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REPRESENTATION OF THE NEUTRON CROSS SECTIONS OF SEVERAL  
FERTILE AND FISSILE NUCLEI IN THE RESONANCE REGIONS\*

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# REPRESENTATION OF THE NEUTRON CROSS SECTIONS OF SEVERAL FERTILE AND FISSILE NUCLEI IN THE RESONANCE REGIONS

J. de Saussure and R. B. Perez

## I. INTRODUCTION

In this paper we discuss some problems related to the measurement, evaluation and representation of the neutron cross sections of the main fertile and fissile nuclides in the resolved and unresolved resonance regions. We restrict our comments to the heavy nuclides most important for nuclear reactor applications and we note here that the resonance structure of light and medium weight nuclides used as moderators, coolants or structural materials has different characteristics and may require a different approach.

For the purpose of organizing our review, we have subdivided our comments around three main topics: (1) the resolved resonance parameters of the fertile nuclides and their uncertainties, (2) the representation of the cross sections of the fissile nuclides in the resolved resonance range, and (3) the treatment of the unresolved resonance range.

In the past ten years or so, little progress has been made in improving the accuracy of our knowledge of the resolved resonance parameters of the fertile nuclides. In our opinion, this absence of progress is due to a lack of adequate methodologies to assess and describe the systematic errors in the resonance parameters resulting from uncertainties in the analysis of the measurements, and to combine relevant information from several sources into a single evaluation. We note recent promising developments in understanding and correcting these problems but we believe that much improvement is still needed if the resolved resonance parameters of the fertile nuclides are to be substantially ameliorated.

to examine the most recent US evaluation, ENDF/B-V, of the cross sections of a fissile nuclide in the resolved resonance region. We find that whereas the  $^{235}\text{U}$  representation conforms to the recommended procedure, the  $^{238}\text{U}$  and  $^{239}\text{Pu}$  representations are inadequate and inconsistent with present state of the art. We recommend that a new analysis of the resolved range of these two isotopes be performed.

Most of our comments are addressed to the ENDF/B treatment of the unresolved resonance range. We feel that this treatment is inadequate and inappropriate. We recommend that the model used for the unresolved range be reexamined and that alternate descriptions be investigated. Most importantly we recommend that validation of the unresolved range evaluations with appropriate transmission and self-indication measurements.

It goes without saying that none of our comments are meant as criticism of ENDF/B-V evaluators: the evaluations were made under a number of practical constraints which explain many of the deficiencies. Rather we hope that some of our observations may lead to a reexamination of some aspects of the evaluation process and to improved future evaluations.

## 11. UNCERTAINTIES IN THE RESOLVED RESONANCE PARAMETERS OF THE FERTILE NUCLEI

### A. Statistical and Systematic Errors

The resolved resonance parameters of the fertile nuclides are usually obtained by least-square shape analysis of time-of-flight transmission measurements, often supplemented by shape or area analysis of capture, scattering or self-indication experiments.<sup>1-4</sup> It is not our purpose here to discuss the measurement or analysis techniques which are described in several recent books.<sup>5,6</sup> Instead, we wish to emphasize one particular aspect of the analysis which we think is important and has perhaps not been properly addressed: the estimation, representation, and utilization of systematic uncertainties.

Experimenters often distinguish between statistical and systematic errors. In a time-of-flight measurement the statistical error in each channel can be obtained in a straightforward way from the number of events observed in that channel. This error is uncorrelated from one channel to the next and can usually easily be propagated through the data analysis to a "statistical error" of the resonance parameters. The statistical errors of the resonance parameters are, of course, generally correlated through the constraints of the model used in the analysis.

Systematic errors, on the other hand, arise in the interpretation and analysis of the experiment: before resonance parameters, or even transmission ratios, can be extracted from the measurements, several inferences must be made about the shape and magnitude of backgrounds, the response of detectors, the homogeneity of transmission samples, and so on. Uncertainties in these inferences result in systematic errors that are often difficult to evaluate and that have complicated correlation patterns.

Modern neutron time-of-flight spectrometers have such high intensities that in many experiments the statistical errors can practically be made arbitrarily small by extending the duration of the measurement. Hence the dominating uncertainty in the resonance parameters of the fertile nuclides is usually the systematic error. Yet most of our methodologies for resonance analysis, for reporting experimental data, and for evaluation are designed for uncorrelated statistical errors.

Many resonance analysis codes cannot properly handle systematic errors; often the code reads or computes an uncorrelated error for each datum, which is used to determine a "weight" for the datum. On the basis of these weights and of some consistency criterion between the model and the data, the program generates errors for the resonance parameters. These errors do not

include properly the systematic uncertainties.<sup>7-9</sup> Experimentalists rarely include information on the correlations between errors and several evaluations of the resonance parameters of the fertile nuclides are essentially weighted mean values of published parameters, with the weights derived from the published errors.<sup>10-11</sup>

We believe that, at present, there is no clear, accepted, and practical approach to estimate and report systematic errors and their correlations and to combine data from different parameters. This situation inhibits the improvement of the data. We shall not illustrate these observations with a couple of examples.

## B. Comparisons of Resonance Parameters

1. The importance of systematic errors has long been recognized by experimenters,<sup>12-15</sup> evaluators and data users.<sup>16-19</sup> In particular, to illustrate the effect of the method of analysis on the values obtained for the resonance parameters, Derrien, Ribon, and L'Heriteau have reanalyzed several transmission experiments.<sup>20-22</sup> An example of this work is shown on Table I, where values of the neutron widths of several  $^{238}\text{U}$  resonances are compared. The values of Carraro and Kolar<sup>2</sup> given in the fourth column were determined using the area analysis program of Atta and Harvey.<sup>7</sup> The errors given include statistical errors and several systematic errors arising from the uncertainty in the transmission sample thicknesses and from several hypotheses used in the resonance analysis.<sup>23</sup> The values in the second column were obtained by Derrien and Ribon<sup>21</sup> by reanalyzing part of the measurements of Carraro and Kolar using the Saclay shape-analysis program. Derrien and Ribon do not characterize the error given in that column, but presumably it is the statistical error generated by their program. Similarly, the last column contains the values obtained by Rahn *et al.*<sup>1</sup> from their measurements, using a combination of area and shape

analysis methods; the errors in that column are not clearly characterized by the authors. The third column lists values obtained by Saclay using shape analysis and part of the transmission data of Rahn *et al.* From an inspection of the data we see that: (1) the same data analyzed by two different methods yield significantly different values for the parameters, (2) the Saclay resonance analysis applied to two different sets of data again yields significantly different parameter values; this in spite of the fact that the analysis program "readjusts" the background in each experiment, (3) it is difficult to give an objective and meaningful interpretation to the errors quoted in each column except that in general these errors are smaller than either the differences between two analyses of the same experiment, or between the same analysis of two sets of data.

2. In Table II values of the neutron and capture widths of the first four large levels of  $^{232}\text{Th}$  are compared. The results of the three latest U.S. measurements are listed in columns 2, 3, and 4; the last two columns give the values of ENDF/B-IV<sup>24</sup> and ENDF/B-V<sup>25</sup> respectively. We were unable to determine from the publication of Rahn *et al.*,<sup>1</sup> whether the errors given were statistical, systematic or a combination of both. Chrien *et al.*,<sup>3</sup> report statistical uncertainties for one of the measurements used in deriving the parameters; these are shown in parenthesis in column 3. The other error is said to "include all statistical and estimated systematic uncertainties." The errors reported by Olsen *et al.*,<sup>4</sup> are statistical uncertainties multiplied by three, because it has been these authors experience "that in order to obtain overlapping parameters with errors from separate fits to the various sample thicknesses or from different transmission measurements requires increasing the least-squares parameter covariance matrix uncertainties by a factor of two to four." It is not clear that the latest evaluation, ENDF/B-V, is more consistent with recent data than the ENDF/B-IV evaluation which, for  $^{232}\text{Th}$ , was completed more than 15 years ago!

