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ANL/NDM-88

An Evaluated Nuclear-Data File for Niobium

by

A.B. Smith, D.L. Smith, and R.J. Howerton

March 1985

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

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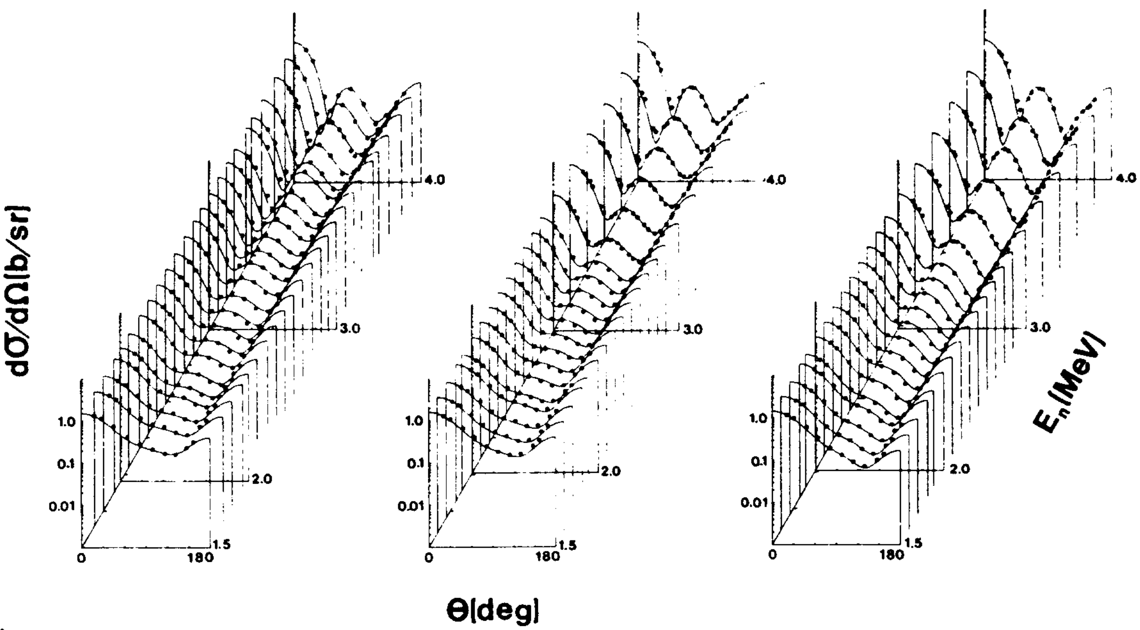

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AN EVALUATED NUCLEAR-DATA FILE FOR NIOBIUM*

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A. B. Smith and D. L. Smith
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Lawrence Livermore National Laboratory

March 1985

EVALUATION, Niobium. Comprehensive neutronic file 0-20 MeV. ENDF/B format.

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TABLE OF CONTENTS

EVALUATED NUCLEAR-DATA FILE FOR NIOBIUM*

by

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ABSTRACT

A comprehensive evaluated nuclear-data file for elemental niobium is provided in the ENDF/B format. This file, extending over the energy range 10^{-11}–20 MeV, is suitable for comprehensive neutronic calculations, particularly those dealing with fusion-energy systems. It also provides dosimetry information. Attention is given to the internal consistancy of the file, energy balance, and the quantitative specification of uncertainties. Comparisons are made with experimental data and previous evaluated files. The results of integral tests are described and remaining outstanding problem areas are cited.

*This work supported by the U. S. Department of Energy.

I. Introduction

The authors have had responsibility for the ENDF/B evaluated niobium file for more than a decade. The first version of this file (1) was privately circulated and widely used in fusion-energy-system calculations. The second version (2) became ENDF/B-IV, and was taken over in its entirety for ENDF/B-V. During the period since these evaluations, there has been a great deal of new experimental and theoretical information, much of it obtained at Argonne (e.g., see ref. 3). This new information makes possible considerable improvement of the evaluation, not only in the context of physical parameters but also in the specification of their uncertainties. Therefore, this new evaluation was undertaken. It is a timely effort as planning for ENDF/B-VI is now underway.

This report is the comprehensive documentation for a new niobium evaluated file. The corresponding numerical values have been transmitted to the National Nuclear Data Center, Brookhaven National Laboratory. Users interested in obtaining copies of the File should contact that Center. The File is primarily oriented toward fusion-energy needs and should be very suitable for fusion-blanket calculations. It is a comprehensive file, containing detailed information throughout the energy range 10^{-11}-20 MeV. However, most attention is given to the higher-energy region of primary fusion interest, i.e., from 100 keV to 20 MeV. Those interested in very detailed resonance properties (e.g., doppler effects in very high temperature systems) may wish to augment the resonance portions of the file. While attention is given to important activation processes (e.g., the (n,n') isomer-activation process used in dosimetry), this is not an activation file. Those interested in a plethora of relatively small activation cross sections are advised to make use of a specialized activation file (e.g., that of ref. 4).

The authors have carefully checked the File using physical tests and specialized integral-benchmark calculations, and are satisfied that file quality and performance are as good as can be obtained with the current state of experimental data and theoretical methods. However, constructive comments are welcome. Of necessity, the evaluation process required a detailed study of the neutron interaction with niobium. From that, areas of significant uncertainty warranting continuing experimental and theoretical attention were identified. These are cited as guidance for future efforts.

II. Resonance Properties

The File employs the resonance-parameter representation to 8 keV. The resonance parameters were explicitly taken from Mughabghab et al. (5). Small backgrounds were added to the 3-1, 3-2 and 3-102 files. These backgrounds were adjusted to give thermal-cross-section values consistent with the experimentally-based results cited in ref. 5, and to provide a reasonably smooth interface with the energy-averaged cross sections at 8 keV. The latter matching was done by calculating the resonance-averaged cross sections over energy increments of 0.5 keV and comparing the results with the energy-averaged values. Inevitably, there will remain a small discontinuity between the energy-averaged and resonance representations. Resonance-parameter uncertainties are complex and thus not quantified in the present evaluation. Some guidance as to resonance uncertainties is given in reference 5.

The neutron-scattering and radiative-capture cross sections implied by the above resonance-parameter representation are illustrated in Fig. 1, where the cross-section values were obtained from the resonance parameters using the code RECENT (6).

