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ANL/NDM-134

An Evaluated Neutronic Data File for Elemental Zirconium

by

A.B. Smith, S. Chiba, and J.W. Meadows

September 1994

ARGONNE NATIONAL LABORATORY,
ARGONNE, ILLINOIS 60439, U.S.A.

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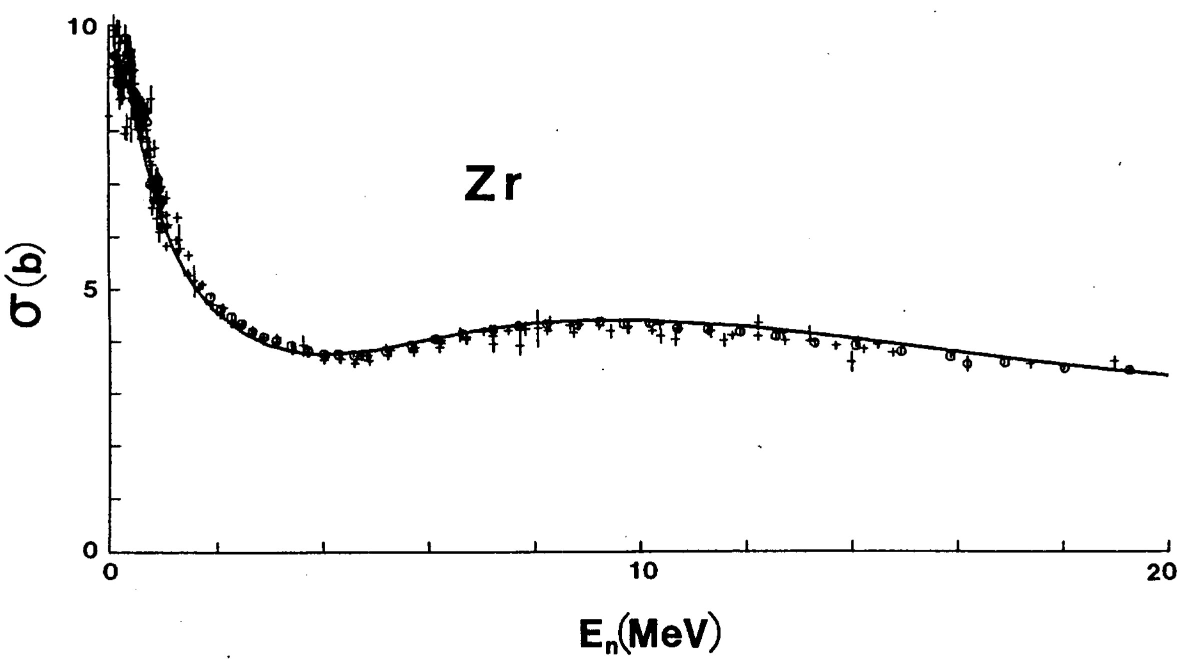

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ANL/NDM-134

AN EVALUATED NEUTRONIC DATA FILE FOR ELEMENTAL ZIRCONIUM*

by

A. B. Smith[a,b], S. Chiba[c] and J. W. Meadows[a]

[a] Argonne National Laboratory
Argonne, Illinois

[b] The University of Arizona
Tucson, Arizona

[c] Japan Atomic Energy Research Institute
Tokai Establishment

September, 1994

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[a] Argonne National Laboratory
Argonne, Illinois

[b] The University of Arizona
Tucson, Arizona

[c] Japan Atomic Energy Research Institute
Tokai Establishment

ABSTRACT

A comprehensive evaluated neutronic data file for elemental tin is derived and presented in the ENDF/B-VI formats. The derivation is based upon measured microscopic nuclear data, augmented by model calculations as necessary. The primary objective is a quality contemporary file suitable for fission-reactor development extending from conventional thermal to fast and innovative systems. This new file is a significant improvement over previously available evaluated zirconium files, in part, as a consequence of extensive new experimental measurements reported elsewhere.

I. INTRODUCTION

The metallurgical and nuclear properties of zirconium have made it a primary structural component of fission-reactor energy systems for more than forty years. This major use continues, including the most advanced and innovative reactor concepts such as the Integral Fast Reactor [1]. With this wide technological application, with very large fiscal impact, it is important to assure that the underlying basic evaluated zirconium nuclear data is updated to the best possible contemporary standards. The present evaluated file has that objective. Considerable improvements over previously-available zirconium evaluated data files are now possible as the result of comprehensive recent microscopic data measurements [2] and improved modeling capability. This new information, together with that previously reported in the literature, is used in the present work.

The present evaluation is comprehensive, including:- i) new resonance representations, ii) energy-averaged total and scattering cross sections, iii) radiative capture processes, iv) (n,2n') and (n,3n') reactions, and v) a variety of (n,X) reactions. The file is formulated on an elemental basis and therefore is directly applicable to practical reactor calculations without extensive isotopic processing. The file does not explicitly deal with certain isotopic reactions encountered in some dosimetry work (e.g., the ^{90}Zr (n,2n') reaction). Those interested in such information should look to special-purpose evaluated files. Finally, the present file has been transmitted to the National Nuclear Data Center, Brookhaven National Laboratory, where it is available to the user community.

II. RESONANCE PARAMETERS

Elemental zirconium consists of the five isotopes ^{90}Zr(51%), ^{91}Zr(11%), ^{92}Zr(17%), ^{94}Zr(18%) and ^{96}Zr(3%). The present evaluation employs the resonance parameters of the individual isotopes as given in the very recent evaluation of Knox and Lubitz [3]. This resonance evaluation extends up to ≈ 90 keV, at which point the transition to energy-averaged behavior is made. The new resonance evaluation of ref. [3] provides improved detail and accuracy relative to prior ENDF/B zirconium evaluations.

III. NEUTRON TOTAL CROSS SECTIONS

The neutron total cross section is the essential envelope to which all other components of the evaluation must conform. The present evaluation follows the procedures successfully employed by this group in a number of prior evaluations (e.g., see ref. [4]), therefore only an outline will be presented here. The energy-averaged neutron total cross sections, extending upward from 90 keV, were obtained by means of the following steps.

The data base available at the National Nuclear Data Center ([5]→[26]) was assembled and augmented with measurements specially made for this evaluation [27]. This composite data base was plotted on a large scale and obviously erroneous data sets rejected. The data was then averaged over energy increments of 50 keV to 1 MeV, 200 keV to 3 MeV, 300 keV to 5 MeV and 500 keV to 20 MeV. The uncertainties were propagated through the averaging procedure. Only one data set (ref. [27]) appeared to give systematic uncertainties. Thus subjective estimates of systematic uncertainties were made for the other data sets (as cited with the relevant references). These judgments were based upon estimates of the quality of the particular measurements involved. The resulting energy-averaged data base is shown in Fig. III.1. The energy-averaged data were then statistically evaluated using the computer code GMA [28]. The calculations employed ENDF/B-V [29] as the initial a priori estimate. The evaluated results included uncertainties and the correlation matrix. The former ranged from ≈ 0.5% to ≈ 1.3%. These are very small uncertainties in the context of the data base, and such small magnitudes are characteristic of the results of statistical evaluations. Therefore, the evaluation uncertainties were doubled for the actual file as the larger values were felt to be far more realistic while, at the same time, maintaining the relative energy dependence of the uncertainties. The statistical-evaluation results displayed very small fluctuations reflecting variations in the underlying data base. These were smoothed by fitting the statistical results with a conventional spherical optical model, varying the ten model parameters real and imaginary strengths (each given a quadratic energy dependence), and the real and imaginary radii and diffusenesses. The results of the model fit were in very good agreement with the values obtained from the statistical evaluation, and the model was then used to generate the explicit evaluated cross sections.

