EXPERIMENTAL S(α,β) DATA FOR MODERATORS WITH ANALYSIS OF CURRENT EVALUATIONS

C. Wendorff, K. Ramic, E. Liu, Y. Danon
Gaerttner LINAC Center
Rensselaer Polytechnic Institute
Troy, NY, USA
wendoc@rpi.edu; ramick@rpi.edu; liue@rpi.edu; danony@rpi.edu

ABSTRACT

New thermal neutron scattering kernels were typically created using Molecular Dynamic simulations of the phonon spectrum that is then used to generate the scattering kernel. For verification and adjustment only microscopic total and inelastic scattering data were typically used. Because of this and due to model approximation the double differential scattering cross section (DDSCS) is not necessarily correct. Multiple experiments have been performed at the Spallation Neutron Source at Oak Ridge National Laboratory to measure the DDSCS of common and important neutron moderators including light water (H_2O), polyethylene (CH_2), and quartz (SiO_2). Using MCNP 6.1 and other tests, ENDF/B-VII.1 and other S(α,β) libraries were compared with the experimental data. Differences between the experimental data and the DDSCS generated from the evaluation were found. Limitations on the modelling and creation of the S(α,β) libraries are also discussed. The experimental data includes some of the highest energy-angle resolution data available for the DDSCS in the thermal region and sheds new light on possible problems in estimating the scattering kernel.

KEYWORDS
Experimental, Thermal Scattering Law, Neutron

1. INTRODUCTION

The double differential scattering cross section (DDSCS) in the neutron transport equation is difficult to calculate in the thermal energy range. The DDSCS is split into two parts, elastic and inelastic scattering. Elastic scattering can be caused by either incoherent or coherent elastic scattering. Incoherent elastic scattering is important in solid hydrogenous material that is usually amorphous. Coherent elastic scattering is important for crystalline material. Discussion on elastic scattering will be revisited later. Incoherent inelastic scattering is the important inelastic process. Incoherent inelastic scattering is defined by the thermal scattering law [1]:

$$\sigma(E \to E', \Omega) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}e^{-\beta/2}S(\alpha,\beta). \quad (1)$$

Where k is the Boltzmann constant and σ_b is the bound cross section of the primary scatterer. E' and E are the scattered energy and incident energy respectively. S(α,β) is defined as the structure factor. It is represented by the momentum transfer and energy transfer variables, α and β.

$$\beta = \frac{E'-E}{kT} \qquad \alpha = \frac{E'+E-2\mu\sqrt{EE'}}{AkT} \quad (2 \& 3)$$

The structure factor, S(α,β), can only be analytically solved for a free gas system where no chemical binding forces are present. The ENDF/B-VII.1 evaluations have relied on outdated phonon spectra to get the underlying structure factor for materials. These evaluations usually model the elastic peak very well but have trouble in representing the inelastic 'wings' as is seen in Figure 1.

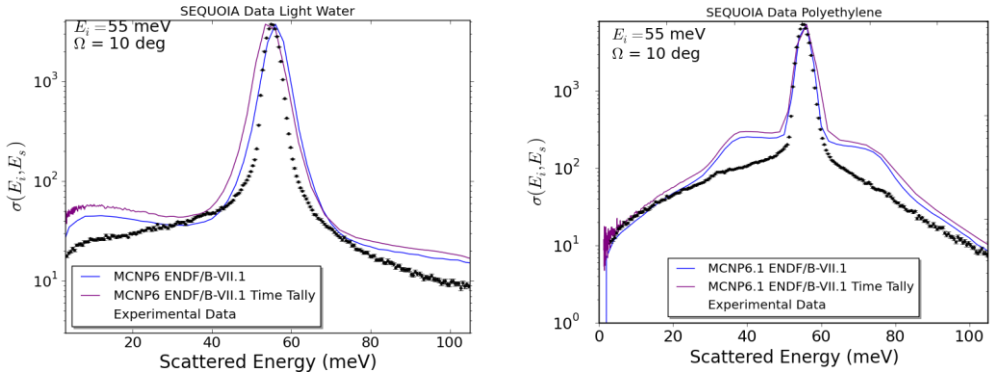

Figure 1: Experimental Comparison with ENDF/B-VII.1 for H_2O (left) and CH_2 (right)

Evaluations have been done using molecular dynamics simulations to create the phonon spectrum. These evaluations use integrated quantities to validate their libraries ignoring the DDSCS. An example of this is seen in Figure 2-Left. The SiO_2 evaluation that was used is a revised version of the ENDF/B-VII.1 evaluation made by Dr. Jesse Holmes [2]. That is why the label is given as ENDF/B-VII.2, a release that does not actually exist.