III. Energy-Averaged Total Cross Section

This portion of the evaluation extends from the upper extreme of the resonance region (8 keV) to 20 MeV. The experimental data base was assembled from the files of the National Nuclear Data Center and from the literature as referenced in CINDA. This data base consists of the citations of refs. 7-27. Brief statements of energy range are given with the references. Each data set was inspected using large-scale plots. Generally, the authors give only statistical uncertainties. Systematic uncertainties were estimated using subjective judgment based upon: the general quality of the author's/institution's work, the method employed in the measurements, and the available documentation. The systematic estimates are cited with the respective references. Some of the data were not in the applicable energy range, appeared qualitatively discrepant with the body of information, or were judged of inferior quality. In these instances, the data were omitted from further consideration, as identified in the references.

It was assumed that the cross section in this energy range behaves in an energy-smooth manner, and the experimental evidence supports that assumption. Therefore, in order to reduce the size of the data base to manageable proportions, the results of each reference were averaged over the energy increments: i) 25 keV (8-500 keV), ii) 50 keV (0.5-1.0 MeV), iii) 100 keV (1.0-5.0 MeV), and iv) 200 keV (above 5.0 MeV). The statistical and systematic uncertainties were carried through the averaging procedure. The resulting energy-averaged data base is shown in Fig. 2. It formed the input to the statistical evaluation procedures developed by Poenitz and implemented via the computer

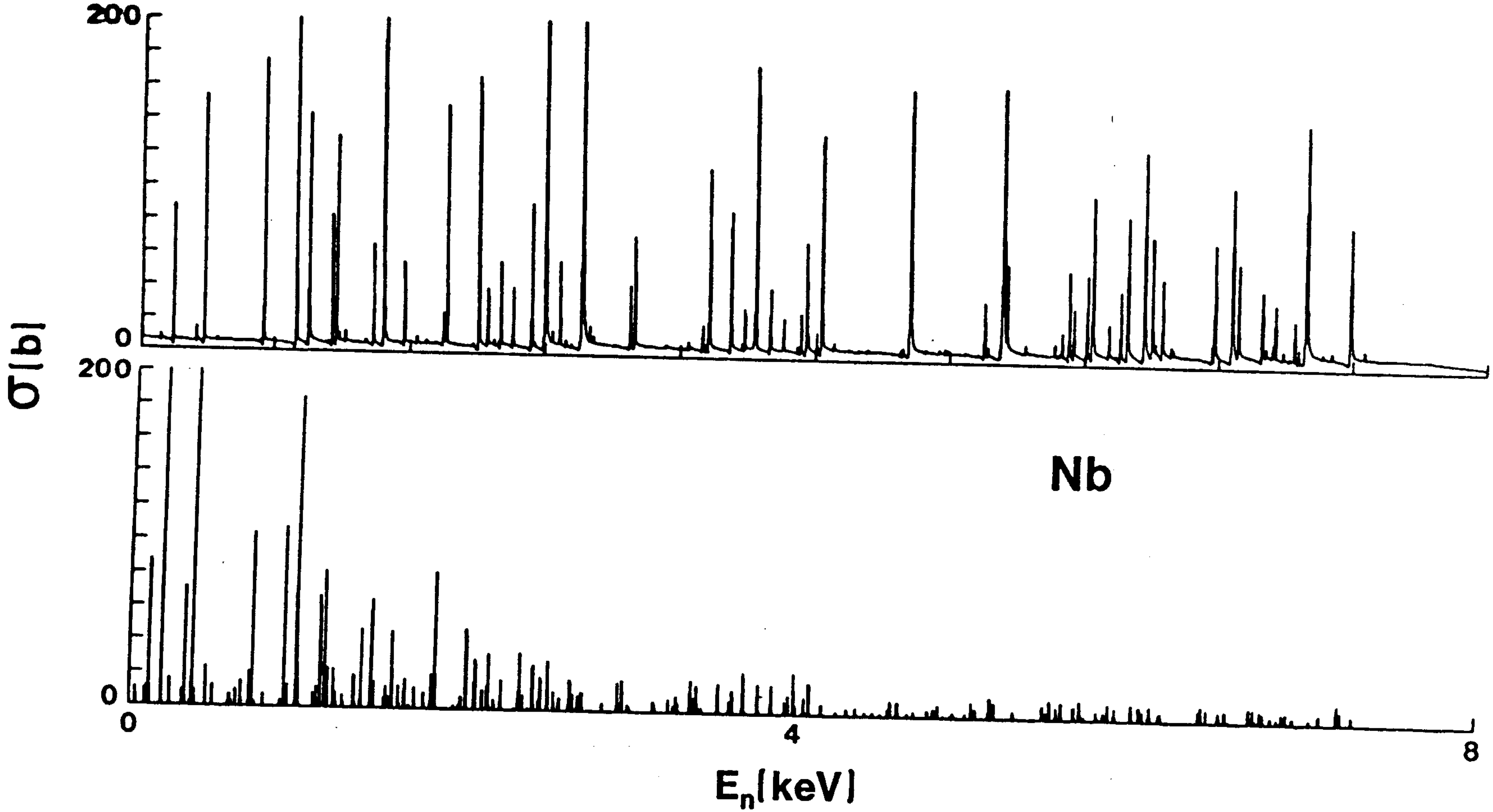

Fig 1. Cross sections implied by the resonance parameters of the File. Upper curve, elastic scattering: lower curve, radiative capture.

program GMA. The method is defined in ref. 28. The output of the procedure is the evaluated cross sections with uncertainties and correlation matrix. The latter were explicitly used to quantify the evaluation uncertainty. The evaluated result fluctuated in magnitude by small amounts dependent on the details of the input data. These fluctuations were smoothed by chi-square fitting a conventional optical model to the evaluated cross sections. The fitting procedure varied ten parameters, real and imaginary strengths, radii and diffusenesses and the four constants associated with the quadratic energy dependencies of both real and imaginary strengths. The resulting optical-model description of the evaluated cross sections was very good, with differences between input and calculated values generally much less than the evaluation uncertainty. The deduced potential is a good vehicle for interpolating and smoothing the experimentally-based evaluation and was used for that purpose. The potential should not be construed as suitable for more general analyses. More appropriate physical models are described elsewhere (29).