It is likely that, particularly for ^{90}Zr (51% abundant), there are significant fluctuations in the total cross section at lower energies. These were not introduced into the evaluation as the data showing such fluctuations is suspect from other points of view (e.g., absolute magnitudes seem anomalous). Fluctuations may have also systematically distorted the lower-energy portions of the data base with self-shielding effects resulting in systematically too small cross sections. The measurements gave very little attention to sample sizes and only one data set considered the self-shielding effects in any detail [27]. In that case they were not large and the results of that particular set of measurements were reasonably consistent with a number of other data sets. This observation, combined with the elemental nature of the samples used in the measurements, suggests that self-shielding is not a serious concern above ≈ 100 keV.

The resulting evaluation is compared with the energy-averaged data base and the evaluation of ENDF/B-VI in Fig. III.1 (see also Fig. IV.1). The present evaluation is very descriptive of the energy-averaged measured values. It is also in good agreement with ENDF/B-VI over the majority of the energy range, with the only

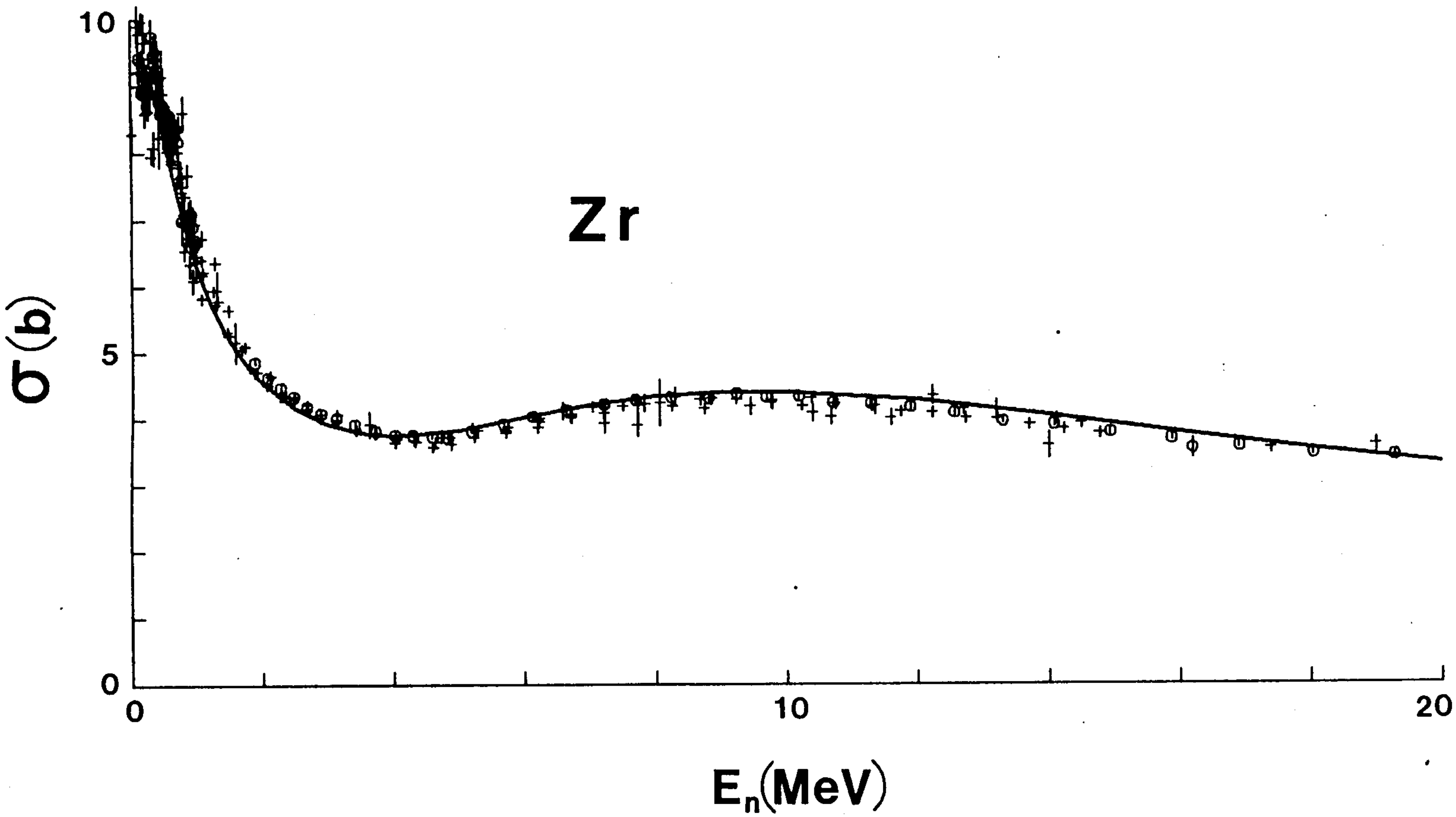

Fig. III.1. Comparison of the energy-averaged measured neutron total cross sections (+) with the present evaluation (heavy curve) and the evaluation of ENDF/B-VI (light curve).

appreciable discrepancies between the two evaluations at the higher energies where ENDF/B-VI is larger by up to ≈ 10%. The latter difference is not surprising as ENDF/B-VI did not have the benefit of recent higher-energy measurements (e.g., those of ref. [27]). As noted above, the present evaluation does not attempt to portray partially-resolved resonance structure below a few-hundred keV, as ENDF/B-VI does, due to the lack and uncertainty of data in this low-energy region.

The present evaluation is probably as good as can be achieved, given the present status of the experimental data. The latter are somewhat unfortunate. There is only one set of data that extends from the low-keV region to ≈ 20 MeV (ref. [27]), and there is no reasonable definition of the expected low-energy structure. In only one case was any detailed attention apparently given to possible self-shielding effects.

--- For significant improvements careful high-resolution measurements are needed, extending from a few keV to 20 MeV and employing a number of sample thicknesses.

Such measurements are technologically simple at a number of facilities.

IV. NEUTRON ELASTIC SCATTERING

The energy-averaged neutron elastic-scattering cross sections of elemental zirconium have recently been studied in detail by the present authors [2]. This study included detailed experimental measurements up to an energy of 10 MeV and a quantitative optical-model interpretation up to 24 MeV. The model of ref. [2] is very descriptive of the experimental data base to more than 20 MeV. Therefore, it was used to obtain the elastic-scattering cross sections of the present evaluation. The model calculations were somewhat renormalized (by the order of a percent) in order to bring the calculated and evaluated neutron total cross sections into exact agreement. The resulting angle-integrated elastic-scattering cross sections are compared with the respective values of ENDF/B-VI in Fig. IV.1. As discussed above, ENDF/B-VI contains some fluctuations at few-hundred-keV energies that the present evaluation ignores due to concern for their reliability. On the energy average, the two elastic-scattering evaluations are in very good agreement at the low energies, and this good agreement extends to at least 15 MeV. There are differences between the two evaluations above 15 MeV, but that is a region that is not of primary applied importance. Fig. IV.1 also shows the total cross section and the nonelastic cross section implied by the evaluated total and elastic-scattering cross sections. In view of the neutron total and elastic-scattering cross-section consistency between the present evaluation and that of ENDF/B-VI, the respective nonelastic cross sections are similar, with some differences at ≈ 2 MeV and above ≈ 15 MeV.