2. EXPERIMENTS

The experiments were done at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL). Light water (H_2O), polyethylene (CH_2), and quartz (SiO_2) were tested. The first experiment was done at the Fine Resolution Fermi Chopper Spectrometer (SEQUOIA); the second at the Wide-Angular Range Chopper Spectrometer (ARCS). An overview of the experiments is given in Table 1.

Table 1: Overview of Experiments at SNS

Moderators	SEQUOIA	ARCS
Light Water (H_2O)	E_I: 55, 160, 250, 600, 1000, 3000, 5000 meV Ω: 3-58° in 1° increments Temp = 300 K	-
Polyethylene (CH_2)	E_I: 55, 160, 250, 600, 1000, 2000 meV Ω: 3-58° in 1° increments Temp = 300 K	E_I: 50, 100, 250, 700 meV Ω: 3-125° in 1° increments Temp = 5, 295 K
Quartz (SiO_2)	-	E_I: 50, 100, 250, 700 meV Ω: 3-125° in 1° increments Temp = 20, 300, 550, 600 C

Both of these instruments are time-of-flight spectrometers. SEQUOIA gives a better energy resolution due to the longer flight path, while ARCS gives a larger angular detector range. An example of comparing the two experimental data sets can be seen in Figure 2-Right. The data sets show good agreement.

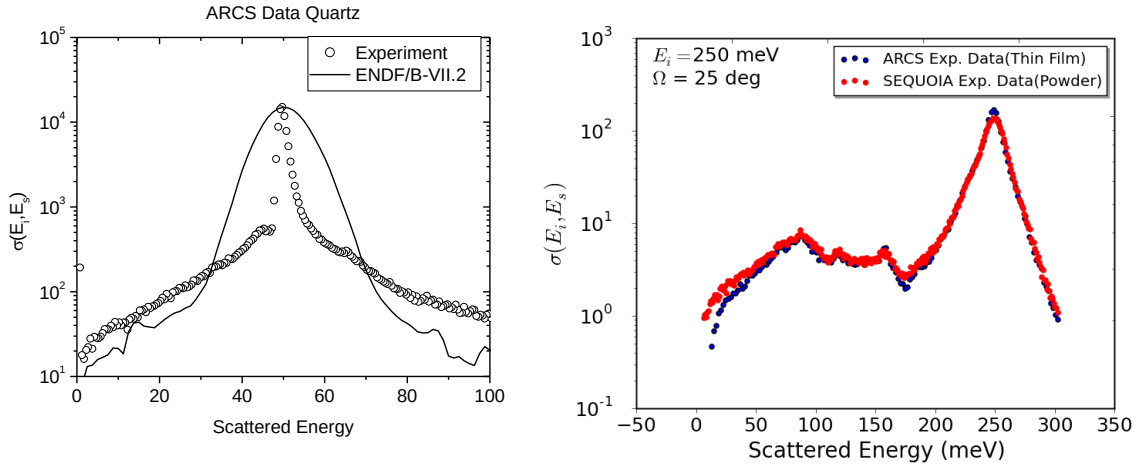

Figure 2: (Left) Comparison with SiO_2 evaluation, (Right) Data from Both Instruments

Figure 2-Right shows that the elastic peak is slightly higher for the ARCS data when normalized to the area under the curve. SEQUOIA has better energy resolution so the elastic peak should be sharper and higher than ARCS. The solution lies in the two forms the moderator sample used: the SEQUOIA CH_2 is in powdered form, while the ARCS CH_2 is in uniform thin films. CH_2 is an amorphous lattice material. But, localized crystalline structure may be present if the sample was created under ideal conditions. If crystalline properties extend to a large enough volume then the elastic peak would have coherent elastic scattering contributions as well as the expected incoherent elastic scattering. The powdering of the material would minimize this effect to a negligible level.