In particular it is noteworthy that the values of the latest measurement, taken in 1971, never overlap within quoted errors either ENDF/B-V or JENDL-4000.

### C. Recommendations

If the evaluations of the resolved resonance parameters of the fertile nuclides are to improve significantly, better methods will be needed to estimate, describe, and use systematic errors and their correlations. We realize that this recommendation is easier to formulate than to implement: Mann and al., for instance, reported more than 700  $^{232}\text{Th}$  and more than 600  $^{238}\text{U}$  resonance parameters. The covariance matrix for these 1300 parameters would consist of more than 800,000 independent entries! Methods must be developed to estimate and describe the essential features of the covariance matrix in a concise form.

In recent years a much greater awareness has evolved of the need for a more complete description of errors and their correlations.<sup>12-15</sup> Larson and Perey<sup>26</sup> have written a computer model for resonance analysis using Bayes' Equations where covariance matrices are explicitly used, but this program has not yet been implemented for the fertile nuclides. Finally the methodology to include covariance matrices to sensitivity calculations is being extended to handle resonance parameters so that the recommended improvements may be forthcoming.<sup>27-28</sup>

## III. RESONANCE ANALYSIS OF THE CROSS SECTIONS OF FISSILE NUCLIDES

### A. The Goals of Resonance Analysis

The main goals of the resonance analysis of the cross sections of the fissile nuclides are:

2. To obtain information on the statistical distribution of the resonance parameters. This information is helpful in determining the basic nature of the fission process and in predicting the structure of the cross sections in the unresolved resonance region. These applications of resonance analysis have been extensively discussed in the literature.<sup>6,29,30</sup>

3. The representation of the low-energy cross sections by an appropriate resonance formalism permits the simultaneous analysis of several partial and total cross-section measurements done at different temperatures under different energy resolution conditions. The use of a unitary formalism insures consistency in the line shapes of the total and partial cross sections.<sup>31</sup>

4. A good resonance formalism allows the concise and precise representation of the details of the complicated resonance structure of the cross sections. This results in an appreciable economy in data storage and data processing.<sup>32</sup>

5. Finally, the resonance parameterization is very convenient for the calculation of Doppler broadened cross sections and of resonance self-protection. Methods have been developed for the rapid calculation of Doppler broadened "line shapes" and for the calculation of self-shielded resonance integrals.<sup>33-36</sup>

#### B. Non-Uniqueness of the Resonance Analysis of the Fissile Nuclides

Several aspects of the analysis of the cross sections of the fissile nuclides makes the interpretation of the resonance parameters somewhat ambiguous:

1. It is well known that the single-level Breit-Wigner resonance formula is a poor approximation for the fissile nuclides, even at low energy. A multi-level formalism is required to describe the interferences in the fission channels, which produce asymmetries in the resonance shapes.

2. The natural widths of the resonances of the fissile nuclides are comparable to the level spacings, so that even at low energy some resonances overlap.

It is not always possible to determine whether a resonance asymmetry is caused by nuclear interference or by a small level in the wing of a resonance.<sup>37</sup> Simultaneous analysis of fission and capture measurements performed at low temperature may help resolve such ambiguities.

4. The bound levels contribute appreciably to the low-energy cross sections. However, the precise position and strength of these levels are not defined uniquely by the data.<sup>38</sup>

5. Most measurements do not separate the contributions of the two-level sequences corresponding to the two possible values of the total angular momentum. Among the fissile nuclides, only for  $^{235}\text{U}$  have measurements of polarization been done over a wide energy range.<sup>39-41</sup>

6. No practical method has been found yet to separate the contributions of the different fission channels which make up the total fission cross section.

In spite of the difficulties mentioned above, multilevel resonance analysis of the cross sections of the fissile nuclides have been performed which yield cross-section curves in excellent agreement with the measurements. However, the good agreement between computed and measured cross sections does not ensure the uniqueness of the parameters obtained: indeed, another interpretation of the resonance structure, or other assumptions concerning the bound levels may lead to a significantly different set of parameters which represents the measurements equally well.<sup>42-44</sup>

### C. Multilevel Resonance Formalisms

Several multilevel formalisms are available to describe the cross sections of the fissile nuclides. The most frequently used are the Reich-Moore and the Adler-Adler formalisms which are specializations of the general dispersion theory of Wigner and Eisenbud.<sup>45-47</sup> Computer programs have been written to analyze measurements with these formalisms and multilevel resonance

work has been performed of the low energy cross sections of all the fissile isotopes.<sup>31,32,45-7</sup>

The most suitable formalism for the resonance analysis of fissile nuclides whose section measurements is the Reich-Moore formalism because it is accurate and yields  $P$ -matrix resonance parameters which are easier to interpret than the parameters used in the Adler-Adler formulation. Furthermore the Reich-Moore representation can readily be transformed into an equivalent Adler-Adler representation, whereas the inverse process of converting Adler-Adler parameters into equivalent Reich-Moore parameters is less straight forward.<sup>33,36</sup>

For describing the cross sections for practical applications the Adler-Adler representation might be more convenient because it is particularly well suited for the calculation of Doppler broadened and self-shielded cross sections, using the Voigt profiles and the generalized J-function.<sup>34-36,57</sup> Recently Froenner has demonstrated a new technique for the direct calculation of Doppler broadened Reich-Moore cross sections which is as fast as the Adler-Adler calculation with Voigt profiles;<sup>58</sup> however, it is not clear that the technique can be used to obtain self-shielded resonance integrals with the generalized J-function approach.

### 3. ENDF-Recommended Procedures and ENDF/B-V Evaluations

In the light of the preceding discussion, the recommendation of the ENDF-B procedures for the treatment of the fissile nuclides in the resolved range appears very reasonable: "the preferred formalism for evaluation purposes is the Reich-Moore multilevel scheme, but it has less flexibility than the Adler method and is therefore better able to distinguish between various grades of experimental data. However, for the purpose of presentation in ENDF/B, Reich-Moore evaluations must be converted to Adler format, since

the latter permits the use of  $\mu$  and  $\chi$ -functions for Doppler broadening, whereas the Reich-Moore scheme requires kernel methods.<sup>49</sup>

The ENDF/B recommendation was followed in the ENDF/B-V evaluation of  $^{233}\text{U}$  (MAT 1397) and the resolved resonance region of this material is represented by equivalent Adler-Adler parameters obtained from the Reich-Moore resonance analysis of Reynolds and Stieglitz.<sup>51</sup> The parameters give an accurate representation of the data, so that the "File 3" contribution of this material is identically zero over the resonance region.

Unfortunately the ENDF/B procedures recommendation was ignored in the evaluations of  $^{235}\text{U}$  and  $^{239}\text{Pu}$ , (MAT 1395 and MAT 1399, respectively.)<sup>61,62</sup> In fact the representations of the resolved resonance range of these two isotopes in ENDF/B-V do not meet any of the goals of resonance analysis as defined in III. A., at the beginning of this section.

In MAT 1395,  $^{235}\text{U}$ , the resolved range extends from 1 to 82 eV and is described by single-level Breit-Wigner parameters for some 130  $J=7/2$  levels, combined with a highly structured File 3 consisting of more than 1300 energy points: the File 3 contribution to the total cross section is illustrated in Fig. 1.

As may be seen on Fig. 1, the "smooth background" File 3 is anything but smooth and the structure should not be ignored in Doppler broadening or in self-shielding calculations. The formalism used to describe part of the cross sections is not unitary so that the consistency in the line shape of the resonances is not insured. Furthermore, the J-value assignments are obviously incorrect.