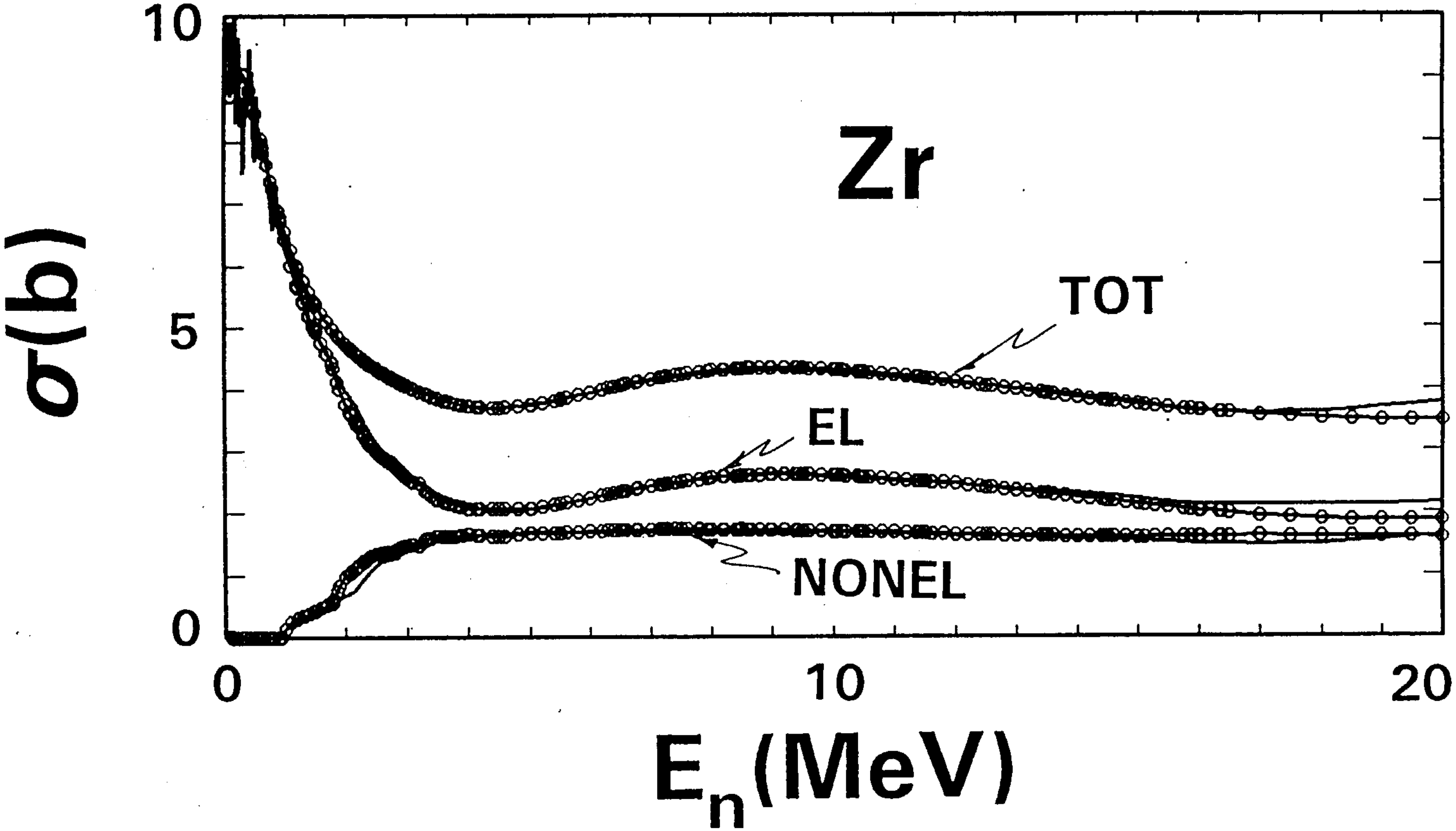

Fig. IV.1. Evaluated total, elastic-scattering and nonelastic cross sections of elemental zirconium. The results of the present evaluation are indicated by curves with symbols, and those of ENDF/B-VI by simple curves.

The model of ref. [2] was also used to generate the evaluated relative elastic-scattering distributions, with the results illustrated in Fig. IV.2. In the numerical file these distributions are expressed in the form of F_l coefficients. The evaluated cross sections and relative angular distributions are consistent with Wick's Limit [30]. The uncertainties of the angle-integrated elastic-scattering cross sections were estimated to be approximately 3% to at least 10 MeV, then increasing to approximately 5% at 20 MeV. These uncertainties are only slightly larger than those of the total cross section. However, as discussed in ref. 2, there are no elemental zirconium elastic-scattering measurements from 10 to 24 MeV.

--- Several high-quality elemental elastic-scattering distributions are needed at incident energies of ≈ 10 → 25 MeV.

If there were a few good experimental angular distributions spread over this energy range there would be more confidence in the model, and thus the present evaluation, above ≈ 10 MeV. Such measurements are technologically viable. The shortage of detailed higher-energy elastic-scattering measurements is considerably mitigated by the availability of a few good isotopic elastic-scattering measurements distributed between 10 and 24 MeV. These isotopic results are well described by the model used for the present evaluation, as discussed in ref. [2].

V. NEUTRON INELASTIC SCATTERING

V.1. Discrete Inelastic Scattering

The evaluation of the discrete inelastic scattering cross sections gave attention to ^{90,91,92} and ^{94}Zr. Contributions from ^{96}Zr were ignored due to the low abundance of the isotope (3%) and the similarity of its excited structure to that of ^{94}Zr. The energies and J^π values of the excited levels were taken from the Nuclear Data Sheets [31] to as high an excitation as possible before J^π assignments become uncertain. The first ten excited levels in the prominent isotope ^{90}Zr, the first five levels in ^{91}Zr, the first eleven levels in ^{92}Zr, and the first ten levels for ^{94}Zr were considered; or a total of 36 discrete inelastic excitations. It is shown in ref. [2] that a specific model gives a very good description of the measured discrete inelastic-scattering results. Therefore that model was used to calculate the individual excitation functions which were normalized by their relative abundances and combined to form the elemental discrete inelastic-scattering file. The calculations were carried out using the optical statistical computer code ABAREX [32]. This code uses the Hauser-Feshbach formula [33], corrected for resonance width fluctuation and correlation effects using the method of Moldauer [34], and includes channel competition from the continuum of levels