The evaluation is very descriptive of the experimental data base, as illustrated in Fig. 2. The evaluation uncertainties are small, often less than 1%, and never exceed 3.5%. The present evaluation is compared with that of ENDF/B-V (30) in Fig. 3. Generally, the band constructed from the present evaluation, ± uncertainty, contains the ENDF/B-V evaluation. There are fluctuations in local regions beyond the band, but they are of small magnitude. At high energies (i.e., above 15 MeV) the present evaluation is slightly lower than that of ENDF/B-V and that is a region where recent data have a relatively large effect. These comparisons, and the evaluation uncertainties, suggest that the neutron total cross section of niobium is very well known in the energy-averaged region. The present evaluation gives confidence as it quantifies this accuracy with an uncertainty file.

IV. Energy-Averaged Elastic-Scattering Cross Section

From 1.0-10.0 MeV, the elastic-scattering evaluation explicitly relies upon the experimental results of refs. 3 and 31. They are in reasonable agreement with sparse previously-reported experimental values but are of better accuracy and provide far more detail. Together with the total cross section and the other explicitly-measured partial cross sections, they define the experimentally-poorly-known inelastic continuum cross section over a very wide energy range. The model of ref. 3 was used to extrapolate the measurements to lower energies. That extrapolation is consistent with the measured values of ref. 32 but the uncertainties of the latter are rather large. In this lower-energy range the elastic-scattering cross section was adjusted to assure absolute file consistency. The adjustments were small but they did

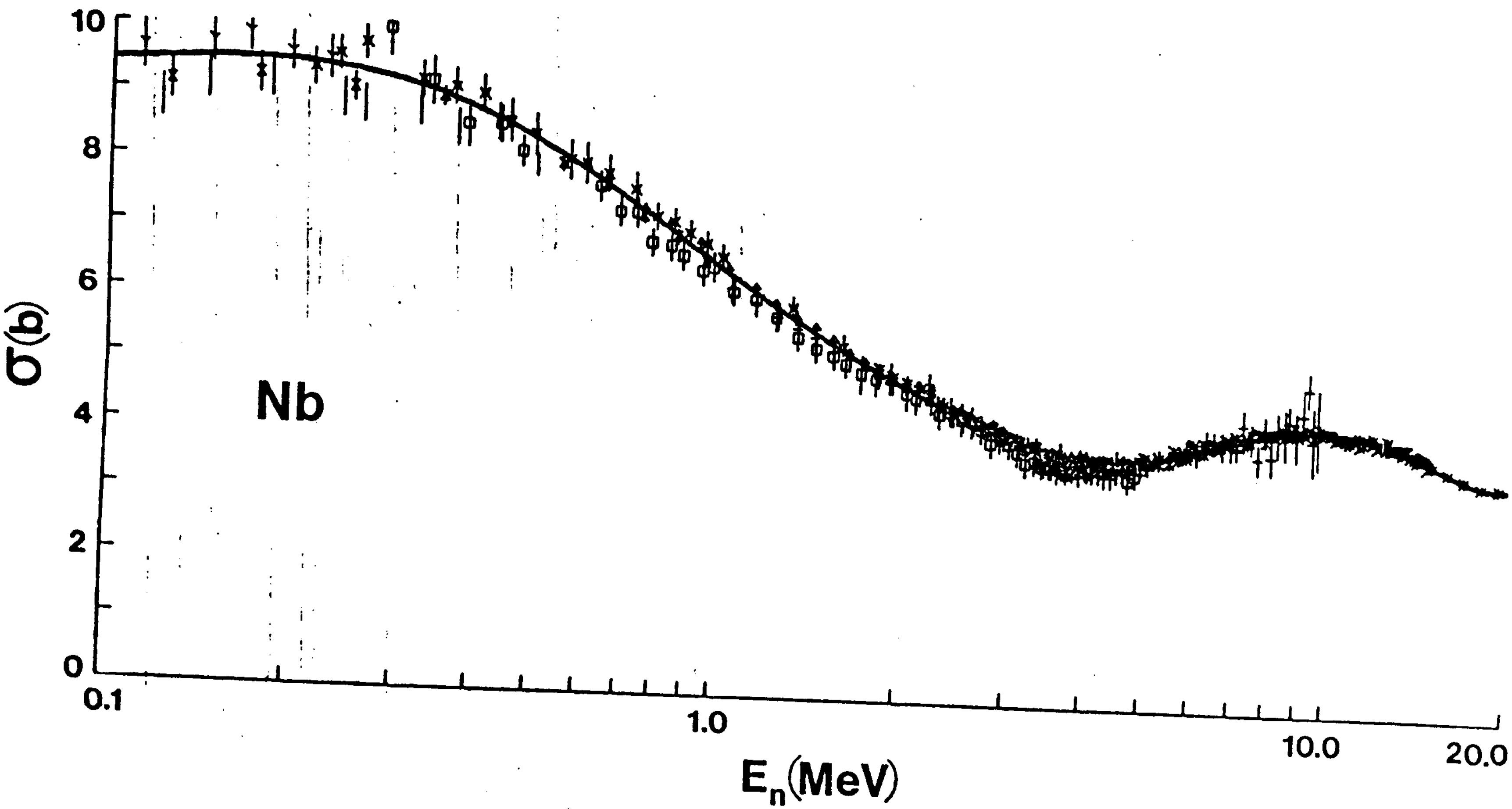

Fig 2. Comparison of the present evaluated neutron total cross sections (curve) with the experimental data base (symbols).

