ORNL Resonance Evaluation for ENDF/B-VII.1*

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INTRODUCTION

Cross-section evaluations in the resonance region are performed at Oak Ridge National Laboratory (ORNL) with the computer code SAMMY [1] based on formalisms derived from the R-matrix theory. Resonance parameters (RPs) obtained in the evaluation, combined with resonance formalism, replicate a regression of the experimental data. The RPs are also used to generate cross-section data for neutron transport calculations in analyses of nuclear reactor design and nuclear criticality safety. In addition to generating RPs, the evaluation also generates the resonance parameter covariance (RPC) data. Several ORNL resonance evaluations, including RPs and RPCs, were incorporated in the recently released US-evaluated nuclear data library, ENDF/B-VII.1. A brief summary of the RPs and RPCs evaluated at ORNL is given.

CODE SAMMY

The computer code SAMMY [1], developed at ORNL, is used in the evaluation of experimental data for the resolved and unresolved resonance energy regions. The data fitting of cross sections is based on the generalized least-squares formalism (Bayesian theory) together with the resonance formalism described by the R-matrix theory. The result of the evaluation is a set of RPs and RPCs that represent the experimental data. The RPCs are used to propagate the uncertainty in the cross section. In SAMMY, the uncertainty in the RPs can be obtained in either of two ways: (a) as a result of the evaluation process in which SAMMY generates a set of RPs that fit the data, together with the corresponding RPC, or (b) by generating the RPC with the retroactive approach because the RPC is no longer available. For example, RPs for many nuclides may be available but the corresponding RPC matrix may not exist. When it is not possible to completely reanalyze the experimental data, the retroactive scheme may be used to generate a realistic approximation of the covariance matrix. Few steps are needed to generate an approximate covariance matrix using the retroactive parameter covariance methodology.

The procedure consists of the following.

1. Select the best available resonance parameter evaluation from the nuclear data libraries.
2. Retrieve resonance parameter uncertainties from the literature [2].
3. Generate total, scattering, capture, fission cross sections for use as “experimental data” in SAMMY.
4. Assign experimental uncertainties to the “experimental data.” Best judgment must be used here in assigning the uncertainty in the “experimental data.” For instance, for uncertainty in the thermal cross-section, resonance capture integral, uncertainty in the scattering radii can be used. Also, uncertainties in the actual experimental data listed in EXFOR [3] or experimental data used in obtaining the resonance parameter in (2) should be included.
5. Run SAMMY code with the option to generate resonance covariance retroactively.
6. Finally, convert the resonance-covariance results from SAMMY into the ENDF format.

A complete ENDF evaluation encompasses several parts that describe neutron interaction in energy ranges other than the resonance region. At the end of the SAMMY evaluation, the RPs and RPCs are converted into the ENDF FILE 2 and FILE 32 format and included in the ENDF.

RP AND RPC EVALUATIONS FOR ENDF/B-VII.1

The isotopes evaluated with SAMMY are displayed in Table I. In addition to the evaluations shown in Table I, RPC evaluations for the actinides ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu were also completed. A description of the methodologies used in the covariance generation for the actinides is given in [4].

Table I. Isotopes Evaluated with SAMMY for ENDF/B-VII.1

Titanium	^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, ^{50}Ti
Chromium	^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr
Nickel	^{58}Ni, ^{60}Ni
Potassium	^{39}K, ^{41}K
Chlorine	^{35}Cl, ^{37}Cl
Manganese	^{55}Mn
Tungsten	^{182}W, ^{183}W, ^{184}W, ^{186}W

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In the RP evaluations of the isotopes of titanium, chromium, nickel, potassium, chlorine, and manganese, the RPCs were generated by evaluating the experimental data. For the tungsten isotopes, the retroactive approach was used to generate the RPCs.

As an example of the use of SAMMY in the RP and RPC evaluation, Fig. 1 shows a comparison of the SAMMY R matrix fit to the data of Guber et al. [5] for natural chromium from 20 keV to 100 keV. The top curve represents the capture cross section, and the other two curves are the total cross sections corresponding to two transmission measurements with thicknesses of 0.026269 at/b (thin sample) and 0.053103 at/b (thick sample), respectively. A full description of the chromium evaluation is given in [6].

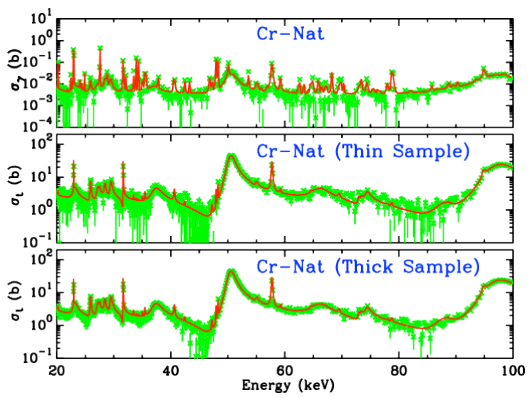

Fig. 1. Comparisons of SAMMY calculations with the measured resonance parameter data for the total and capture cross sections of natural chromium in the energy region 20 keV to 100 keV.

The percentages of uncertainty in the averaged total and capture cross section calculated with the RPC for an energy bin of 10 keV from 20 keV to 100 keV for a flat flux weight are shown in parentheses in Table II for ^{52}Cr isotope. The average cross-section uncertainty for the total cross section is approximately 1% to 2%, whereas for the capture it is approximately 4% to 8.5%.

Table II. Average Total and Capture Cross Section Calculated with the RP and RPC for ^{52}Cr

Energy Range (keV)	Total (% Uncertainty) (barn)	Capture (% Uncertainty) (millibarn)
20–30	1.95 (1.5)	15.68 (7.0)
30–40	1.46 (1.4)	7.73 (4.0)
40–50	2.41 (1.2)	7.40 (7.4)
50–60	13.72 (1.0)	8.87 (8.0)
60–70	1.99 (1.1)	1.19 (8.5)
70–80	0.85 (1.8)	1.92 (8.0)
80–90	0.17 (1.9)	1.99 (7.9)
90–100	14.30 (0.9)	16.36 (6.0)

For the remaining isotopes listed in Table I, a thorough description is given in [7].

CONCLUSION

Evaluations were performed at ORNL with the computer code SAMMY for the resonance regions included in ENDF/B-VII.1. As an example, the results of calculations performed with the RP for natural chromium and RPC for ^{52}Cr are presented.

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