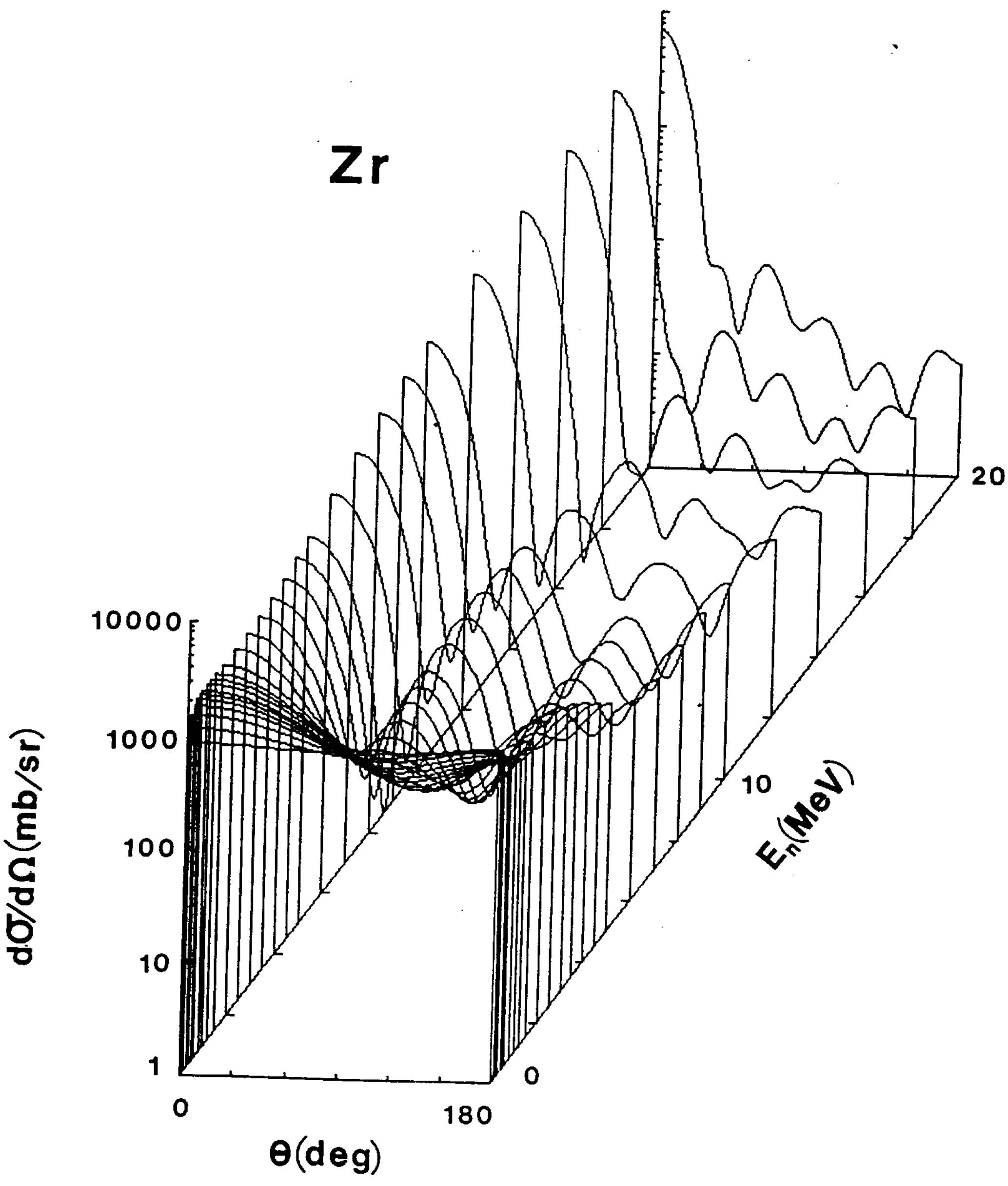

Fig. IV.2. Differential elastic-scattering cross sections of elemental zirconium as given in the present evaluation. The values are given in the laboratory coordinate system calculated using the statistical formulation of Gilbert and Cameron [35]. The details of the calculational method are setforth in ref. [2]. The onset of the continuum is at the lowest energy in ^{91}Zr, and at higher energies for the other isotopes. The cumulative contributions of each of these discrete levels is shown in Fig. V.1.1. Generally they fall in three groups separated by the prominent excitations of the first few levels of the ^{90}Zr isotope.

The discrete inelastic cross sections of the evaluation are all due to compound-nucleus processes. Thus the angular distributions of the emitted neutrons are symmetric about 90^0 and closely approach isotropy. Therefore the evaluation assumes the isotropy of the emitted neutrons. This will not be strictly true at higher energies as there will be some direct-reaction components. However, ^{90}Zr is magic in neutron number so direct-reaction contributions will be small, are poorly known, and therefore were ignored. The estimated uncertainty associated with the discrete inelastic-excitation cross sections is ≈ 10% in regions of prominent magnitude. The ENDF/B-VI discrete inelastic-scattering cross sections are in far less detail than the present work so direct comparisons are not possible.

V.2. Continuum Inelastic Scattering

There is very little experimental knowledge of the continuum inelastic scattering from elemental or isotopic zirconium. Therefore, the present evaluation determined the continuum inelastic cross section from the difference between the nonelastic cross section following from the total and elastic-scattering cross sections and the sum of other reaction cross sections. This procedure assures the internal consistency of the file. The resulting continuum inelastic-scattering cross sections behaved in a physically reasonable manner as illustrated in Fig. V.2.1. There is some small structure in the illustrated inelastic cross sections as a physical result of the onset of reaction channels and as an artifact of the energy mesh used in the representation. The continuum inelastic scattering rises from a threshold at ≈ 2.8 MeV to ≈ 1.75 b, then rapidly decreases with the onset of the prominent (n,2n') process, and finally asymptotically approaches a relative small magnitude at higher energies. The latter component is due to pre-compound processes. The uncertainties are probably in the order of 10% in regions of appreciable cross section, reflecting the uncertainties of the various components involved in the subtraction process. The comparable ENDF/B-VI inelastic cross sections are illustrated in Fig. V.2.1. The total inelastic-scattering cross sections of ENDF/B-VI are similar to those of the present evaluation up to ≈ 15 MeV while the continuum contribution of ENDF/B-VI is smaller. Above ≈ 15 MeV the inelastic scattering cross sections of ENDF/B-VI behave in an unphysical manner and should not be taken seriously.

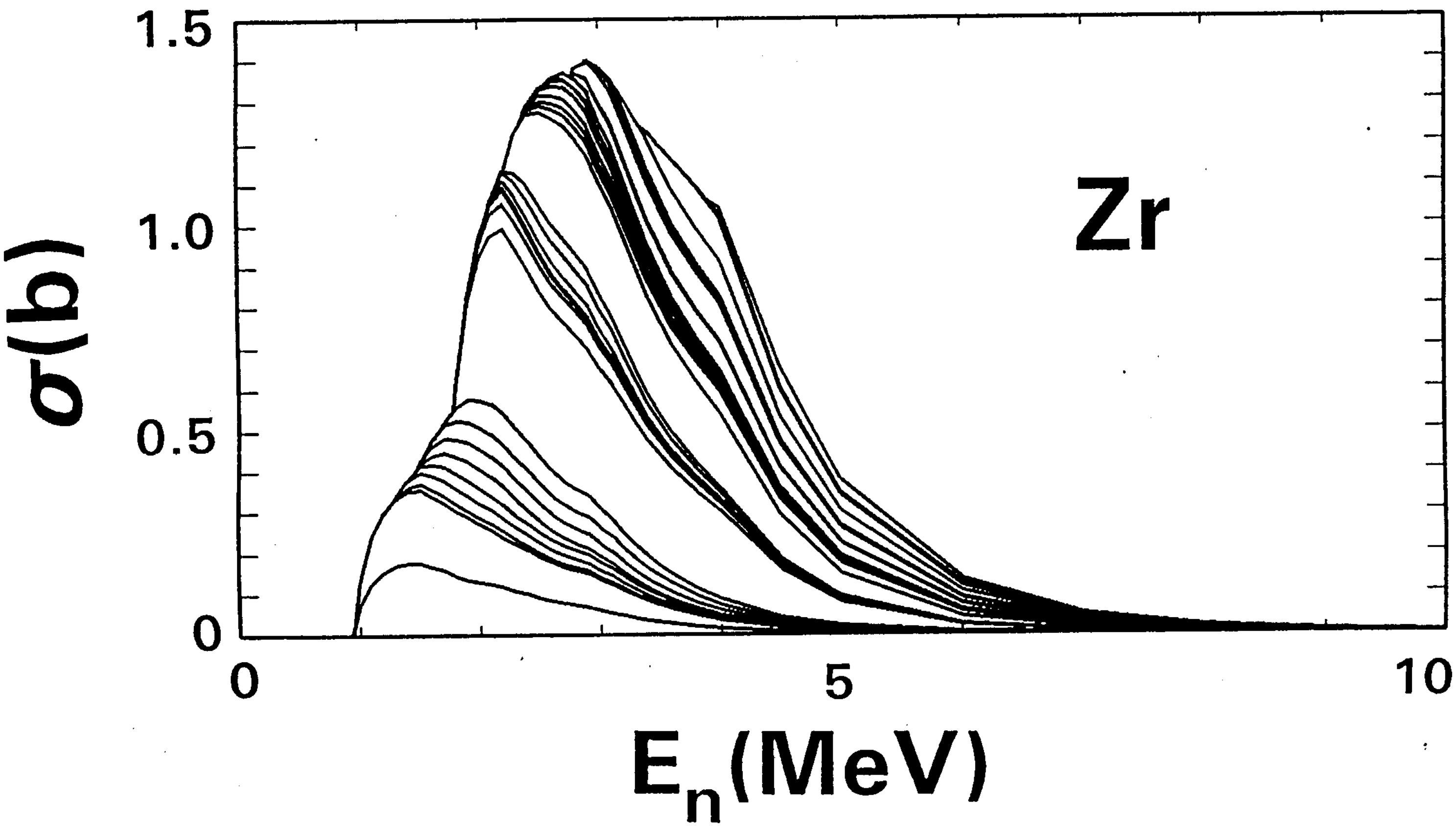

Fig. V.1.1. Cumulative sums of the evaluated discrete inelastic-scattering cross sections of elemental zirconium.