3. SIMULATIONS

Monte Carlo simulations were created in MCNP 6.1 to compare thermal scattering libraries and the experimental results [3]. Input files were created for each of the experimental instruments, ARCS and SEQUOIA. The models have the same physical dimensions as the instruments [4,5]. This was done to recreate the time-of-flight binning. To recreate the energy resolution, two Gaussian shaped probability functions were introduced into the input file's source card. The first was a staggering of the initial time to the creation of the incident neutron. The full width at half maximum (FWHM) for the Gaussian distribution was set to one microsecond. One microsecond corresponds to the length of the proton pulse incident on the spallation source at the SNS. The second is a broadening of the incident neutron's energy. This was to better match the range of energies leaving the neutron choppers. The FWHM was found using a numerical algorithm. These values were found to be in good agreement with the recorded values for the energy resolution [6]. Figure 3-Left shows an example of comparing the data with two simulations of the ENDF/B-VII.1 evaluation. The simulation matches very well with the experimental data in the elastic peak.

To create a thermal scattering law evaluation from experimental data, the instrument resolution needs to be removed. The resolution affects the elastic peak. The experimental DDSCS is a sum of the elastic and inelastic DDSCS. Removing the elastic piece from the experimental DDSCS is needed. CH_2 is a hydrogen based amorphous material. The elastic peak is defined by the incoherent elastic DDSCS [7].

$$\frac{\partial^2\sigma}{\delta E\prime\delta\Omega}(E \to E', \mu, T) = \frac{\sigma_b}{4\pi} e^{-2WE(1-\mu)}\delta(E - E') \tag{4}$$

where μ is the cosine of the scattering angle; W is the De-Bye Waller factor; and σ_b is the bound scattering cross section of the primary scatterer. Figure 3-Right shows the effect of the process.

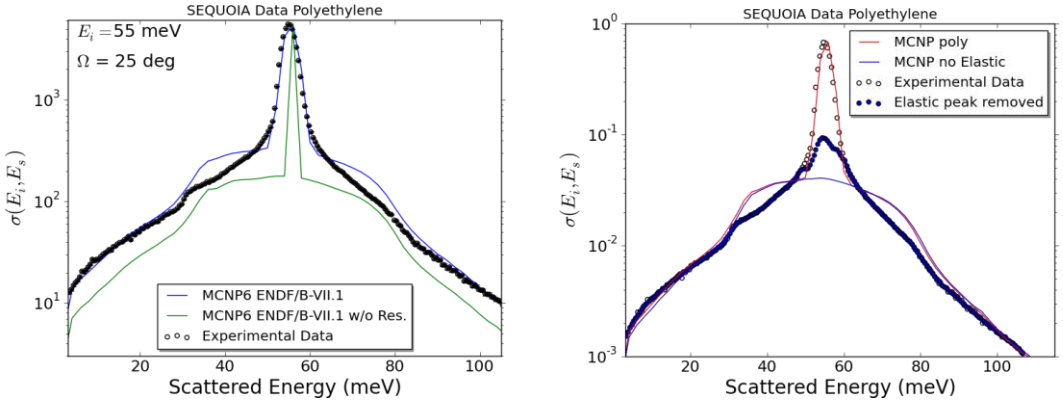

Figure 3: (Left) CH_2 Example of Simulation, (Right) Energy Resolution Removed

Theoretically, that which is left is the experimental incoherent inelastic DDSCS. Eq. (1) gives the relationship between the DDSCS and S(α,β). These S(α,β) values can be placed into ENDF format. These ENDF style evaluations are then processed through NJOY 2012 to create ACE files usable in MCNP 6.1.

4. ANAYLSIS AND RESULTS

The current ENDF/B-VII.1 release shows that there is good agreement in the elastic peak for most of the angles when normalized to the maximum of the elastic peak. Figure 4 show the comparison between our experimental data and the ENDF/B.VII.1 release. Two separate incident energies are shown.