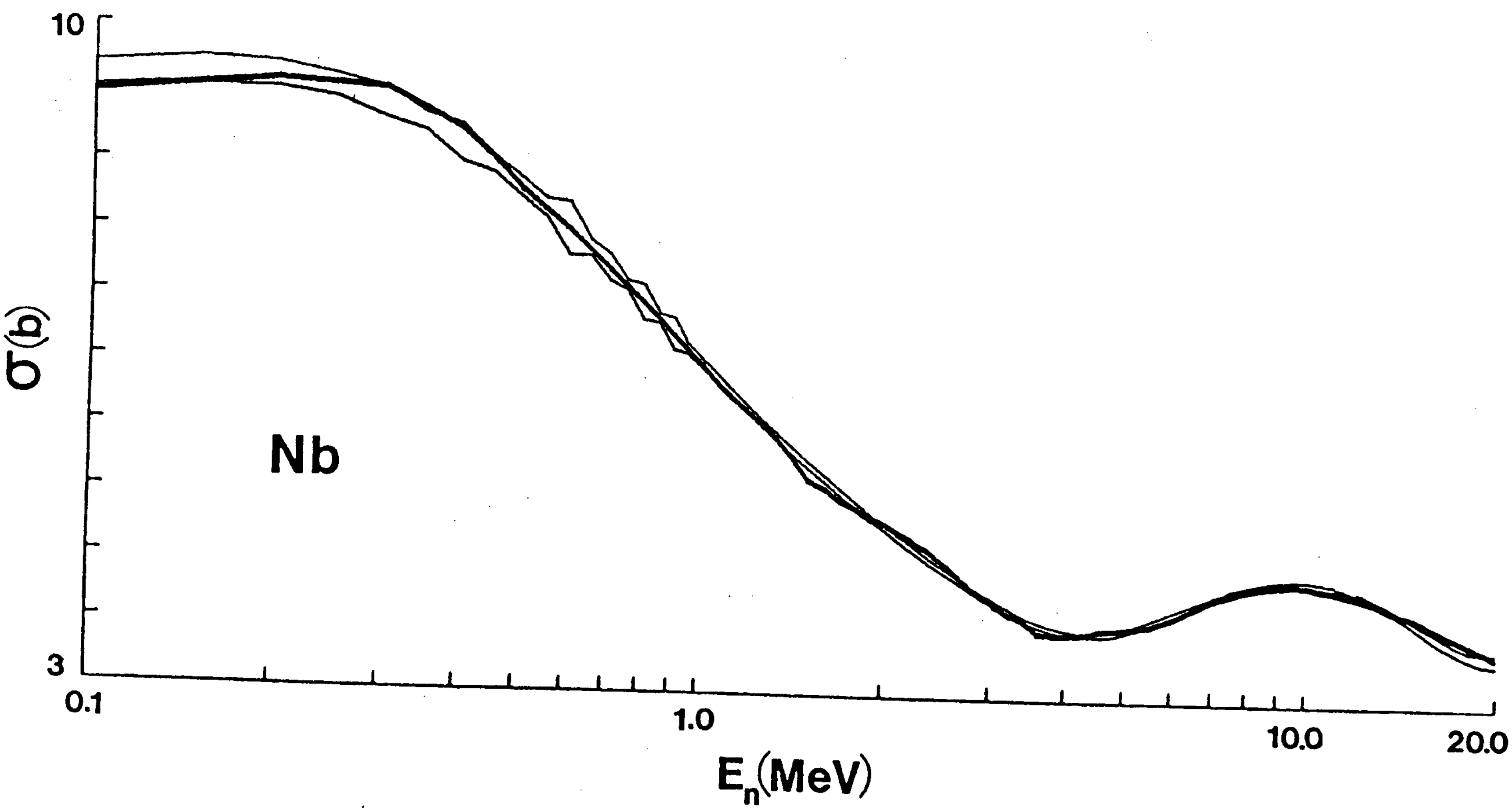

Fig 3. Comparison of the present neutron total cross sections with those of ENDF/V-V. The ENDF/B-V values are indicated by the heavy curve. The band of the present evaluation, ± its uncertainty, is indicated by the light curves.

result in some fluctuating artifacts due to partially resolved resonance structure in the radiative-capture cross section. Such artifacts are unavoidable when correlating data obtained with very different energy resolutions. In the present case, the artifacts are of negligible practical concern. Above 10 MeV, the evaluation is based upon the model of ref. 29. That model is soundly based upon the experimental results of ref. 31 and the total cross section to 20 MeV. This higher-energy model does have some interesting physical properties: e.g., evidence of a "fermi-surface anomoly" as discussed in ref. 31. From 10-20 MeV, the elastic scattering, together with the total and other measured partial cross sections, essentially define the total inelastic-scattering cross section which consists nearly entirely of the continuum component.

The present evaluated elastic-scattering cross sections are compared with those of ENDF/B-V in Fig. 4. There are modest differences, particularly at the higher energies. The principle advantage of the new evaluation is the superior accuracy that leads to improved definition of, particularly, the continuum inelastic-scattering cross section. Over the range 1-10 MeV, where the evaluation is based on careful measurements, the elastic cross-section uncertainty is 3%. At lower energies the estimated uncertainties are 5%. The uncertainty increases at higher energies to approximately 5% (10-15 MeV) and 7% (15-20 MeV).

The differential elastic-scattering distributions are represented by Legendre expansions, explicitly derived from the experimental values over the 1-10 MeV range, and from the above-outlined model extrapolations at higher and lower energies. The energy-dependent trends of these distributions are illustrated in Fig. 5. Detailed discussion of these distributions in the context of the model and experimental data are given in refs. 29 and 31. All the differential evaluated elastic-scattering distributions are consistent with the values of "Wick's Limit" (33) implied by the above total cross section.

V. Discrete Inelastic-Scattering Cross Sections

The experimental-data base was assembled from the files of the National Nuclear Data Center and the literature as referenced in CINDA (see refs. 3 and 34-47). These data consist of the results of (n,n') measurements and of cross sections deduced from (n;n',gamma) measurements. The latter provide superior resolution of excited-level structure but the deduced cross sections are far from consistent, often differing by 100% or more. Some of these discrepancies are traceable to erroneous level structure and/or branching ratios. Even with correction, the uncertainties persist and re-interpretation of many of the experimental results is not practical due to uncertain definition of the