Many man-years of efforts have been expended to determine the spin of the levels of  $^{235}\text{U}$ , to develop appropriate multilevel formalisms and data analysis computer programs and to perform high quality resonance analyses of the cross sections of  $^{235}\text{U}$  and  $^{239}\text{Pu}$ . It seems surprising that all this

work has been done in the ENDF/B-V representation of these two important isotopes. Stage ENDF/B-III is intended to define the best available representation of the unresolved resonance region to be used in reactor designs and data testing. The present work is a first step in the evaluation of  $^{238}\text{Pu}$ , MAT 1399, also represented with single-level parameters.

It seems appropriate here to recommend that new ENDF/B-type evaluations of the unresolved ranges of  $^{238}\text{U}$  and  $^{239}\text{Pu}$  be performed, incorporating all the relevant information, and in particular the polarization data for  $^{235}\text{U}$ ,<sup>61</sup> and using the multilevel scheme recommended for fissile nuclei in the ENDF/B procedures.

## IV. COMMENTS ON THE ENDF/B UNRESOLVED RESONANCE REGION FORMALISM

### A. Introduction

A considerable amount of effort has gone into improving processing methods for the unresolved resonance region but probably less into validating the model used to represent the cross sections in that region.

It seems to us that the central question about the ENDF/B representation of the unresolved resonance region is whether or not that representation leads to a correct estimate of resonance self-shielding. Ultimately this question should be answered by comparing computed self-shielding factors as a function of energy, temperature, and dilution with values derived from self-indication measurements or from other clean experiments. We know of no such tests performed with ENDF/B-V. Admittedly there are few good self-indication and Doppler effect measurements<sup>63-70</sup> and these are perhaps difficult to interpret, but these difficulties will have to be addressed, or new measurements will have to be done if the unresolved resonance model is to be properly validated.<sup>71</sup>

We now wish to examine as an example the ENDF/B-V  $^{238}\text{U}$ , MAT 1398,<sup>72</sup> representation of the unresolved resonance cross sections. Our comments are not intended to be critical of the evaluation per se, or of the procedures and the followed accepted ENDF/B procedures. We wish rather to raise some questions about the model, which we hope may lead to an improved representation of the unresolved resonance region and to improve future evaluations.

We confine our description of MAT 1398 to the energy range 4 to 45 keV to avoid complications associated with the inelastic-scattering competitive width, which are irrelevant to our discussion. The low energy end of the unresolved resonance region is also the region where resonance self-shielding effects are most important.<sup>73</sup>

In the next subsection we review the unresolved resonance treatment of MAT 1398 in the interval 4 to 45 keV and we comment on the model. In subsection C we report on a study of the influence of the choice of unresolved resonance parameters on the calculation of self-shielding factors in  $^{238}\text{U}$ . In subsection D we report on another study where we have treated the  $^{238}\text{U}$  resolved range from 1 to 4 keV with exactly the same methodology used in the unresolved range. We then compare the self-shielding factors computed "exactly" with the resolved resonance parameters with those computed "statistically" with the unresolved resonance formalism. Finally in subsection E we recommend the investigation of other techniques to treat the unresolved resonance region.

#### B. The MAT 1398 Unresolved Resonance Region in the Interval 4 to 45 keV

The unresolved resonance parameters were generated on the basis of criteria discussed in File 1 of MAT 1398 and described below:

Average resonance parameters are given for neutron angular momenta  $\ell=0$ , 1 and 2. Since the  $^{238}\text{U}$  ground state has spin zero, the  $^{239}\text{U}$  compound states to be formed with spin values  $J = |\ell \pm 1/2|$ .

The average value of the level spacing  $D(i,J)$ , the reduced neutron widths  $\Gamma_n^0(i,J)$  and the capture widths  $\Gamma_{n\gamma}^0(i,J)$  for each  $(i,J)$  series. The reduced neutron widths are assumed to have a Wigner distribution, the reduced capture widths are assumed to have a Porter-Thomas distribution and the capture widths are taken to be constant. The average value of all the parameters is taken to be constant over the interval 4 to 45.18 keV (as given in Table III except for  $\Gamma_{n\gamma}^0$  which is assumed to be constant) and the widths  $\Gamma_n^0$  are adjusted at 19 energy points to fit the evaluated average capture cross section,  $\sigma_{n\gamma}$  at these 19 energies. At these 19 energy points the value of  $\Gamma_n^0$  ( $\lambda=1, J=3/2$ ) was assumed to be  $\Gamma_n^0(i,J=1/2)$ . The 19 energies, the corresponding values of  $\Gamma_n^0$  ( $\lambda=1/2$ ) and of the computed average capture cross section are listed in Table IV.

There is not theoretical or logical justification for such a model although this model conforms to usual ENDF/B procedure. From the theoretical point of view, there is no reason to expect the variation in the locally averaged cross section to be due entirely to a variation in the locally averaged  $\lambda=1$  reduced neutron widths. There is no reason either to expect a small sample of the reduced neutron widths to have a Porter-Thomas distribution around their locally averaged values.

The model is also logically inconsistent. By specifying average resonance parameters and their distributions, we specify only the probability distribution of the average cross sections, not the actual values. By fitting the local reduced neutron widths to the locally average values of the capture cross section, on the other hand, we imply that the most probable value of the average cross-section is the actual value. Furthermore the magnitude of the fluctuations of the locally averaged capture cross section is determined by the width of the averaging intervals and there is no compelling rationale for selecting these widths. The widths of the averaging intervals should probably be interpreted as being of

of the average capture cross section as the intervals between successive energy points. The unresonance parameters are defined: as can be seen from Table II, the intervals are considerable in magnitude.

Because of the lack of theoretical justification and because of these gross inconsistencies, the model should be viewed at best as an ad hoc parameterization of the average capture cross section. Because of the way it is constructed, the model will reproduce exactly the evaluated locally averaged capture cross sections but there is no reason to expect it to provide correct values of the self-shielding factors, since the parameterization is not unique and since no self-shielding information was utilized.

#### 4. Influence of the Choice of Unresolved Resonance Parameters on the Calculation of Self-Shielding Factors in <sup>238</sup>U

In this subsection we investigate now the self-shielding factors change when the average s-wave and p-wave reduced neutron widths are modified so as to keep the average capture cross section unchanged. We show that, particularly at the low energy end of the unresolved resonance region, the uncertainties in average unresolved resonance parameters would lead to significant uncertainties in the computed self-shielding factors even if the average infinitely dilute capture cross section were known exactly.<sup>74</sup>

For simplicity of notation we shall refer from now on to the average s-wave reduced neutron width as G<sub>0</sub> and to the average p-wave reduced neutron width for J=1/2 as G<sub>1</sub>. We shall also abide by the Version V choice that the average p-wave reduced neutron width for J=3/2 is exactly half of G<sub>1</sub>, although there is no physical reason for this relation to hold for averages over a relatively small number of levels.

