Validation of Multiple-Scattering Corrections in the Analysis Code SAMMY

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Many analyses of neutron-induced cross section data in both the resolved-resonance region (RRR) and the unresolved-resonance region have been accomplished using the computer code SAMMY,[1] developed over the span of two decades at Oak Ridge National Laboratory. Accurate analyses in the RRR have significant requirements beyond "merely" using the correct R-matrix formulation with reasonable spin assignments for resonances: It is also necessary to properly include in the calculations all those experimental effects which cause the quantities being measured to differ noticeably from the quantities one wanted to measure. For example, the finite temperature of the measurement requires computation of Doppler broadening; spread in beam width and in flight-path-length requires computation of resolution broadening. These effects and many others are included in the SAMMY code.

For analyses of capture (or other reaction) measurements, one important experimental effect is the multiple-scattering correction: When a neutron reaches the sample, it is often first scattered by one or more of the nuclei in the sample before it is captured by yet another nucleus. At each scattering, the neutron loses energy. What may therefore be seen in the measurement is not only the resonance peak, but also an additional (smaller) peak at a higher energy; the center of this single-scattering peak corresponds to 90-degree scattering with the exact position determined by kinematics alone. Double- and higher-multiple-scattering peaks also may be visible in the data.

Analytic calculation of the full multiple-scattering correction is not practical, since each additional scattering introduces an additional six-fold embedded integration. The single-scattering correction can be calculated with high accuracy for specific geometries. Double- and higher-multiple-scattering corrections can be calculated with modest accuracy using crude approximations to decouple the integrations. The approximations and computational techniques used in SAMMY will be described in some detail.

Because the computation is complicated, and experimental verification of the results is inconclusive due to the presence of other measurement effects, it is important to have an independent method of testing the validity of the SAMMY approximations and computational techniques. Monte-Carlo simulations provide such a method. A Monte-Carlo code SAMSMC has been created, which uses the exact same Doppler-broadened cross sections and geometric information as are used for input to the SAMMY multiple-scattering calculation. Both SAMMY and SAMSMC permit the existence of more-than-one type of nuclide in the sample, and both calculate non-isotropic scattering as needed.

Both codes provide values of Y0 (the self-shielded capture yield), Y1 (the single-scattering correction to the capture yield), and Y2 (the double- and higher-multiple-scattering correction); the "measured" value is the sum of these three: Y = Y0 + Y1 + Y2. (Of course the actual measured value includes resolution broadening and other effects which are neglected in these calculations.) Generally, values for Y1 are one-or-more orders of magnitude smaller than the

maximum value of Y0 (at the peak of the resonance), and values for Y2 are significantly smaller than the maximum value of Y1.

Comparisons between results for Yi (i = 0, 1, 2) from SAMMY vs those from SAMSMC will be shown for a variety of samples, including (but not limited to) ^{58}Ni, natural Sm plus heavy water, various isotopes of Ba, natural Si, LiCl, and isotopic Cl.

Results from the comparisons undertaken so far indicate that agreement between SAMMY and SAMSMC for the value of Y0 is excellent (as expected, since this is a trivial quantity to calculate). Agreement for Y1 is also good. Agreement for Y2 is, again as expected, not as good, since the calculation of Y2 involves crude approximations. Nevertheless, the general shape (as a function of energy) of SAMMY's Y2 calculation is similar to the shape of SAMSMC's Y2 simulation. This therefore suggests one simple possibility for ad-hoc improvement in the SAMMY calculation of Y2: a multiplicative factor for Y2 could be determined by the analyst using SAMSMC/SAMMY comparisons, and provided as input into the SAMMY analysis. This possibility will be explored further.

1. "Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations," N. M. Larson, ORNL/TM-9179/R5, Oak Ridge National Laboratory, Oak Ridge, TN (November, 2000).