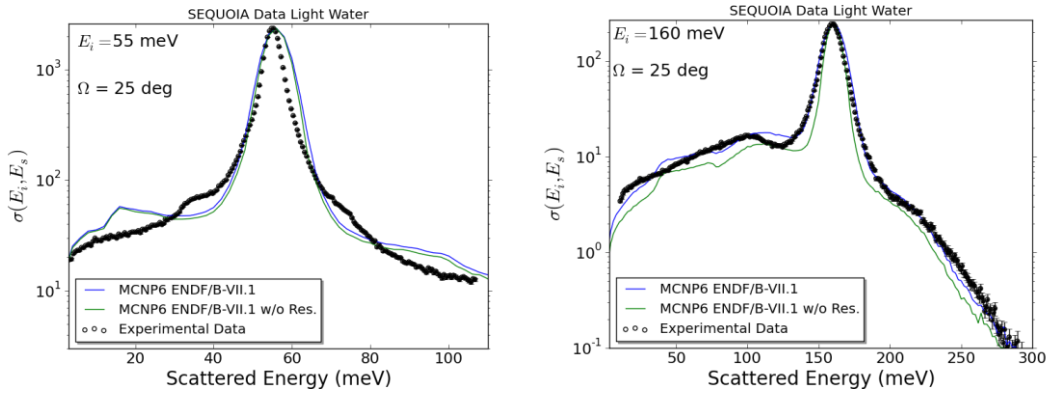

Figure 4: Light Water Experimental Data Comparison with ENDF/B-VII.1

Liquid H_2O does not have an elastic scattering component. Resolution broadening does little to change the DDSCS. The peak that exists around the incident energy is quasi-elastic scattering. Solid CH_2 does have an elastic scattering component. The dependence on energy resolution is represented in Figure 5.

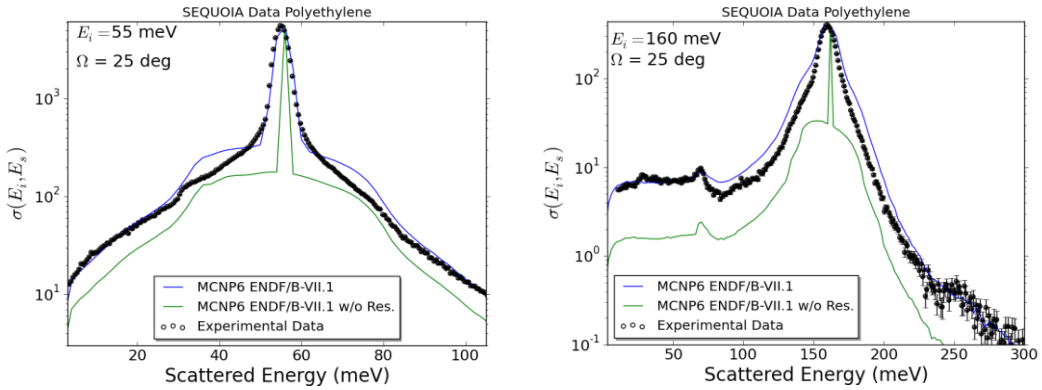

Figure 5: Polyethylene Experimental Data Comparison with ENDF/B-VII.1. The plots demonstrate the effect of the resolution function

Figure 6 is useful to see the washing out of underlying structure that the energy resolution can cause. As angle size increases the ENDF/B-VII.1 evaluation matches the experimental DDSCS much better. This has been noticed for thin films and small angle scattering already [1]. It can be seen by comparing Figure 5 and Figure 1-Right. New evaluations were created by the Comisión Nacional de Energía Atómica (CNEA) in Argentina. Figure 6 shows the comparison at two different incident energies for H_2O.

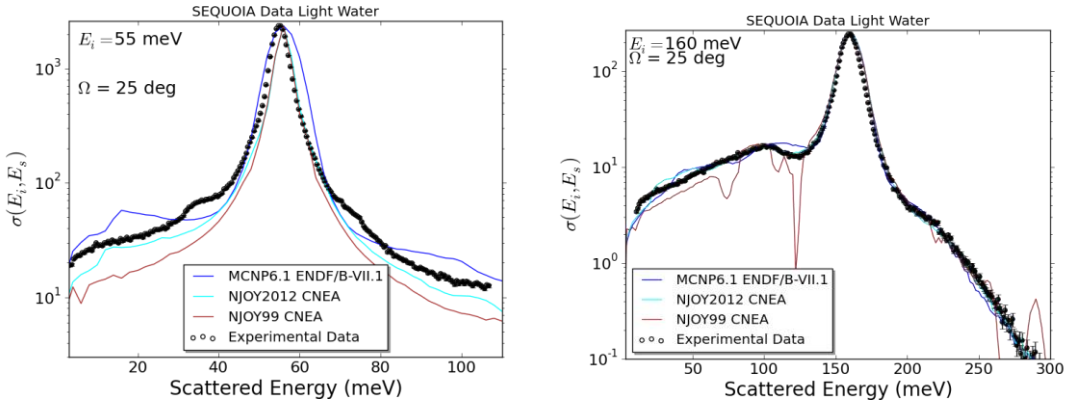

Figure 6: CNEA and Experimental comparison

CNEA's original ACE file was created with NJOY 99. Running their ENDF format data through our NJOY2012 gave a much better fit. In some places it performs better than the ENDF/B-VII.1 library.