As stated in the previous subsection, the values of the unresolved resonance parameters of MAT 1398 below 45 keV were obtained by a fit to an evaluated average capture cross section. Such a fit is not unique, since several sets

The same resonance parameters may yield the same average capture cross-section.
 The resonance parameters of the average resonance parameters were kept constant at the
 values given in Table III, except for GNI which was adjusted in the fit.
 In the context of the unresolved resonance region model described in the
 previous subsection, we interpret the average reduced neutron widths as local
 averages over an energy width roughly equal to the separation between successive
 levels at which they are defined. For instance, as can be seen in Table IV
 from 4 to 5 keV the resonance parameters are redefined every 250 eV. Hence,
 the J=1/2 parameters which have a spacing of 20 eV are averaged over  $N=250/20=$ 
 12.5 levels. Hence, the local averages have a "sampling error" which, for a
 Porter-Thomas distribution, is  $\delta GNO/GNO = \sqrt{2/N} = .4$ . Hence, there is no reason
 to expect the average s-wave reduced neutron width to be constant from one
 250-eV interval to the next and the fluctuations in the average capture cross
 section to be due entirely to fluctuations in the average p-wave reduced
 neutron widths.<sup>75</sup>

We have varied the average s-wave reduced neutron width GNO over the
 range 1.26 to 2.95 meV ( $\pm 40\%$  of the ENDF/B-V value of 2.10 meV). For each
 change in GNO we have searched for the correlated change in GNI which would
 leave the average capture cross section unchanged. For each correlated pair
 of GNO-GNI values we have computed the infinitely dilute average total cross
 section,  $\langle \sigma_t \rangle$  and the capture self-shielding factor  $f_\gamma$  for several dilution
 cross sections  $\sigma_0$  and for several effective temperatures. We define here
 the capture self-shielding factor as<sup>76,77</sup>

$$f_\gamma = \frac{1}{\langle n\gamma \rangle} \frac{\left\langle \frac{n_f}{\sigma_t + \sigma_0} \right\rangle}{\left\langle \frac{1}{\sigma_t + \sigma_0} \right\rangle} \quad (1)$$

were the averages are taken over the probability distribution of the resonance parameters as specified by ENDF/B procedures. The values of  $f_Y$  and  $\langle\sigma_t\rangle$  were calculated by the probability table method,<sup>73,79</sup> using the computer code PAPIN.<sup>80</sup> The values of  $f_Y$  corresponding to an energy of 4 keV, effective temperatures of 100, 1000, and 2000°K, and dilutions of 1, 10, and 100 b are shown in Table V. The errors given in the table are absolute statistical errors from the Monte Carlo calculations, however, since each calculation was done with the same series of random numbers, the uncertainty in the ratio or difference of two values shown in the table is much smaller than implied by these errors.

It can be seen from Table V that two different pairs of correlated values of GNO and GNI, yielding the same infinitely dilute average capture cross section, correspond different values of the computed capture self-shielding factors. At 4 keV to the assumed  $\pm 40\%$  uncertainty in GNO and GNI corresponds an uncertainty of  $\pm 10\%$  in  $f_Y$  for 300°K and for a dilution of 10b, and an uncertainty of the same magnitude in the change in  $f_Y$  between 1000°K and 2000°K. Note that since the infinitely dilute average capture cross section is the same for all the correlated values of GNO and GNI, the self-shielded average capture cross section is strictly proportional to  $f_Y$ . Note also that at 4 keV, the changes in the correlated values of GNI corresponding to the  $\pm 40\%$  variation in GNO are comparable to the changes in GNI with energy, specified by MAT 1398 and shown in Table IV.

It can also be seen from Table V that the correlated changes in GNO and GNI induce changes in the computed infinitely dilute average total cross section  $\langle\sigma_t\rangle$  so that in principle a good knowledge of  $\langle\sigma_t\rangle$  could reduce the uncertainty in GNO and GNI. However  $\langle\sigma_t\rangle$  is not a directly measured quantity; it must be inferred from good resolution transmission measurements as a function of energy and thickness, and it is not clear that it can be obtained with sufficient precision to reduce the uncertainty in GNO.

average (Dopler) free capture self-shielding factors  $f_{\gamma}$  are very close to 1 for all dilutions larger than 1 and for all temperatures above 300°K so that the self-shielding factors  $f_{\gamma}$  are not sensitive to the choice of GNO and GNI.

However, the quantity which is relevant for Doppler effect calculations is the change in  $f_{\gamma}$  with temperature, and this quantity is quite sensitive to the choice of unresolved resonance parameters. This is illustrated in Table II where we report the computed changes of  $f_{\gamma}$  for 100 K and 300 K at 40 keV for several dilutions and for several pairs of correlated values of GNO and GNI.

#### D. The Unresolved Treatment of the Resolved Range for MAT 1398

As a test of the validity of the unresolved resonance region treatment of MAT 1398, the exact same methodology was used over the energy range 1-4 keV which is described by resolved resonance parameters.

The range 1-4 keV was divided into 13 intervals of approximately 250 eV. The average capture cross section  $\langle \sigma_{n\gamma} \rangle$  for each interval was obtained as:

$$\langle \sigma_{n\gamma} \rangle = \frac{1}{\Delta E} \int \sigma_{n\gamma}(E) dE \quad (2)$$

where the integration is over the width  $\Delta E$  of the interval, and  $\sigma_{n\gamma}(E)$  is computed from the resolved resonance parameters and the background File 3. Using the values of the average resonance parameters given in Table III, appropriate values of the average p-wave reduced neutron widths GNI were obtained by fitting  $\langle \sigma_{n\gamma} \rangle$  defined in (2). The capture self-shielding factors  $f_{\gamma}$  were then obtained using Eq. (1) of the previous section. These values can be compared to the corresponding values  $f_{\gamma}^*$  computed by the resolved resonance methodology:<sup>76</sup>

$$\sigma_{n,\gamma} = \frac{2\pi^2 \Gamma_{n,\gamma}}{\Gamma_{n,\gamma} + \Gamma_{\text{res}}}$$

$$\sigma_{n,\gamma}^* = \frac{2\pi^2 \Gamma_{n,\gamma}^*}{\Gamma_{n,\gamma}^* + \Gamma_{\text{res}}}$$

$$\sigma_{n,\gamma}^{\text{self}} = \frac{2\pi^2 \Gamma_{n,\gamma}^{\text{self}}}{\Gamma_{n,\gamma}^{\text{self}} + \Gamma_{\text{res}}}$$

(3)

where the energy dependent cross sections are computed from the resolved resonance parameters.

Some results of this comparison are presented in Table VII. The first column of the table gives the neutron energies for which the unresolved resonance parameters were defined. The second column gives the limits of the energy interval  $\Delta E$  over which the capture cross section was averaged, see Eq. (2). The width of these intervals were selected to correspond approximately to the corresponding width of MAT 1398 in the range 4 to 5 keV. The third column of Table VII gives the average capture cross section, computed from Eq. (2); the fourth column gives the reduced p-wave neutron width for  $J=1/2$ , GNI. The next 3 columns give the values of  $\sigma_{n,\gamma} > f_{\gamma}$ ,  $\sigma_{n,\gamma} > f_{\gamma}^*$ , and their ratio, respectively, for a dilution  $\sigma_0=10b$ . The last 6 columns give the corresponding information for dilutions  $\sigma_0=50b$  and  $\sigma_0=100b$ . At the bottom of the table the self-shielded cross sections have been added over intervals of 1 keV and 3 keV, respectively.

For our purposes here, we view the self-shielding factors  $f_{\gamma}$  computed with actual resolved cross sections as correct. We see from Table VII that over 250-eV intervals the values of  $f_{\gamma}^*$  obtained with the unresolved resonance statistical model may differ appreciably from the values of  $f_{\gamma}$ ; for a dilution of 10b the difference between  $f_{\gamma}^*$  and  $f_{\gamma}$  exceeds 30% in 25% of the intervals. For a dilution of 50b, it exceeds 20% again in 25% of the intervals.<sup>81</sup> Of course, when the self-shielded group cross sections are summed over wider intervals of 1 keV or 3 keV, the differences between the resolved and unresolved calculations become relatively less important; nevertheless even for intervals of 1 keV differences of the order of 5% remain.

It is perhaps particularly noteworthy that over 1-keV intervals the unimodal resonance model appears to overestimate systematically the self-shielding capture cross section. If it can be assumed that from 4 to 10 keV the cross sections are of the same sign as in the interval 1 to 4 keV, then this effect would reduce the longstanding discrepancy between measured and computed values of the capture rate in  $^{238}\text{Pu}$ -containing assemblies.<sup>64,65</sup>

## E. Discussion

The results presented in this section suggest the need for additional validation of the ENDF/B treatment of the unresolved resonance region. In particular, we suggest that because of the non-uniqueness of the unresolved resonance representation it would be desirable to test that the representation leads to correct estimates of the self-shielding, with self-indication and thick-transmission measurements.