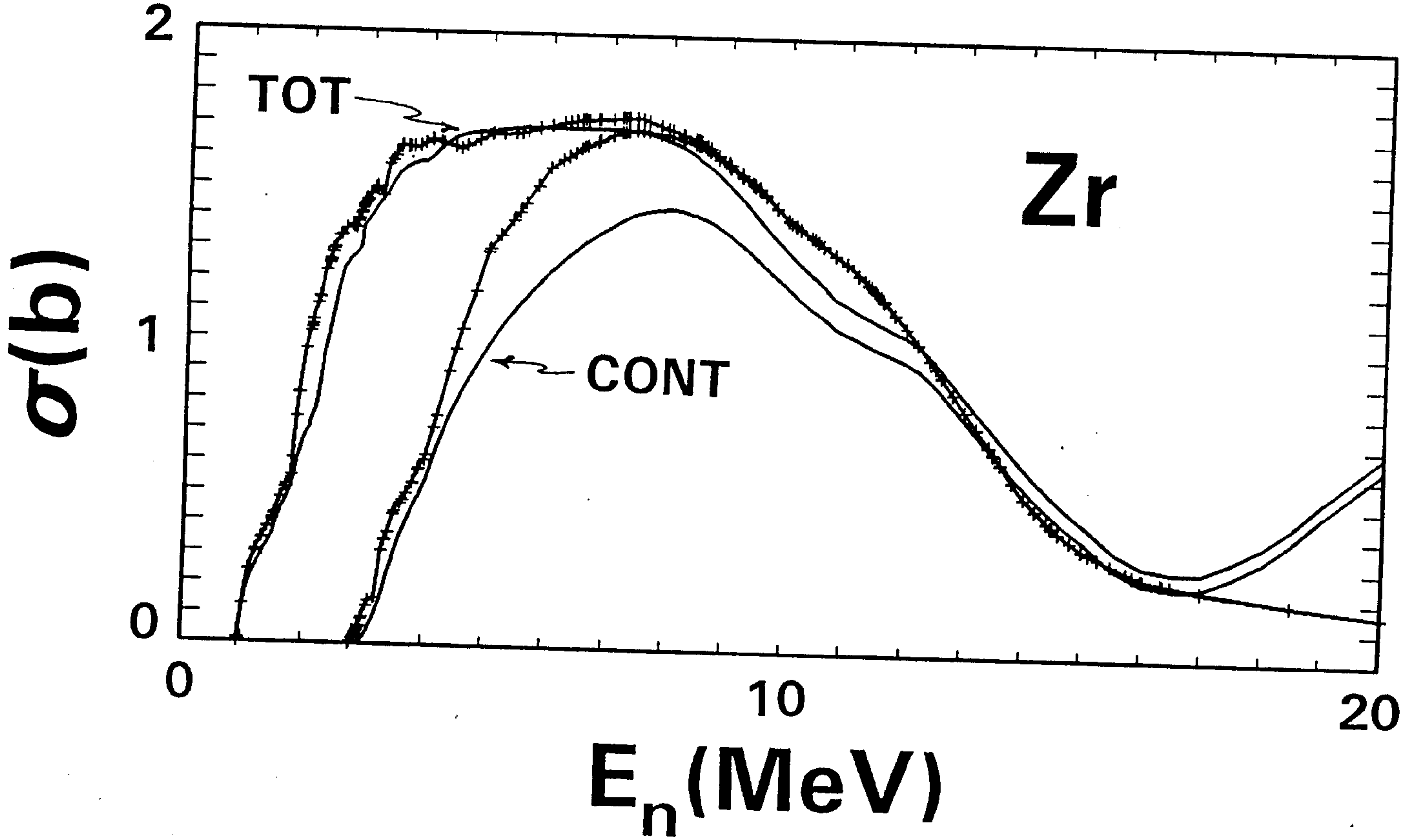

Fig. V.2.1. Evaluated total inelastic-scattering and continuum inelastic-scattering cross sections of elemental zirconium. The present evaluated results are indicated by curves with "+" symbols and the comparable values from ENDF/B-VI by simple curves.

Below ≈ 10 MeV continuum inelastic scattering is primarily due to compound-nucleus processes and thus the neutron emission is symmetric about 90^0 and approaches isotropy. Therefore, the present evaluation assumes isotropic emission of the continuum inelastic neutrons. This assumption is less suitable at higher energies where anisotropic pre-compound processes are dominant. The continuum neutron-emission spectra were assumed to consist of two Weisskopf distributions with the temperature following a $(E/a)^{1/2}$ energy dependence, where is "E" is energy and "a" the level density parameter [36]. The prominent contribution is due to compound-nucleus processes and "a" was taken from ref. [36]. The second component, attributed to pre-compound processes, was assumed to have an intensity 2.5% that of the primary compound-nucleus contribution, with a temperature 3.5 times larger. These simple assumptions have been successfully used elsewhere ([37], [38]). The alternative is extensive isotopic model calculations the results of which are themselves uncertain, particularly when adjusted for consistency with experimental results. In addition, the present file is primarily directed toward fission-reactor needs where there is essentially no interest in the details of high-energy neutron-emission spectra. In any event, the present representations are considerably better than those of ENDF/B-VI.

VI. NEUTRON RADIATIVE CAPTURE

The experimental (n,γ) data base was assembled from the files of the National Nuclear Data Center. Above the resonance region (≈ 90 keV) it is very limited, consisting of only five sets of elemental data (refs. [39]→[43]), two of which are less than a quarter of a century old. In addition, there are a few experimental isotopic (n,γ) results. The latter are fragmentary, and do not give a clear picture of the elemental (n,γ) cross section, therefore they contribute nothing to the evaluation.

Given the above data situation, the evaluation is a matter of subjective judgment. The general energy-dependent trend of the cross section below ≈ 500 keV was estimated using a simple dipole calculation, normalized to the fragmentary experimental information [44]. Above ≈ 500 keV, the two recent sets of data (refs. [39] and [40]) were used to determine the evaluation. The result matches reasonably well to the calculations, and the two sets of data are in good agreement. The result is also consistent with the measured values of ref. [42], but the latter have large uncertainties. The data of ref. [43] is higher, and has a somewhat different energy dependence. The latter measurements are very old, and were made relative to the sum of the σ_f and σ_{cap} of ^{235}U. These reference values at the time of the measurements were approximately 6% larger than corresponding contemporary values. But the difference between the results of ref. [43] and the evaluation considerably exceeds that amount. The evaluation simply excepts the two more recent experimental sets as being representative of reality.

The present evaluation is compared with that of ENDF/B-VI and with the experimental data base in Fig. VI.1. The present evaluation is 15-20% lower than that of ENDF/B-VI, with a somewhat similar energy dependence. Given the weak experimental data base, the estimated uncertainties associated with the present evaluation are rather large, approximately 10% to 2 MeV, 15% from 2 - 4 MeV, and larger at higher energies. These relatively large uncertainties are mitigated in applications by the small value of the cross section (≈ 10 mb).

For over thirty years, zirconium has been widely used as a cladding material in fission-reactor systems. It is shocking that the corresponding energy-averaged capture cross section is not experimentally better known. The only saving grace is that it is clearly small.

--- Before the elemental (n,γ) evaluation can be substantively improved, there will have to be several good measurements extending from ≈ 0.1 to 4 MeV.

These must have accuracies of at least 10%, sufficient detail to reasonably define the energy-dependent shape, and employ prompt-detection techniques. An alternative is detailed measurements of the isotope (n,γ) cross sections. However, that alternative is not particularly attractive as the desired data base is much larger, in many cases fundamental physical problems are encountered in activation measurements, and there is the concern for obtaining good isotopic samples.