The process described in section 3.2 is shown in Figure 7 for two angles.

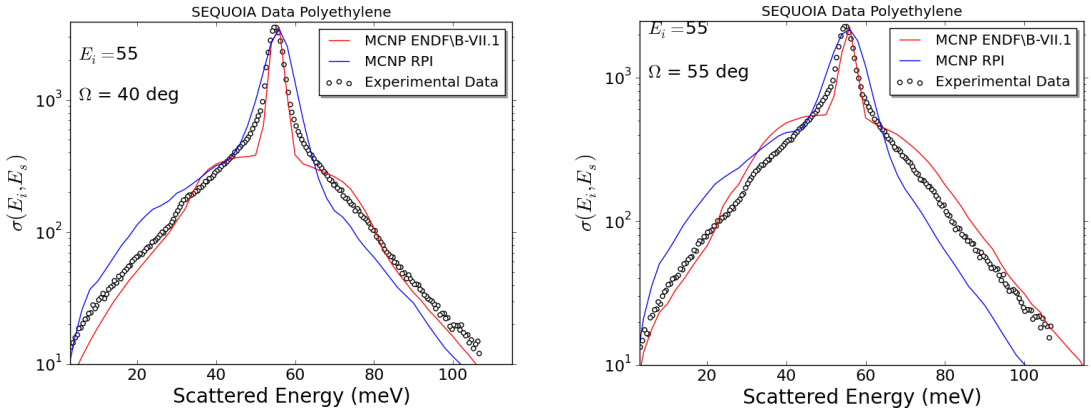

Figure 7: Comparison with RPI Thermal Scattering Law Evaluation

The agreement for the MCNP RPI line is reasonable but leaves room for improvement. The elastic peak is slightly too wide, and the inelastic wings average out in integration. This process used the given De-Bye Waller factor from the ENDF/B-VII.1 library. A new De-Bye Waller factor will be needed to calculate a better evaluation.

5. CONCLUSIONS/FUTURE WORK

The experimental data from SEQUOIA and ARCS show some of the most detailed DDSCS to date. This allows for comparisons with current Thermal Scattering Law libraries. Comparisons yield a good representation of the elastic peak for CH_2 and H_2O. The SiO_2 library shows major discrepancies with the collected experimental data. The limited agreement shown in the results of using the experimental data to create a thermal scattering law evaluation supports the feasibility of using the experimental data for more than validating evaluations. Improving the De-Bye Waller factor and normalization procedures are part of the future work.

ACKNOWLEDGMENTS

Research at Oak Ridge National Laboratory's Spallation Neutron Source was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. A specific thank you is given to the instrument scientists of the ARCS and SEQUOIA machines for their continued assistance. Funding for this work has been provided by the DOE-NCSP.

REFERENCES

1. R. E. MacFarlane, et al, *The NJOY Nuclear Data Processing System*, pp 165-186, pp 493-544, Los Alamos National Laboratory, Los Alamos, New Mexico, USA (2012).
2. J. Holmes, *Development of ENDF Thermal Neutron Scattering Libraries for Silicon Dioxide and MCNP Criticality Testing with an ICSBEP Benchmark*, Appendix A, North Carolina State University, Raleigh, North Carolina, USA (2011).
3. T. Goorley, et al., "Initial MCNP6 Release Overview", Nuclear Technology, 180, pp 298-315 (2012).
4. A. Kolesnikov, M. Stone, "SEQUOIA Fact Sheet," https://neutrons.ornl.gov/sites/default/files/06_G00806H_Instrument_17.pdf (2014).
5. D. Abernathy, A. Christianson, "ARCS Fact Sheet," https://neutrons.ornl.gov/sites/default/files/06_G00804F_Instrument_18.pdf (2014).

6. G.E. Granroth, A.I. Kolesnikov, L.M. DeBeer-Schmitt, T.E Sherline, *SEQUOIA Operations Manual for Users*, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA (2013).
7. M. Herman, A. Trkov, et al, *ENDF-6 Formats Manual*, Brookhaven National Laboratory, Upton, New York, USA (2009).