Our specific comments were limited to MAT 1393, but it should be clear that validation is also needed for the  $^{235}\text{U}$  and  $^{239}\text{Pu}$  unresolved representations.<sup>61,62</sup> In fact, the fissile isotopes unresolved range starts at a much lower energy (82 eV for  $^{235}\text{U}$  and 300 eV for  $^{239}\text{Pu}$ ) where self-shielding effects might be more important.<sup>34</sup>

We were not able to find the original justification for the current ENDF/B treatment of the unresolved resonance region which consists of fitting the average infinite dilute capture cross section with an energy dependent p-wave strength function. For  $^{238}\text{U}$  this approach was first used by T. A. Pitterle for the ENDF/B-II evaluation (MAT 1107).<sup>85</sup>

Early treatments of the unresolved resonance region were based on energy independent average resonance parameters.<sup>86</sup> Brissenden and Durston<sup>87</sup> introduced a numerical treatment based on the construction of a "ladder" of artificial resonances randomly selected from the appropriate energy independent

probability distributions. As pointed out by Brissenden,<sup>96</sup> in this approach any of the possible ladders is equally probable so that the statistical sampling error can be estimated, but cannot be reduced, by sampling over many possible ladders. Keiser and Kien<sup>97</sup> and Adkins and Dyos<sup>90</sup> computed the uncertainties in Doppler coefficient calculations due to the statistical sampling error. Dyos and Stevens<sup>91</sup> have shown that when the partial inelastic neutron rate integral of  $\Sigma_{in}$  between 4 and 5 keV is computed by the statistical approach, the probable statistical sampling error is about 10%. In order to reduce this statistical error several authors have proposed to select from all possible pseudo-resonance ladders, one particular ladder which yields fine group average cross sections that are consistent with those evaluated from low resolution measurements.<sup>87,92-94</sup> This can be achieved by a forced sampling technique.<sup>92</sup> Note that this technique is not strictly equivalent to the ENDF/B treatment discussed above.<sup>95</sup>

Other treatments of the unresolved resonance region have been proposed. In a previous paper,<sup>36</sup> the authors suggested that the statistical treatment be replaced by using directly the cross sections obtained from high resolution measurements. We discussed methods for the broadening and unbroadening of the resonance structure, even if a proper resonance analysis of the structure cannot be performed. S. Pearlstein<sup>97</sup> suggested a somewhat different approach based on representing the data by the probability table method. Pearlstein also discussed a technique for Doppler broadening and unbroadening of data where resonance parameters are not available. Gur and Yiftah,<sup>98</sup> on the other hand, have suggested the direct parameterization of the resonance self-shielding factors.

We recommend that the present ENDF/B treatment of the unresolved resonance region be reexamined, and perhaps replaced by one of the alternate treatments just reviewed. Before leaving this topic we make three more observations:

(1) There is an inherent statistical sampling error associated with any

placement of the unresolved resonance region which specifies probability distributions for the cross sections, rather than the actual cross sections. It is important that this error be recognized and properly accounted for. The "resolved" and "unresolved" ranges refer to different methods of treating the resonance structure of the cross sections: there is no sharp difference in the data. The decision as to where to stop the resonance analysis of the data and where to start the "unresolved" range is largely an arbitrary decision of the evaluator or analyser of the data. We have discussed this in more detail previously,<sup>9</sup> and as an example, in Figs. 2 to 4 we show examples of the cross sections of  $^{235}\text{U}$  below 60 eV (the resolved range) and of  $^{235}\text{U}$  above 100 eV. (the unresolved range). Clearly the  $^{235}\text{U}$  data above 100 eV are just as "resolvable" as the  $^{235}\text{U}$  data below 60 eV!

Whenever resonance self-shielding is important, the gross features of the resonance structure can be observed in high-resolution data. These gross features dominate the resonance self-shielding effects and can be represented fairly accurately by any resonance parameterization. The smaller resonances which constitute a "noisy background" in the cross section could be accounted for by one statistical ladder or by a File 3 smooth contribution. Such a representation would appear preferable to the present ENDF/B approach.

## V. CONCLUSIONS

In this paper we have discussed several aspects of the measurement, analysis and evaluation of the cross sections of the fertile and fissile nuclides in the resonance regions.

In the resolved range, for the fertile nuclides we think that the principal requirement for improved evaluations is for a practical methodology to deal with systematic errors and their correlations. For the fissile nuclides  $^{235}\text{U}$  and  $^{239}\text{Pu}$ , the ENDF/B-V evaluations are not consistent with ENDF/B procedures recommendations and fall short of the goals of resonance

...but the evaluations of these two isotopes should be performed. In the self-shielded resonance region we show that the ENDF/B representation is not justified and is not theoretically justified. A better representation may be available, and a validation of the representation with experimental self-shielding and transmission measurements is certainly required.

Our emphasis has been on the shortcomings of the latest evaluations, because this is the goal of a critical review, however, it would be unfair to conclude this review without mentioning that, if many problems remain, nevertheless much progress has been achieved in recent years in improving the evaluations of the heavy nuclides. We shall illustrate this observation with two examples:

(1) A longstanding discrepancy between the computed and directly measured values of the self-shielded resonance integral of  $^{238}\text{U}$  has been considerably reduced if not entirely removed.<sup>82,83,99-101</sup> The problem was due to an incorrect uncertainty assignment to an early measurement<sup>103</sup> of the capture width of the 6.68 eV level in  $^{238}\text{U}$ , and was solved by a reexamination of that uncertainty assignment,<sup>100</sup> and by a series of new high quality measurements and analyses of the low energy cross sections of  $^{238}\text{U}$ .<sup>100-102</sup>

(2) In all previous ENDF/B versions several heavy nuclides, particularly  $^{232}\text{Th}$ ,  $^{233}\text{U}$  and  $^{238}\text{U}$ , had "negative cross sections" in the resolved region.<sup>104,105</sup> This problem resulted from an improper treatment of the contribution of the levels with energies outside the resolved range, and from the use of the single level Breit Wigner approximation, which is acceptable only in the vicinity of a resonance energy. In the ENDF/B-V representations of the heavy nuclides these negative cross sections appear only for  $^{242}\text{Pu}$ .

Finally, in concluding, we stress that the shortcomings discussed in this review are being actively addressed by the nuclear cross section community and we feel confident that further improvements in measurements and evaluations are forthcoming.

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Table I.

Resonance Widths for Large Resonances Between 1450 eV and 1760 eV

Energy	Shape analysis of Geel data (2 thicknesses) $\Gamma_n$ , meV	Shape analysis of Columbia data (3 thicknesses) $\Gamma_n$ , meV	Geel published values [Ca 71] $\Gamma_n$ , meV	Columbia published values [Ra 72] $\Gamma_n$ , meV
1473.1	114 ± 2	108 ± 2	125 ± 8	125 ± 10
1522.3	215 ± 4	236 ± 3	260 ± 15	240 ± 15
1597.5	309 ± 6	352 ± 4	351 ± 40	355 ± 25
1622.3	97 ± 2	88 ± 2	116 ± 15	68 ± 14
1637.4	50 ± 1	46 ± 2	60 ± 5	50 ± 8
1662.0	201 ± 4	214 ± 4	241 ± 20	171 ± 20
1687.3	98 ± 2	97 ± 2	104 ± 9	92 ± 10
1709.0	81 ± 2	77 ± 2	94 ± 7	86 ± 8
1755.2	121 ± 3	116 ± 3	135 ± 10	105 ± 10
$\sum \Gamma_n$	1286	1334	1486	1292

In the shape analysis of Geel data the adjusted background parameters  $a$  were negligible ( $\leq 10^{-3}$ ).