VII. (n,2n') AND (n,3n') PROCESSES

The five naturally-occurring zirconium isotopes have widely varying (n,2n') and (n,3n') Q-values, as given in Table VII-1. All of the (n,2n') thresholds are well below 20 MeV, so all of the isotopic components were considered in the evaluation.

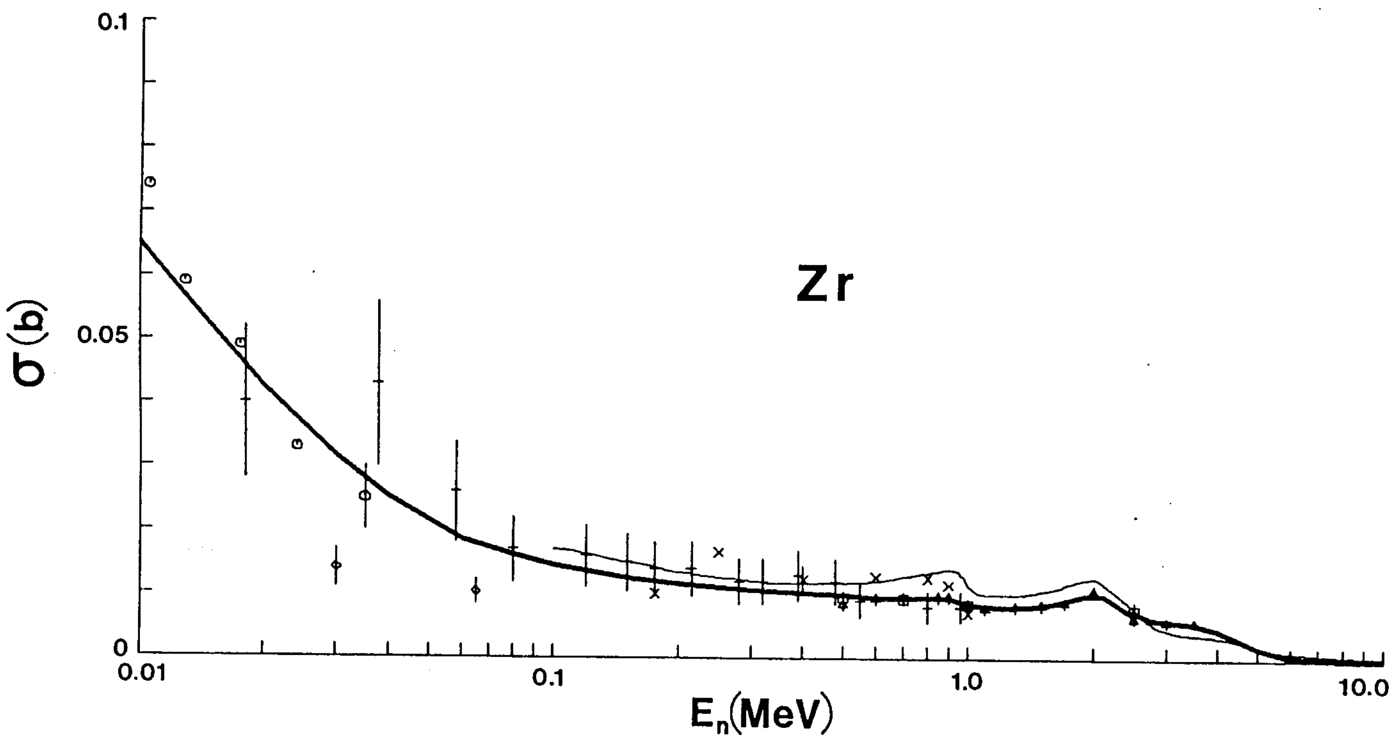

Fig. VI.1. Measured and evaluated (n,γ) cross sections of elemental zirconium. Symbols indicate measured values. The heavy curve denotes the present evaluation, and the light curve that of ENDF/B-VI. In the present evaluation, the resonance representation extends to 90 keV, thus the indicated curve is only a qualitative extrapolation to the lower energies.

Table VII.1. (n,2n') and (n,3n') Q-values for the naturally-occurring Zirconium isotopes (in MeV).[a]

Isotope	Reaction (n,2n')	(n,3n')
^{90}Zr	-11.976	-21.287
^{91}Zr	-7.200	-19.176
^{92}Zr	-8.635	-15.835
^{94}Zr	-8.219	-14.951
^{96}Zr	-7.853	-14.324

a. Taken from the Lawrence Livermore National Laboratory tabulation of R. Howerton [45].

The threshold for the ^{90}Zr (n,3n') process is above 20 MeV, and that for the ^{91}Zr (n,3n') process very nearly 20 MeV, so both processes were ignored in the evaluation. Contributions from the remainder of the (n,3n) processes were included.

The experimental measurement of elemental zirconium (n,2n') and (n,3n') cross sections requires prompt-detection techniques. There have been only two such measurements, both of the (n,2n') cross section, and neither of them extends above ≈ 15 MeV. One of these [46] is an old measurement resulting in a single point at 14 MeV. The other set of data is reasonably contemporary and extensive, extending from threshold to ≈ 15 MeV [47]. These two sets of experimental data are shown in Fig. VII.1. There are no similar elemental (n,3n') measurements.

There have been a number of measurements of the activation cross sections resulting from the (n,2n') reaction on various of the zirconium isotopes ([48]→[88]). Not all of the isotopes are amenable to activation studies of the (n,2n') process. The results are most prolific for the 78.4 hr. ground-state activity of ^{89}Zr, which should be equivalent to the ^{90}Zr (n,2n') cross section. These ^{89}Zr activation results are summarized in Fig. VII.2. There are additional scattered activation results for some of the other isotopes, notably the ^{96}Zr activation cross sections. There is essentially no reliable and reasonably extensive experimental information on the (n,3n') cross sections at energies of less than 20 MeV.

In view of the sparse nature of the above experimental data base, considerable reliance had to be placed upon calculational