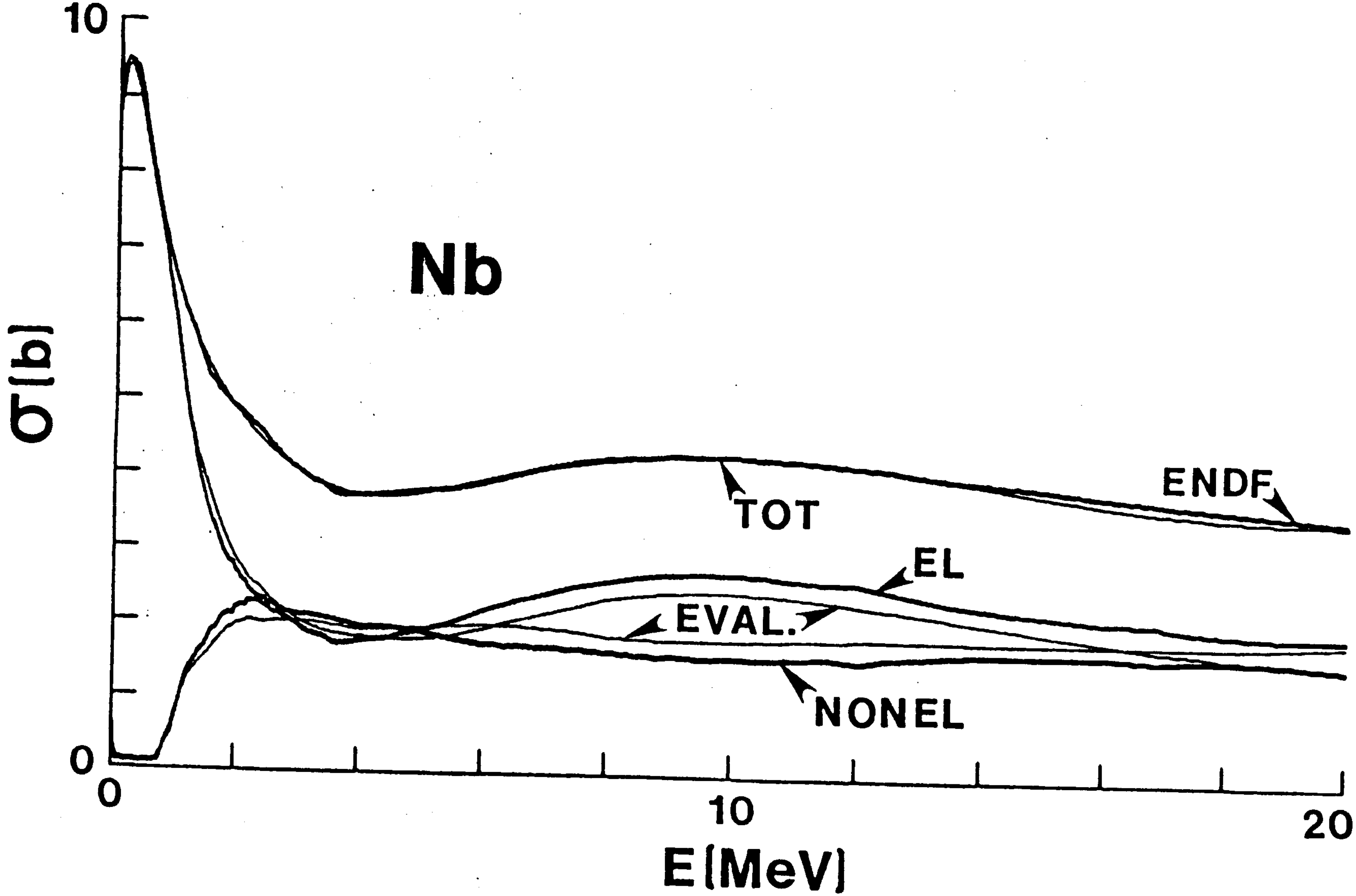

Fig 4. Comparisoon of evaluted elastic-scattering and nonelastic cross sections. The ENDF/B-V evaluation is indicated by the heavy curves, that of the present work by light curves.

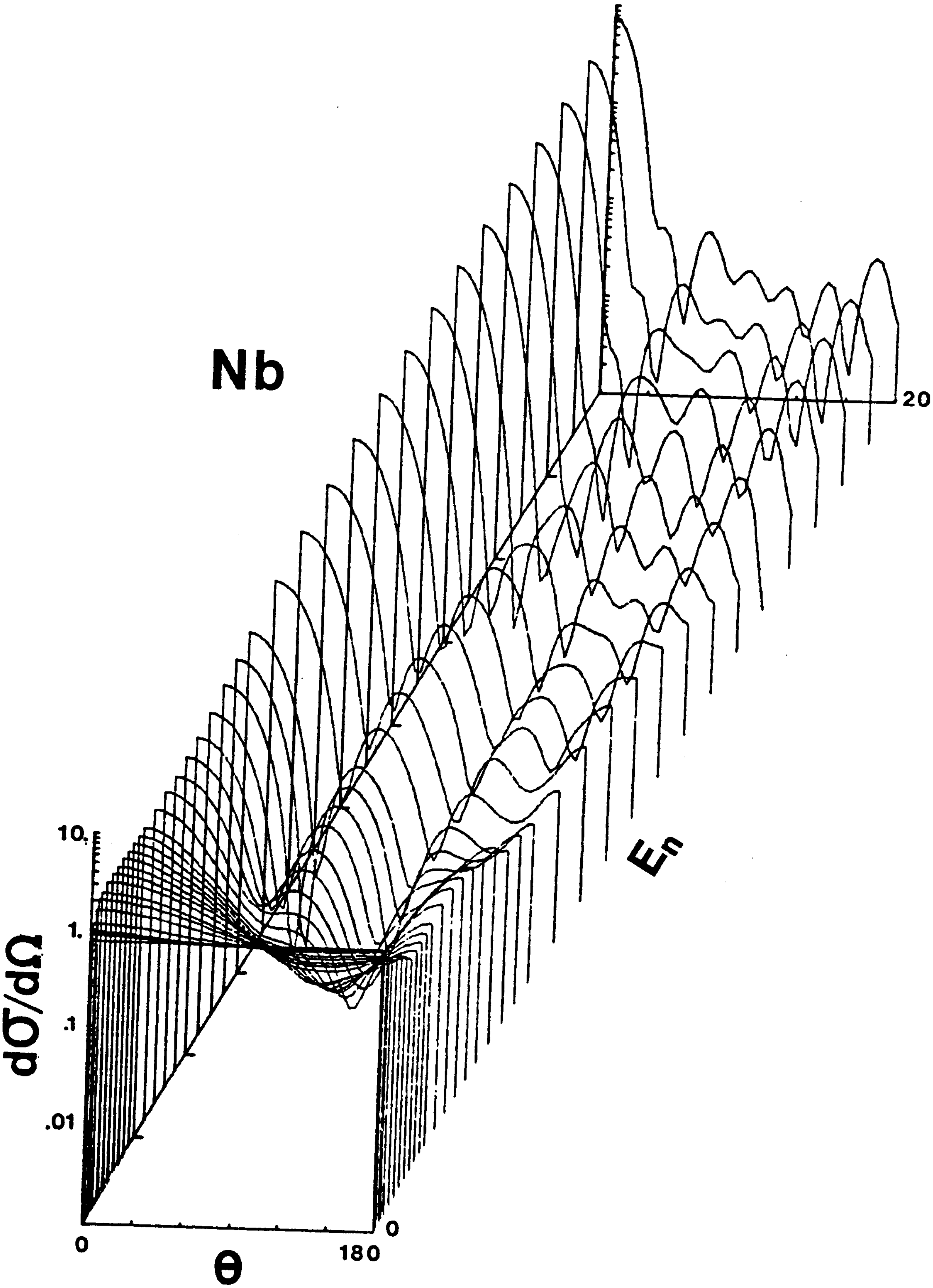

Fig 5. Evaluated differential-elastic-scattering angular distributions as given by the present evaluation.

measurements. Thus, cross-section values deduced from (n;n',gamma) measurements were only used to guide the evaluation near threshold where they are more reliable. Several (n,n') data sets are relatively consistent (e.g., refs. 41, 42, 43, 46 and 3). Due to their unambiguous nature and relative consistency, the (n,n') results were given primary consideration in this evaluation.