In the shape analysis of Columbia the adjusted background parameters  $a$  were equal to:

- 0.0011 for 0.084 at/b sample;
- 0.010 for 0.0348 at/b sample;
- 0.027 for 0.0084 at/b sample.

Table II. Comparison of  $^{232}\text{Th}$  Resonance Widths (meV)

Level Energy eV		Rahn <i>et al.</i> (1972)	Chrien <i>et al.</i> * (1979)	Olsen <i>et al.</i> (1980)	ENDF/B-V (1979)	ENDF/B-V (1993)
21.8	$\Gamma_n$	$1.91 \pm .09$	$2.1 \pm .1 (.02)$	$2.08 \pm .02$	2.02	2.06
	$\Gamma_\gamma$	$20 \pm 2$	$24.5 \pm 1.5 (.2)$	$25.3 \pm .4$	23.0	25.9
23.5	$\Gamma_n$	$3.24 \pm .24$	$3.7 \pm .2 (.02)$	$3.82 \pm .04$	3.88	3.74
	$\Gamma_\gamma$	$25 \pm 2$	$26.0 \pm 1.5 (.2)$	$26.9 \pm .4$	25.0	25.9
59.5	$\Gamma_n$	$3.9 \pm .2$	$4.0 \pm .3 (.03)$	$3.86 \pm .06$	4.04	4.0
	$\Gamma_\gamma$	$25 \pm 2$	$25.0 \pm 2.0 (.3)$	$24.6 \pm .9$	23.2	25.9
69.2	$\Gamma_n$	$44.0 \pm 2$	$41.2 \pm 3.0 (.3)$	$43.2 \pm .2$	44.0	42.0
	$\Gamma_\gamma$	$25 \pm 2$	$22.6 \pm 2.0 (.4)$	$24.1 \pm .3$	21.9	25.9

\*The error in parenthesis is statistical only.



	(A)	(B)	(C)
	0.000000-02	0.90010	17.95
	0.000000-01	0.92122	17.79
	0.000000-02	0.91852	17.55
	0.000000-02	0.91503	17.49
	0.000000-02	0.91171	17.36
	0.000000-02	0.90850	17.25
	0.289960-02	0.81958	16.62
	0.277070-02	0.76900	16.25
	0.230820-02	0.69385	15.76
	0.171720-02	0.70499	15.75
	0.139710-02	0.71516	15.65
	0.123100-02	0.67502	15.30
	0.114000-02	0.62891	14.92
	0.104070-02	0.51001	14.21
	0.094000-02	0.48521	13.96
	0.083910-02	0.45301	13.72
	0.074730-02	0.43601	13.63
	0.065770-02	0.40000	13.30
	0.057270-02	0.37387	13.12

Temperature Self-shielding Factors at 4 keV

$\sigma_{\text{th}} = 17.35\text{b}$   
 $\sigma_{\text{th}} = 17.35\text{b}$

Temperature (K)	Doppler Broadening (K)	Doppler Width (K)	T=300°K		
			$\sigma = 1\text{b}$	$\sigma_0 = 10\text{b}$	$\sigma_0 = 100\text{b}$
1000	1.00	15.3	.60 ± .01	.68 ± .01	.83 ± .02
1000	1.00	15.3	.65 ± .01	.64 ± .01	.65 ± .02
1000	1.00	15.3	.32 ± .01	.60 ± .01	.83 ± .02
1000	1.00	15.3	.48 ± .01	.57 ± .01	.81 ± .02
1000	1.00	20.7	.46 ± .01	.55 ± .01	.79 ± .02
T=1000°K					
1000	1.00	15.3	.70 ± .01	.77 ± .01	.92 ± .01
1000	1.00	15.3	.56 ± .01	.73 ± .01	.91 ± .01
1000	1.00	15.3	.62 ± .01	.70 ± .01	.89 ± .01
1000	1.00	15.3	.59 ± .01	.67 ± .01	.88 ± .01
1000	1.00	20.7	.55 ± .01	.65 ± .01	.86 ± .01
T=2000°K					
1000	1.00	15.3	.76 ± .01	.82 ± .01	.95 ± .01
1000	1.00	15.3	.72 ± .01	.72 ± .01	.93 ± .01
1000	1.00	15.3	.69 ± .01	.76 ± .01	.92 ± .01
1000	1.00	15.3	.66 ± .01	.74 ± .01	.91 ± .01
1000	1.00	20.7	.63 ± .01	.71 ± .01	.90 ± .01

Table VI. Temperature Dependence of  $^{238}\text{U}$  Capture Self-shielding Factors at 40 keV

$\sigma_{\text{th}} / \text{b}$	$\sigma_{\text{eff}} / \text{b} = f_{\text{eff}}(\sigma_{\text{th}}) \sigma_{\text{th}}$		
	$\tau_1 = 1 \text{ b}$	$\tau_1 = 10 \text{ b}$	$\tau_1 = 100 \text{ b}$
0.01	.017	.017	.0038
.01	.020	.018	.0041
.1	.018	.019	.0043
.1	.02	.020	.0045
.1	.021	.020	.0047

Table VII.  $^{238}\text{U}$  Self-shielded Capture Cross Sections From 1 to 4 e (b)

$E$ eV	$\sigma_{\text{unsh}}^{\text{a}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{b}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{c}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{d}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{e}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{f}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{g}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{h}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{i}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{j}}}$	$\frac{\sigma_{\text{unsh}}}{\sigma_{\text{unsh}}^{\text{k}}}$
1000	100-1100	3.044	9.47	1.075	.77	1.26	1.535	1.57	1.1	1.15	1.0
1500	150-1500	2.113	1.00	.631	.625	.96	1.001	1.003	1.0	1.0	1.0
1500	1500-1500	1.912	2.14	.708	.771	.92	1.076	1.077	1.0	1.0	1.0
1750	1500-1750	2.087	6.82	.971	.77	1.32	1.303	1.063	1.0	1.0	1.0
1750	1750-2100	1.747	5.52	.558	.71	.75	.818	.941	1.0	1.0	1.0
2250	100-2100	1.610	4.33	.824	.77	1.03	1.051	1.04	1.0	1.0	1.0
2500	100-2600	1.630	5.93	.915	.971	1.76	1.169	.919	1.0	1.0	1.0
2750	2600-2900	1.250	2.24	.660	.902	.82	.865	.955	1.0	1.0	1.0
3000	2900-3100	.985	2.54	.404	.712	.65	.646	.827	1.0	1.0	1.0
3250	3100-3400	1.455	6.07	.911	.932	.98	1.123	1.133	1.0	1.0	1.0
3500	3400-3500	1.210	3.71	.755	.616	1.16	.933	.823	1.0	1.0	1.0
3750	3500-3700	1.099	2.80	.631	.657	1.03	.843	.795	1.0	1.0	1.0
4000	3700-4000	1.094	3.03	.699	.699	1.00	.856	.856	1.0	1.0	1.0
<hr/>											
1000	100-1100	3.963	3.779	3.963	3.779	1.05	5.683	5.325	1.07	6.007	1.07
1500	150-1500	2.883	2.993	2.883	2.993	.96	3.761	3.713	1.07	4.113	1.07
1750	1500-1750	3.016	1.94	3.016	1.94	1.01	3.759	3.567	1.06	4.113	1.06
2250	1750-2250	3.672	1.00	3.672	1.00	1.02	13.199	12.655	1.04	15.007	1.04