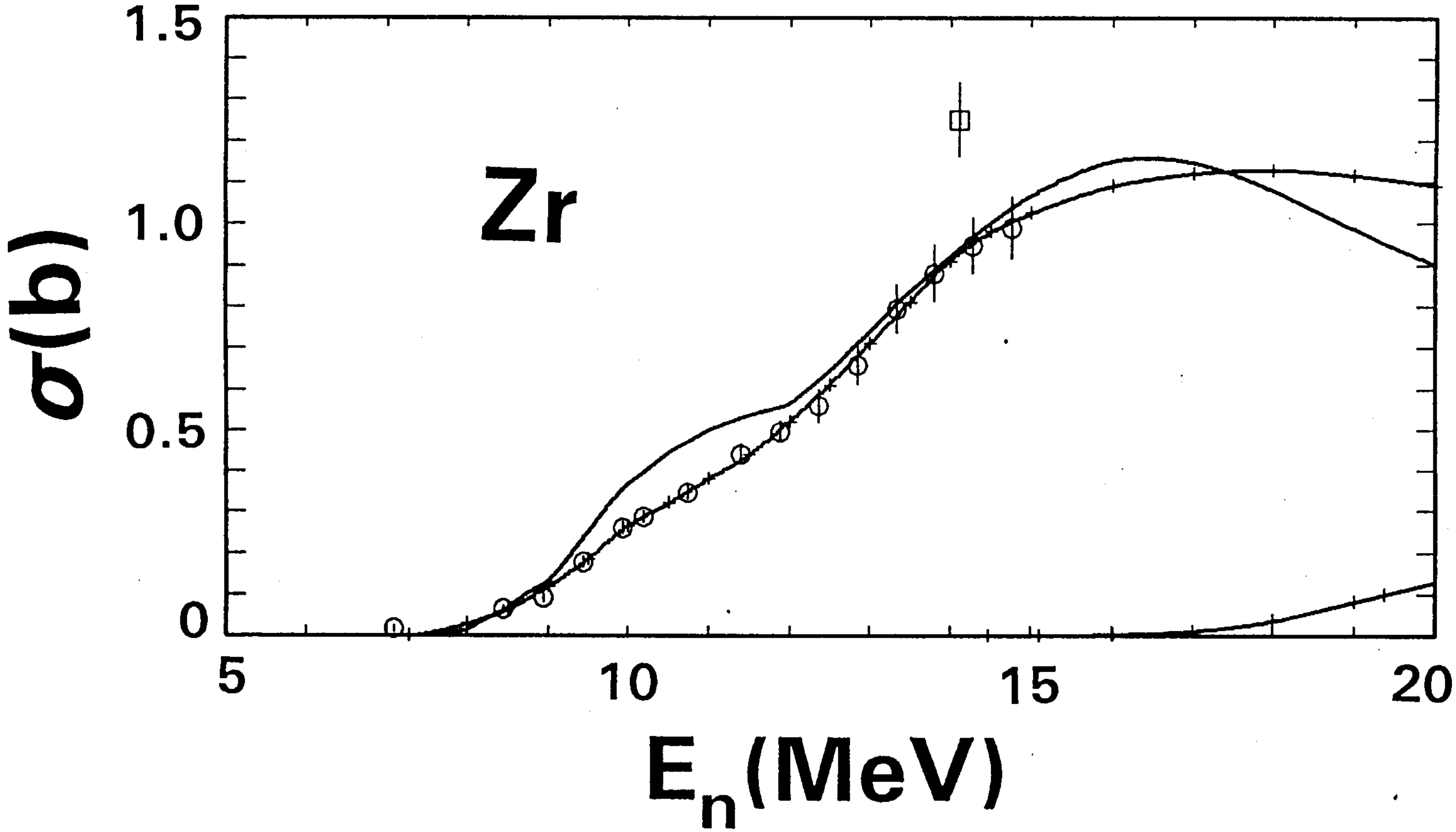

Fig. VII-1. (n,2n') (upper data) and (n,3n') (small high-energy data) cross sections of elemental zirconium. The measured values of ref. [47] and given by "O" symbols and that of ref. [46] by "□". The curves with "+" symbols indicate the results of the present evaluation, and the simple curve that of ENDF/B-VI.

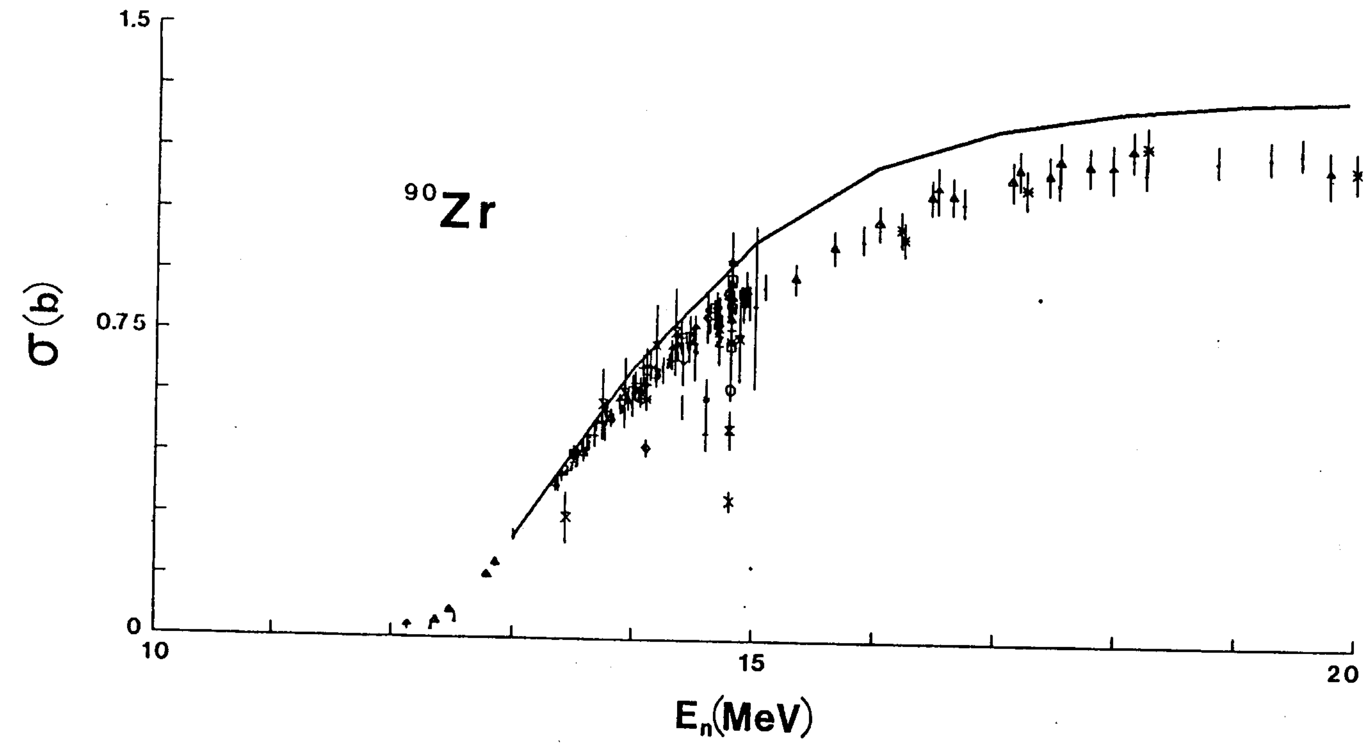

Fig. VII.2. The ^{90}Zr (n,2n') cross section. The symbols indicate the results of activation measurements resulting in the 78.4 hr ground-state half life, and the curve denotes results of CADE calculations, as discussed in the text.

extrapolations. The calculations were made using the statistical and Hauser-Feshbach computational codes CADE [89] and GNASH [90], treating each isotope separately, and combining the isotopic components to obtain the elemental values. An illustrative comparison of measured and calculated results is given in Fig. VII-2. In this example the calculated shape is relatively consistent with the measured values but approximately 15% larger. Qualitatively similar results were obtained with GNASH, with the primary differences between the two types of calculated results above ≈ 15 MeV. Both calculational vehicles give a more pronounce inflection in the elemental cross sections at ≈ 12 MeV than indicated by the experimental results of ref. [47] (and similar to ENDF/B-VI). One should note that the prominent contribution to the (n,2n') cross section is ^{90}Zr. That isotope is magic in neutron number and it is known that nuclear models in this mass region have properties that are not characteristic of the "global" behavior implied by the general calculational codes.

In view of the above, the (n,2n') elemental evaluation is based on the experimental information of ref. [47] up to ≈ 15 MeV and extrapolates to 20 MeV using the model results normalized to the measured values in the 14 → 15 MeV region. The experimental value of ref. [46] was abandoned as being anomalously higher than the measurements of ref. [47] and the results of the calculations. The resulting evaluation is shown and compared with that of ENDF/B-VI in Fig. VII.1. The estimated uncertainties in the present (n,2n') evaluated cross sections are ≈ 10% in regions of significant magnitude. The present evaluation differs from that of ENDF/B-VI as the threshold is approached and at high energies.

In the absence of experimental (n,3n') cross sections the evaluation had to rely upon the predictions of the models. The result is shown in Fig. VII.1. The uncertainties are probably large, perhaps 25% of more, but the thresholds are all at relatively high energies and the (n,3n') cross section is significant only above ≈ 17 MeV. Thus the relatively large uncertainties are not a concern in most applications. There is no comparable file in ENDF/B-VI.

It was assumed that the neutrons emitted in both (n,2n') and (n,3n') processes are distributed isotropically. The corresponding neutron-emission spectra are represent by simple temperature distributions in the manner outlined in Section V.2 for the continuum inelastic scattering. The angular-dependence and spectral-emission used in the evaluation are both approximations to the physical reality, but suitable for the large majority of the applications of the file.

It is remarkable that that the experimental knowledge of the elemental zirconium (n,2n') and (n,3n') cross sections is so sparse.