The evaluation uses 23 excited levels, extending to approximately 2.0 MeV, taken from ref. 38. That reference provides detailed level information which is relatively consistent with widely accepted compilations (e.g., ref. 48), and ref. 38 is selective of inelastic-neutron-scattering processes. However, there remain uncertainties in J-pi assignments and other evidence suggests that the level density of ref. 38 is an under-estimate above excitations of approximately 1.5 MeV (49). Even with these limitations, the levels of ref. 38 are a good basis for calculations, defining the relative energy-dependent shapes of the individual excitations. The details of these calculations are described elsewhere (3,49). The calculations assume the optical potential of ref. 49 and the compound-nucleus reaction process. The calculated cross sections were compared with the experimental (n,n') values, grouped to comparable resolutions where necessary, and normalized to the experimental values to obtain the evaluated cross sections. This method was successful to excitations of approximately 1.5 MeV, but for higher-energy excitations the normalizations became large, and above excitations of 1.9 MeV the evaluation is based entirely upon experimental observation. The derivation of the individual excitation cross sections is briefly outlined below.

The excitation of the 30.4(1/2-) keV level was entirely based upon calculation. This particular excitation is further discussed in Sec. XI of this report. The cross sections are very small and will have negligible impact on neutronic calculations. The estimated uncertainties are approximately 20%.

The excitations of the 687(3/2-), 744(7/2+), 808(5/2+) and 810 (5/2-) keV levels were compared with the collectively observed cross sections. The agreement was reasonably good, but was improved by renormalizing the calculated results by a factor of 1.08. The major contribution is from the 744 keV level. The uncertainty for the composite of levels is estimated to be approximately 10% over the energy region of appreciable magnitude.

The calculated collective excitation of the 950(13/2+) and 979(11/2+) keV levels was in good agreement with the experimental value and thus the calculations were accepted for the evaluation with no renormalization. The contributions of the two components are approximately equal and the uncertainties are approximately 10%.

The calculated excitation of the 1082(9/2+) keV level is in agreement with observation and thus was accepted for the evaluation. The cross sections are not large and the uncertainties are approximately 20%.

The cummulative calculated excitations of the 1297(9/2+), 1315 (5/2-), 1334(17/2+), 1369(3/2-) and 1395(5/2+) keV levels is in agreement with observation and thus the calculations were accepted for the evaluation. The cross sections of some of the components of this group are very small. The collective estimated uncertainty is approximately 15%.

The calculated excitation of the sum of 1483(3/2-), 1491(17/2+),and 1499(7/2+) keV levels was smaller than observation by 30-40%, thus the calculations were multiplied by 1.4 to obtain the evaluation. This large normalization factor may reflect the omission of levels in the calculations. The cumulative evaluation uncertainty for these levels is approximately 20%.

The calculated sum of 1603(15/2+), 1665(3/2-), 1680(5/2+), 1682(5/2+) and 1686(15/2-) keV excitation cross sections was again lower than the observation and a normalization factor of 1.3 was used to obtain the evaluation. The estimated cumulative evaluation uncertainty is approximately 15%.

The calculated sum of the excitations of the 1910(7/2+), 1915(7/2-), 1947(5/2+) and 1949(5/2-) keV levels was very much smaller than observed, probably due to missed levels in the calculational model. The discrepancy was so large that the calculations were abandoned and the evaluation was based upon a subjective assessment of the observations. A similar subjective assessment was used for the evaluation of the observed "level" at 2155 keV. There is experimental evidence for "levels" at approximately 2535 and 2500 keV (3,41) but the cited experimental cross sections are not very consistent and thus the evaluation relies upon a continuum representation for these and higher-lying levels.

Generally, this portion of the evaluation assumes a compound-nucleus reaction mechanism, thus the high-energy discrete-level inelastic-scattering cross sections are very small. There may be a significant direct-reaction component to the excitation of some of these levels (e.g., due to the coupling of a 1g 9/2 proton to the 2+ first-excited state of Zr-92). These precompound processes are discussed in Sec. VI of this report. The cumulative evaluated discrete-inelastic-scattering cross sections are illustrated in Fig. 6. Their magnitudes are cumulatively consistent with the other partial cross sections (see, for example, Fig. 4). A number of experimental comparisons are made in ref. 49. With the compound-nucleus assumption and many open channels, the inelastic-neutron emission is essentially isotropic and the evaluation explicitly assumes that. Those wishing to predict the few-percent