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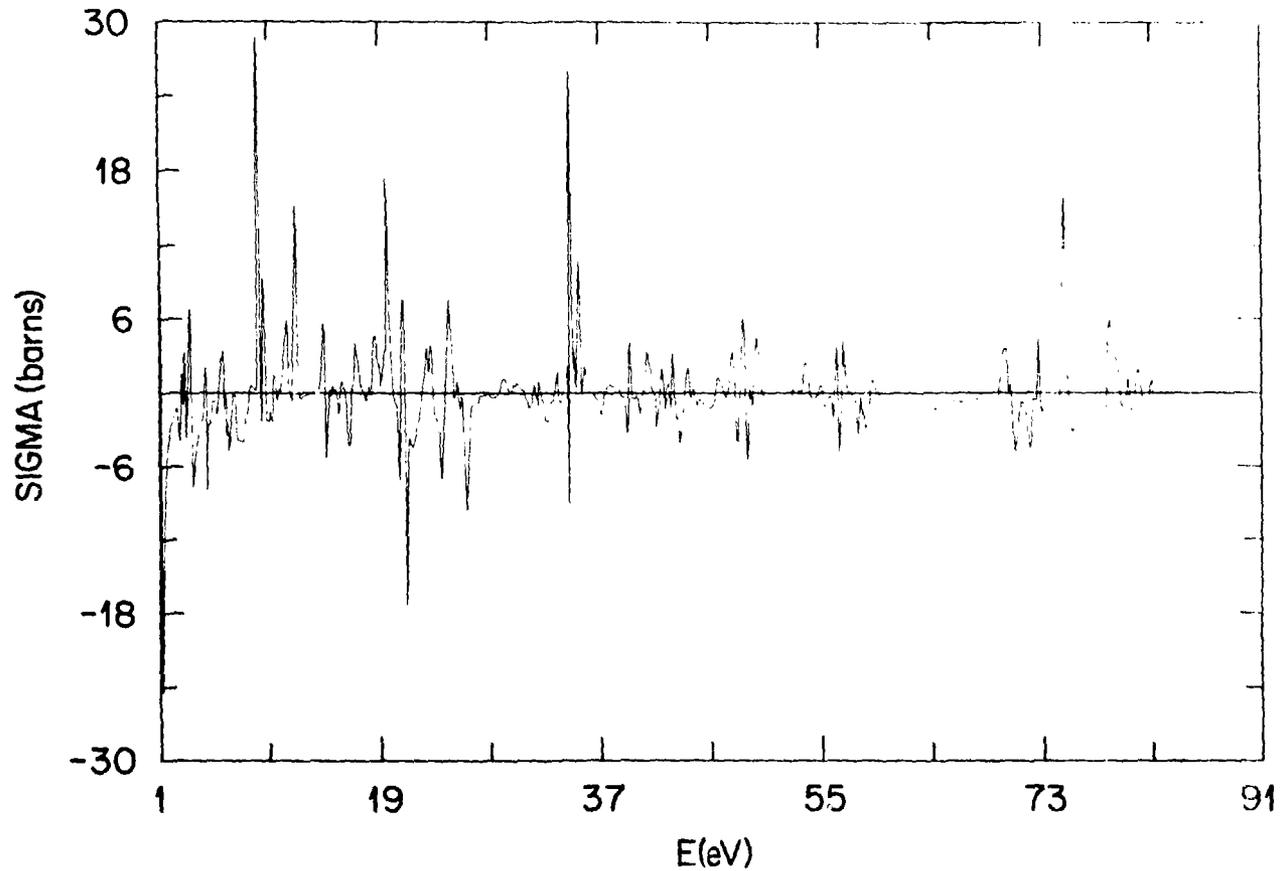


Fig. 1. The "smooth" MF=3 contribution to the ENDF/B-V representation of  $^{235}\text{U}$  over the resolved resonance range: 1 eV - 81 eV.

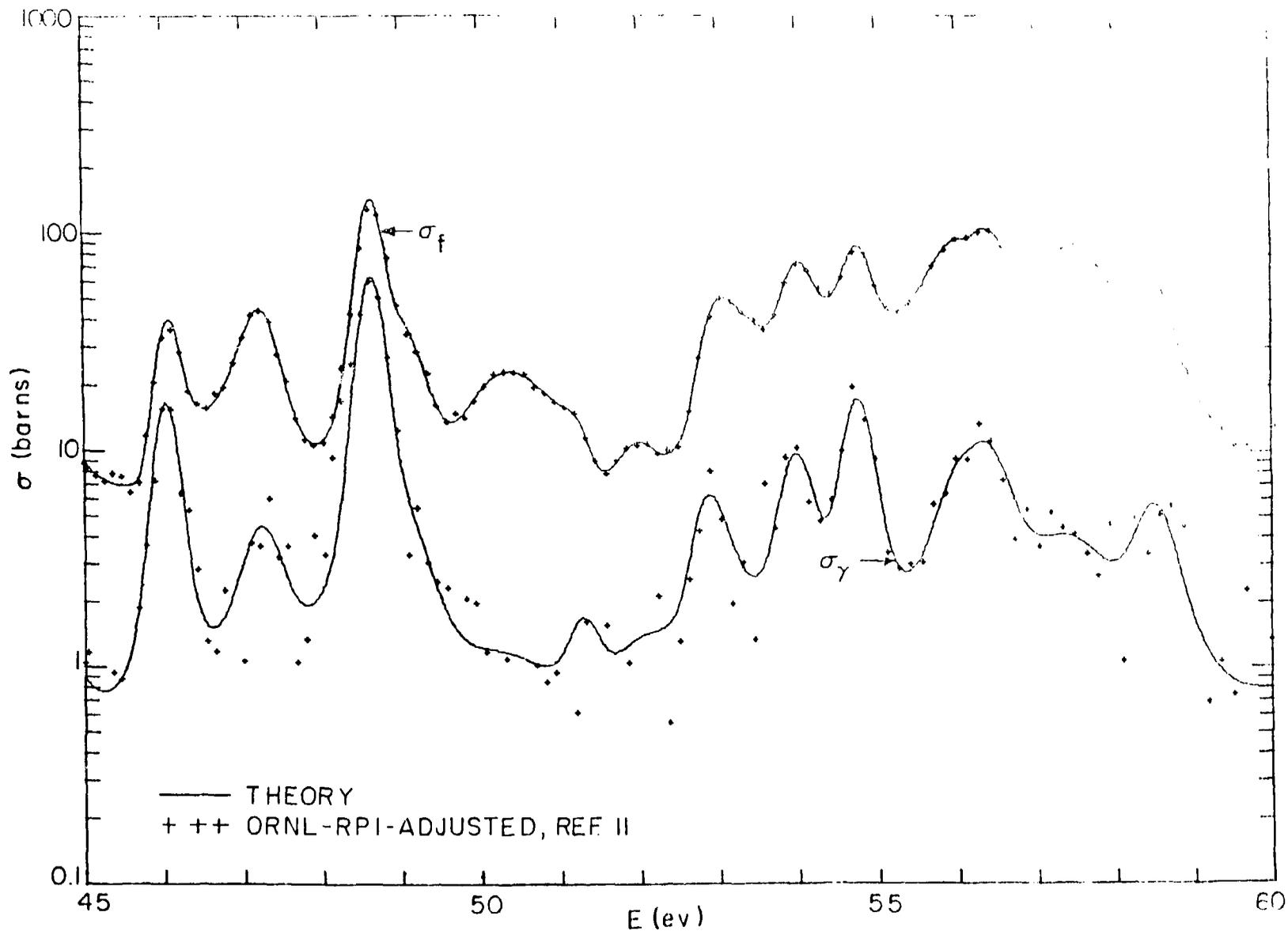


Fig. 2. U-233 fission and capture cross sections in the resolved resonance range 45 to 60 eV. The solid lines are from a multi-level analysis of Reynolds and Steiglitz used in ENDF/B-V. The figures illustrates that even in the "resolved range," the resonances are not truly resolved.