--- If there is to be a significant improvement in the (n,2n') evaluation, extensive new prompt-detection measurements must be undertaken, extending from threshold to 20 MeV or above.

The accuracies of the present evaluation are probably beyond the capability of calculational prediction alone.

VIII. CHARGED-PARTICLE-EMITTING PROCESSES

There are a number of open zirconium (n,X) reaction channels at incident energies of ≤ 20 MeV. For the present evaluation, the respective thresholds were taken from the LLNL tabulation of R. J. Howerton [45].

VIII.1. The (n,p) and (n;n',p) Processes

The thresholds for these two reactions in the five isotopes are given in Table VIII.1.

Table VIII.1. Thresholds for the (n,p) and (n;n',p) reactions in the isotopes of zirconium.

Isotope	Thresholds (in MeV) (n,p)	(n;n',p)
90	1.518	8.452
91	0.769	8.798
92	2.884	9.499
94	4.144	10.437
96	6.298	11.622

VIII.1.1. The (n,p) Process

The (n,p) reaction in the zirconium isotopes leads to residual activities, and many of the corresponding activation cross sections have been measured. The National Nuclear Data Center provides ≈ 100 citations. Many of these results refer to metastable activities that are not directly the reaction cross sections, and the large majority of the activation results are concentrated about an incident energy of 14 MeV. The energy dependence of the cross section is not well defined. In addition, there is one proton-production measurement at 14.8 MeV [91]. With this experimental data primary reliance was placed upon the results of GNASH calculations [90]. The calculated isotopic energy-dependent shapes of the cross sections appeared to be reasonably consistent with the sparse experimental information. The calculated cross section magnitudes were subjectively normalized to the experimental information where the latter was reasonably available (generally about 14 MeV). The normalization factors ranged from ≈ 10% to 50%, with the largest value for the ^{90}Zr isotope. This trend is not surprising as ^{90}Zr is magic in neutron number, and it is known that model potentials at N = 50 are anomalous [2]. The adjusted calculated isotopic cross sections were combined to obtain the elemental result for the evaluation. The energy-dependent shape of the elemental result is probably quite good but the normalization uncertainty may be 20% or more.

--- The elemental (n,p) evaluation will probably not be improved until good activation and proton-production experimental results spanning a wide energy range are available.

The present (n,p) evaluation and that of ENDF/B-VI have a similar energy dependence but the latter is ≈ 40% smaller in the plateau region.

VIII.1.2. The (n;n',p) Process

There are a few activation studies of the (n;n',p) reaction but it is physically impossiblė to separate this activation process from that due to the (n,d) reaction. There is available a single proton-production measurement at 14.8 MeV [91] as noted above. With this fragmentary experimental information, the evaluation relied upon the isotopic GNASH calculations, with the results were combined to obtain the elemental evaluation. The evaluation may be uncertain by as much as 50% or more, but this is of little concern in most applications as the cross sections do not become of significant size until above ≈ 14 MeV. The emitted neutrons were assumed to be isotropically distributed and to be due primarily to compound-nucleus processes. The emitted neutron spectrum were determined in the same way as descried for the continuum inelastic scattering in Section V.2. ENDF/B-VI has no (n;n',p) information.

VIII.2. The (n,α) and (n;n'α) Processes

The thresholds for these two processes in the five isotopes are given in Table VIII.2.1.

Table VIII.2.1. Thresholds for the (n,α) and (n;n',α) processes.

Isotope	Thresholds (in MeV) (n,α)	(n,n',α)
90	-1.751	6.752
91	-5.664	5.509
92	-3.393	3.003
94	-2.048	3.794
96	-0.482	5.030

The relevant experimental data base is analogous to that of the (n,p) and (n;n',p) reactions, above, only weaker. For example, the National

Nuclear Data Center gives ≈ 40 citations of (n,α) activation measurements, nearly all of which are clumped about 14 MeV. The evaluation followed the same procedure outlined above for the (n,p) and (n;n',p) processes, normalizing the GNASH calculations to the measured values where possible. The normalization factors were smaller than in the (n,p) case. This is a bit surprising as the α-particle potential is not as well known as the proton potential. The improved agreement between the measurements and the calculated results suggests that the (n,α) and (n;n',α) evaluation uncertainties are smaller than in the (n,p) and (n;n',p) cases. As for the (n,p) and (n;n',p) cases,

--- The (n,α) evaluation will probably not be improved until more comprehensive and high-quality experimental results are available.

The (n,α) evaluation of ENDF/B-VI is similar to that of the present work, while ENDF/B-VI contains no (n;n',α) information.

VIII.3. The (n,d) and (n;n',d) Processes

Activation measurements of the (n,d) cross section are very sparse and the (n,d) and (n;n'p) processes can not be distinguished from one another. There is only a single deuteron-production measurement at 14.8 MeV [91]. There is even less experimental information on the (n;n',d) process. What experimental information is available suggests very small cross sections and the (n;n',d) thresholds are generally above 15 MeV. In view of this experimental situation, the present evaluation relies entirely upon GNASH calculations, with the additional assumption of isotropic neutron emission in the (n,n',d) process and compound-nucleus emission spectra. There is no comparable information in ENDF/B-VI.

VIII.4. The (n,t) and (n;n',t) Processes

The experimental situation for these reactions is more marginal than for the (n,d) and (n;n',d) processes, the thresholds are at higher energies, and the cross sections smaller. Therefore the present evaluation relies entirely upon GNASH calculations. The results may have large uncertainties (e.g., 100%), but this will be of negligible concern in most applications. There is no comparable ENDF/B-VI information.

VIII.5. The (n,^{3}He) and (n;n',^{3}He) Processes

The situation here is even more acute than for the reactions of Title VIII.4, above. For completeness these reactions are included in the evaluation using entirely the calculated GNASH results. The evaluation should be used only for qualitative guidance. There is no comparable ENDF/B-VI information.

IX. SUMMARY COMMENTS

The present evaluation provides a nuclear-data base suitable for many applications. It makes use of the most recently available information to improve the quality and coverage of the evaluation in a manner that may have a significant economic and safety impact on nuclear-energy systems. It supersedes ENDF/B-VI, much of which dates back nearly a quarter of a century. This does not mean that the present file is perfect. There are many shortcomings that will be alleviated only with high-quality measurements so as to provide explicit information and also for tests of the validity of calculational extrapolations. Success will require a coordinated measurement and calculational effort.

Some of the measurements necessary for significant improvement in the present evaluation include:

1. Total cross sections, with good resolution, from ≈ 10 keV to 20 MeV. The present data base is particularly poor below 1 MeV where there are no reliable high-resolution measurements reasonably defining what must be some significant cross-section fluctuations. The desired measurements are straightforward with a large white-source facility. However, they must be made with care, providing, accuracies of ≈ 1%, and with attention to possible self-shielding perturbations.

2. The present elastic-scattering evaluation is largely based upon a model interpolation from 10 to 24 MeV. This is a region where the potential is expected to change due to dispersion effects that are not defined by present measurements. Three or four high-quality elemental differential elastic scattering measurements are needed, distributed between ≈ 10 and 25 MeV. Such measurements are difficult but technologically possible.

3. The experimental knowledge of energy-average radiative-capture from ≈ 0.1 to 5 MeV is very marginal. Several good elemental measurements throughout this energy range are needed. They will require conventional prompt-detection techniques.

4. The elemental (n,2n') processes should be carefully measured from near threshold to at least 20 MeV. Concurrently the (n,3n') process should be studied. Prompt-detection techniques will be required but are feasible.

5. There are a great number of reported (n,p) and (n,α) activation measurements. However, they lack systematic energy and isotopic coverage. Detailed measurements extending from ≈ 8 to 20 MeV would be useful for the evaluation and for the testing of model capabilities used in extrapolation. It would also be useful to have some proton- and alpha-particle production measurements at more than the presently available single energy of 14.8 MeV.

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