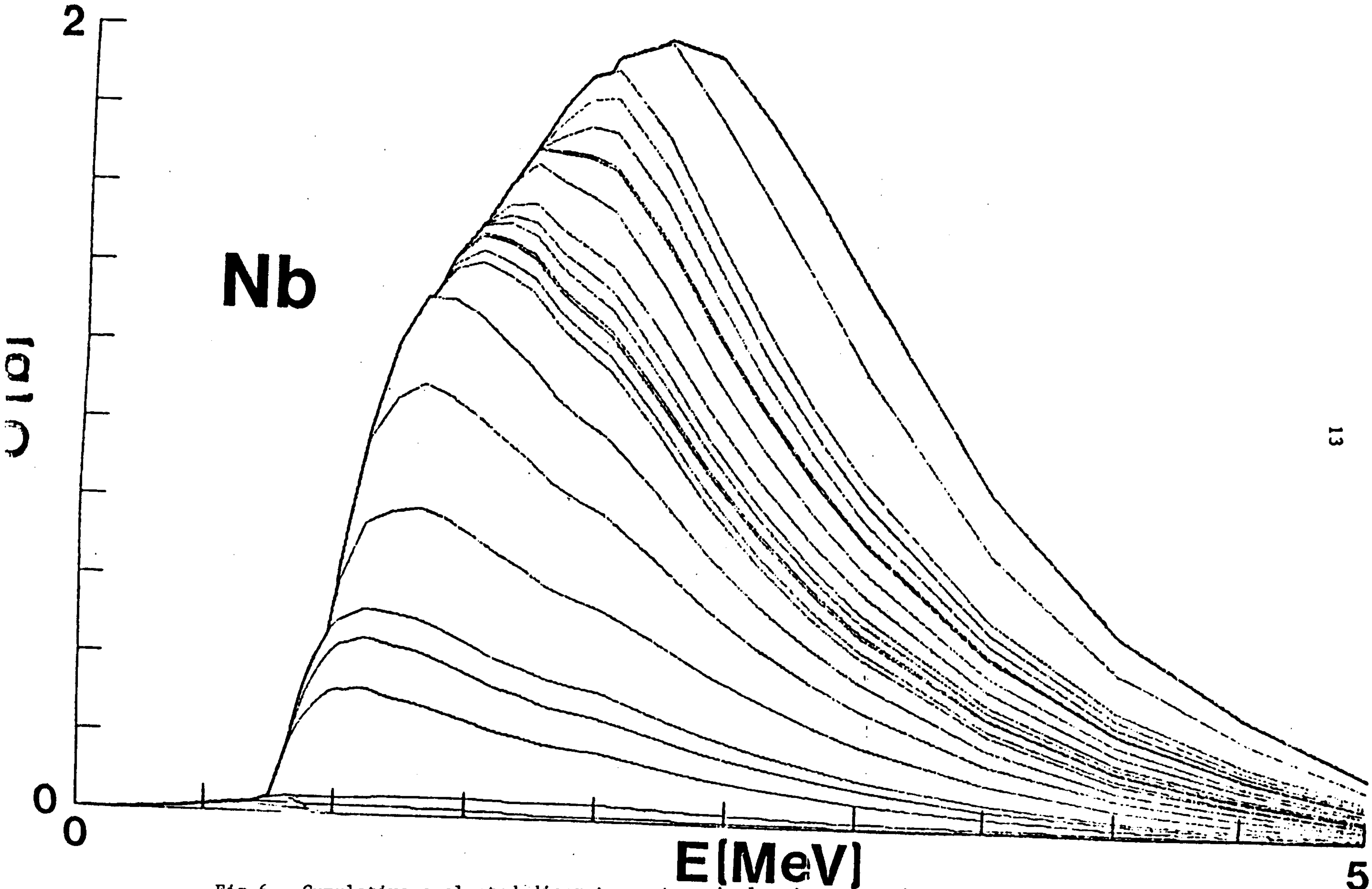

Fig 6. Cumulative evaluated discrete-neutron-inelastic-scattering cross sections of niobium.

anisotropy are encouraged to carry out straightforward compound-nucleus calculations using the above cited J-pi values. A number of uncertainty guidelines are cited in the above text. The numerical file quantifies these in the context of total inelastic-scattering uncertainties.

VI. Continuum Inelastic-Scattering Cross Section

The evaluated continuum inelastic-scattering cross section was defined as the difference between the total cross section and the sum of the other partial cross sections (predominently elastic, discrete-inelastic and (n,2n) cross sections). This definition assures explicit consistency of the File over most of the energy range. There is very little experimental information on which to base the evaluated data as most of the measurements pertain to emission cross sections near 14 MeV, which include a very large (n,2n) component. The evaluation is consistent with the fragmentary information available below the (n,2n) threshold (50,51,59). The cross-section energy dependence is illustrated in Fig. 7. Clearly, the compound-nucleus contribution is largely absorbed in the (n,2n) process above approximately 10 MeV, and the cross section remaining at higher energies is largely due to precompound processes.

The evaluation assumes that continuum-inelastic-scattered neutrons are emitted isotropically. This is a crude approximation at higher energies where the cross section is largely due to the precompound processes which are known to be anisotropic. The fragmentary experimental information available below the (n,2n) threshold shows significant anisotropy only at very forward angles where the solid angle contributing to the overall cross section is small (50,51). Near 14 MeV, the anisotropy of the emission neutrons is not well defined but is clearly peaked forward and is energy-angle correlated. There is no experimental information in the range 9-14 MeV or above 15 MeV. ENDF/B-V procedures do not permit representation of continuum-neutron energy-angle correlation, and many processing codes will not handle such anisotropy. ENDF/B-VI procedures will allow such a representation, but we feel that the simple assumption of isotropy is practically justified and the available experimental information does not well define the more complex formulation.

There is some experimental knowledge of the energy distribution of continuum-inelastic-scattered neutrons (50-59). Most of this information deals with approximately 14-MeV neutron-emission spectra which include large (n,2n) components. The limited experimental information available below the (n,2n) threshold (e.g., refs. 50, 51, and 59) was examined. These experimental results are generally well described by a simple maxwellian of the form SQRT(E)*EXP(-E/T), with only a very small higher-energy component. The experimental results extend over the limited incident-neutron energy range of approximately 6-9 MeV and thus do not reasonably define the energy dependence of the "temperature" T. At an incident energy of 6.0 MeV, T is taken to be 0.76 MeV. For energies of 8.0 MeV and greater, the continuum inelastic scattering has an ever-increasing component of the precompound process. For incident neutron energies of 12 MeV and greater, the entire continuum inelastic scattering is assumed to be precompound and the spectra are appropriate to that process. The result is reasonably consistent with the measured values and with the results of model calculations including both compound and precompound processes (e.g., the calculations of Strohmaier (60)). The manner of derivation precludes any fluctuating structure in the emission spectrum. Some recent measurements do indicate considerable structure corresponding to excitations of several MeV (57). However, the experimental evidence is not clear at the present time and its energy dependence is completely unknown. For these reasons, fluctuating structure was not included in the present evaluation. At a future date, better experimental evidence may warrant consideration of such fluctuations in the evaluation but the requisite measurements must be reasonably definitive as the phenomenon is doubtless peculiar to the individual nucleus and not consistent with extrapolation based upon energy-averaged models.

VII. (n,2n) and (n,3n) Processes

VII-1. The (n,2n) Process

The experimental data base is limited to the values of refs. 61-65, primarily to refs. 61 and 64. The most comprehensive measurements were made using the tank technique. The experimental results are remarkably consistent, as illustrated in Fig. 8. Below approximately 12 MeV, there have been no new data since 1975 and the experimental results are well represented by the careful evaluation of Philis and Young (66). Above 14 MeV there are the recent and comprehesive results of Veeser et al. (61). These latter data are consistent with the lower-energy work of refs. 63 and 64, and with several isolated-energy values. Therefore, the present evaluation is based upon the measured values of ref. 61 above 12-14 MeV.