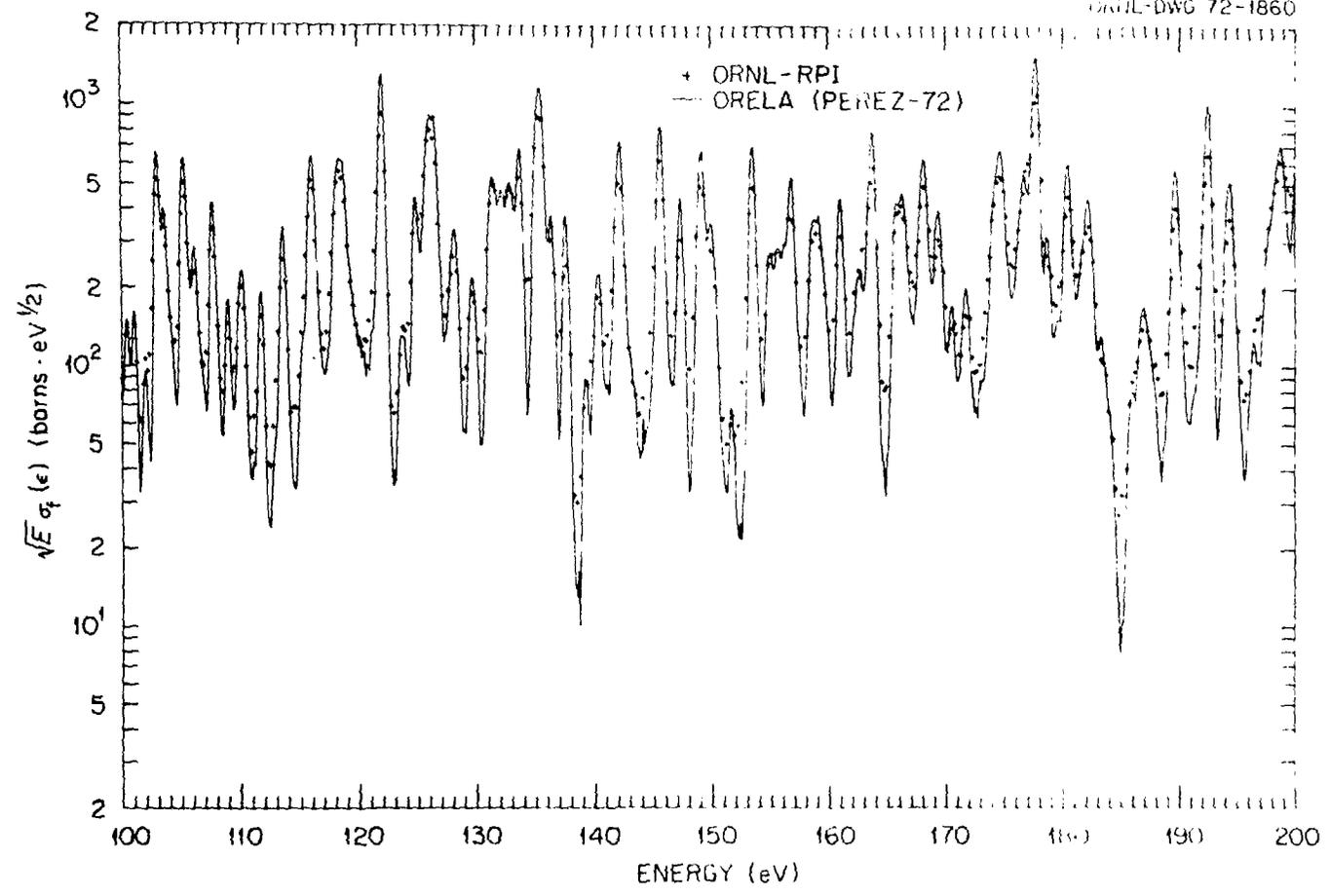


Fig. 3. U-233 fission cross section between 100 and 200 eV. The figure shows a comparison between two sets of experimental data. In the ENDF/B-V, this range is treated as "unresolved." The figure illustrates that the resonances are just resolved in the <sup>233</sup>U between 45 and 60 eV.

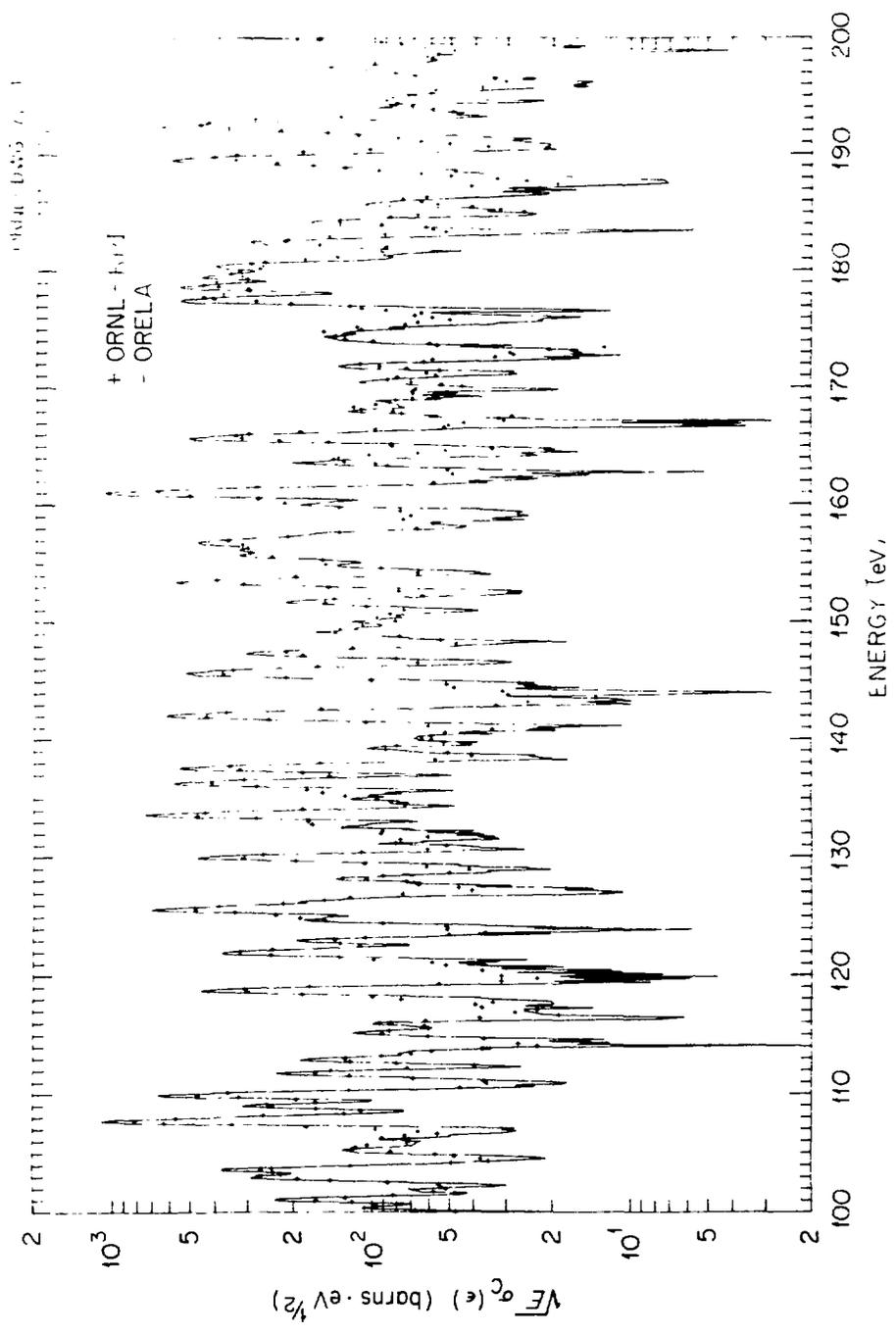


Fig. 4. U-235 capture cross section between 100 and 200 eV.  
(See Legend of Fig. 3.)

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