Improvements to Thermal Neutron Scattering Law of CH_2

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INTRODUCTION

MCNP [1], as a widely accepted simulation tool, depends heavily on evaluated nuclear data found in current ENDF libraries [2]. Modeling CH_2 (polyethylene), as one of the prominent moderators, is of high importance for many applications such as spent fuel storage or shipping systems.

Current thermal scattering $S(\alpha,\beta)$ evaluations are based on theoretical calculations of the phonon spectrum that are usually adjusted to match the energy dependent total scattering cross section. Double differential scattering data is not always available and thus rarely used in the evaluation. In this work double differential scattering measurements were used to obtain a phonon spectrum that can be used to generate a thermal scattering evaluation. This procedure resulted in better agreement with the experimental total cross section of CH_2 and better agreement with double differential scattering experiments.

THEORY AND MEASUREMENTS

The inelastic neutron scattering in CH_2 can be represented as: [3]

$$\sigma(E \to E', \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}S(\alpha,\beta,T), \tag{1}$$

where E and E' are energies of the incoming and scattered neutrons, μ is the cosine of the scattering angle, σ_b is the bound scattering cross section of the material, kT is the moderator equilibrium temperature in eV (25 meV at around 300 K), $S(\alpha,\beta)$ is the scattering law, and α and β are respectively the momentum transfer and energy transfer parameters. $S(\alpha,\beta)$ is directly proportional to density of states, as seen in eq. 4.

The experimental measurements of generalized density of states (GDOS) were performed at Spallation Neutron Source using the ARCS (wide angular-range spectrometer) [4]. The data analysis was performed using software present at ARCS analysis station, where the experimental data for all users is automatically reduced to a form that can be easily converted to energy dependant structure dynamic factor, $S(Q,\omega)$. The transformation from $S(Q,\omega)$ to $S(\alpha,\beta)$ is:

$$S(\alpha,\beta) = kT\exp\left(\frac{-\hbar\omega}{2kT}\right)S(Q,\omega) \tag{2}$$

$$\alpha = \frac{Q^2\hbar^2}{2MkT}, \beta = \frac{-\hbar\omega}{kT}, \tag{3}$$

where M is the mass of the scattering material.

The software used to obtain GDOS from the experimental data is the DAVE suite available from the National Institute of Standards and Technology [5]. Specifically MSLICE, part of DAVE suite, was used to deduce the GDOS. The transformation from $S(Q,\omega)$ to GDOS is:

$$G(\omega) = S(Q,\omega)\cdot\left[1 - exp\left(\frac{-\omega}{kT}\right)\right]\cdot\frac{\omega}{Q^2}, \tag{4}$$

where $G(\omega)$ is GDOS, ω is frequency of the scattered neutron in meV, and Q is the momentum transfer.

The obtained GDOS has been further used with NJOY2012 to generate new 300 K thermal scattering libraries for CH_2. NJOY2012 has also been used to generate a total scattering cross section for CH_2, as well as to create files to be used with MCNP for validation of double differential scattering cross section (DDSX) measurements.

RESULTS AND ANALYSIS

The performed experiments produced unique experimental GDOS and provided the DDSX measurements on CH_2. The comparison between experimental DDSX, the current ENDF library, and the library generated in this work can be seen in Figure 1. The comparison was made by full simulation of the experiment, including the energy resolution of the ARCS detector. The experimental data were measured at neutron incident energies of 50, 100, 250 and 700 meV, with the horizontal detector coverage from 28^o to 135^o. The sample was at 5 K.

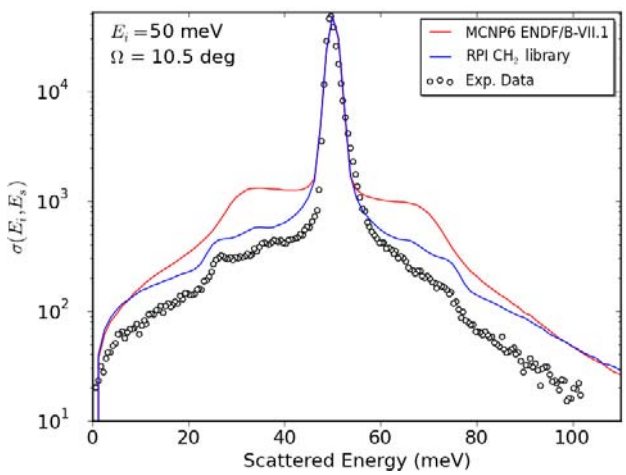

Fig. 1. Double differential scattering cross section comparison at a scattering angle of 10.5 degrees and the 50 meV incident energy of the neutron.

Although there is room for improvement, Figure 1 shows that the newly created CH_2 thermal library created in this work improves upon the current ENDF library.

The total scattering cross section for CH_2 has also been calculated and compared to an experimental cross section.

Since both total cross section values for ENDF and RPI libraries were produced by NJOY2012, they need to be calculated in the following manner, in order to be compared with the experimental values:

$$\sigma_{CH_2,t} = 2 \times (\sigma_{H,s}^{NJOY2012} + \sigma_{H,a}^{ENDF}) + \sigma_{C,t}^{ENDF}. \qquad (5)$$

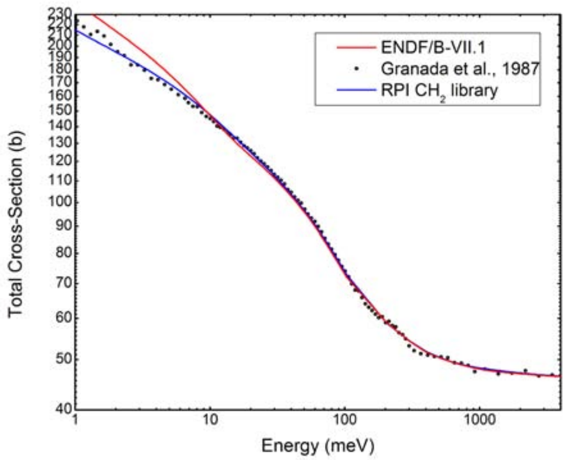

Fig. 2. Total scattering cross section of CH_2, with this work improving upon ENDF library in the lower energy region.

Figure 2 shows that below approximately 10 meV there is a mismatch between measured total scattering cross section and the current ENDF library. For most of the region below 10 meV the library created in this work agrees slightly better with the experiment. Benchmarks against a critical system, that contains CH_2, show slightly improved *C/E* values compared to the current $S(\alpha, \beta)$ in ENDF/B-VII.1.

CONCLUSIONS

With the current technology and instruments available at Spallation Neutron Source at Oak Ridge National Lab, and elsewhere in the world, essential quantities, such as density of states and double differential scattering cross sections, were measured and those measurements are used to create new and improved thermal scattering libraries.

ACKNOWLEDGMENTS

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