-VIII.0 provides practically the only thermal scattering law (TSL) data for nuclear-grade graphite, and JENDL-5 adopts them. However, it has recently been pointed out that the TSL evaluation for nuclear-grade graphite employed in ENDF/B-VIII.0 have several concerns [1]. Under these circumstances, we newly evaluated TSL for nuclear-grade graphite.

The inelastic scattering component due to lattice vibration was evaluated based on the phonon density of states computed with first-principles lattice dynamics simulations. The simulations were performed for ideal crystalline graphite. This is based on the assertion in Ref. [1] that the vacancies in nuclear-grade graphite are larger in size than the crystals and other non-vacant region are highly crystalline. This is also in contrast to the modelling in ENDF/B-III.0 evaluation, in which carbon atoms are randomly removed from the crystal. The present evaluation and that of ENDF/B-VIII.0 were compared with the double-differential cross sections we have recently measured in the Materials and Life Science Experimental Facility (MLF) in the J-PARC in the temperature up to 500 K.

The coherent elastic scattering component due to crystal structure was evaluated based on neutron scattering and transmission experiments we recently performed in the MLF in J-PARC. The intensities of the individual Bragg peaks were evaluated through comparison with the experimental angular distribution of scattered neutrons. The sum of the inelastic and coherent elastic scattering components evaluated by the methods described above reproduced the experimental total cross sections well in the incident energy range above 10 meV. Below 10 meV, however, the experimental values were significantly underestimated. To resolve this discrepancy the small-angle neutron scattering (SANS) component was quantified. By adding the SANS component, the evaluated values reproduced the experimental total cross sections well.

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[1] I. Al-Qasir et al., Ann. Nucl. Energy 161, 108437 (2021).