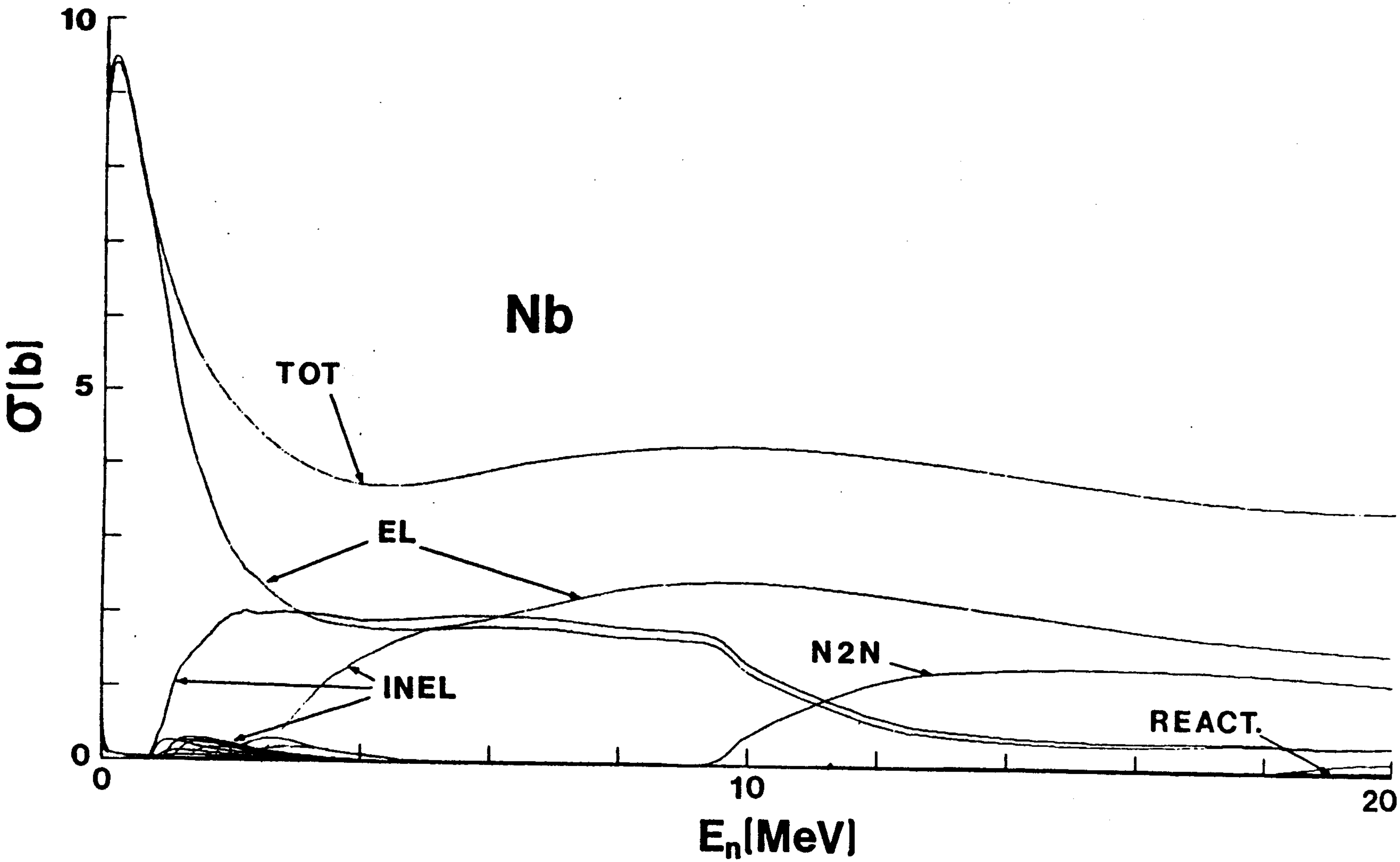

Fig 7. Comparison of the evaluated continuum-inelastic-scattering cross section with the other evaluated cross sections.

The estimated cross-section uncertainties vary with energy, with the smallest uncertainty approximately 6% near 14 MeV. In view of the good agreement between the experimental values of refs. 61 and 64, the evaluation of ref. 66 was used below 12 MeV but with approximately a 30% reduction in the cross-section uncertainty. Above 12 MeV the present evaluation becomes increasingly larger than that of ref. 66, the difference amounting to approximately 39% at 20 MeV. The present evaluation is generally larger than that of ENDF/B-V by 10-15% (see Fig. 8). It was assumed that the reaction mechanism was essentially the compound-nucleus process, and thus the neutron emission is isotropic. The neutron-emission spectrum is represented by a simple maxwellian of the form SQRT(E)*EXP(-E/T). The "temperature" T was adjusted, in concert with the continuum-inelastic-scattering process, to give a good representation of the measured and calculated 14 MeV emission spectrum, as outlined in Sec. VI above. At 14 MeV, T=0.97 MeV, and it was assumed to have a SQRT(E) energy dependence.

VII-2. The (n,3n) Process

This reaction has a high energy threshold (approximately 16.9 MeV) and a small cross section, thus is of minor applied interest. There appears to be only one experimental data set (61), as illustrated in Fig. 8. The evaluation is a subjectively-constructed curve through these few experimental values. The estimated cross-section uncertainties are large, 15-20% near 20 MeV, and they increase as the energy decreases. The present evaluation is considerably different from that of ENDF/B-V in the threshold region. This is not surprising as the only experimental information has become available since the ENDF/B-V evaluation was completed. It was assumed that the (n,3n) neutron emission is isotropic and that the emission spectrum is a maxwellian with a constant "temperature" T=0.5 MeV.

VIII. Radiative-Capture Cross Section

The experimental data base was assembled from the files of the National Nuclear Data Center and from the literature. This resource consists of the data of refs. 67-82. Where possible, the reported experimental data were renormalized to ENDF/B-V standards, and one large data set (ref. 67) was renormalized in accord with a private communication from the author. Large-scale plots of these data were inspected and it was concluded that the results obtained over the last 15 years are in reasonable agreement. Results from some of the earlier work appeared to be less suitable. Therefore, the

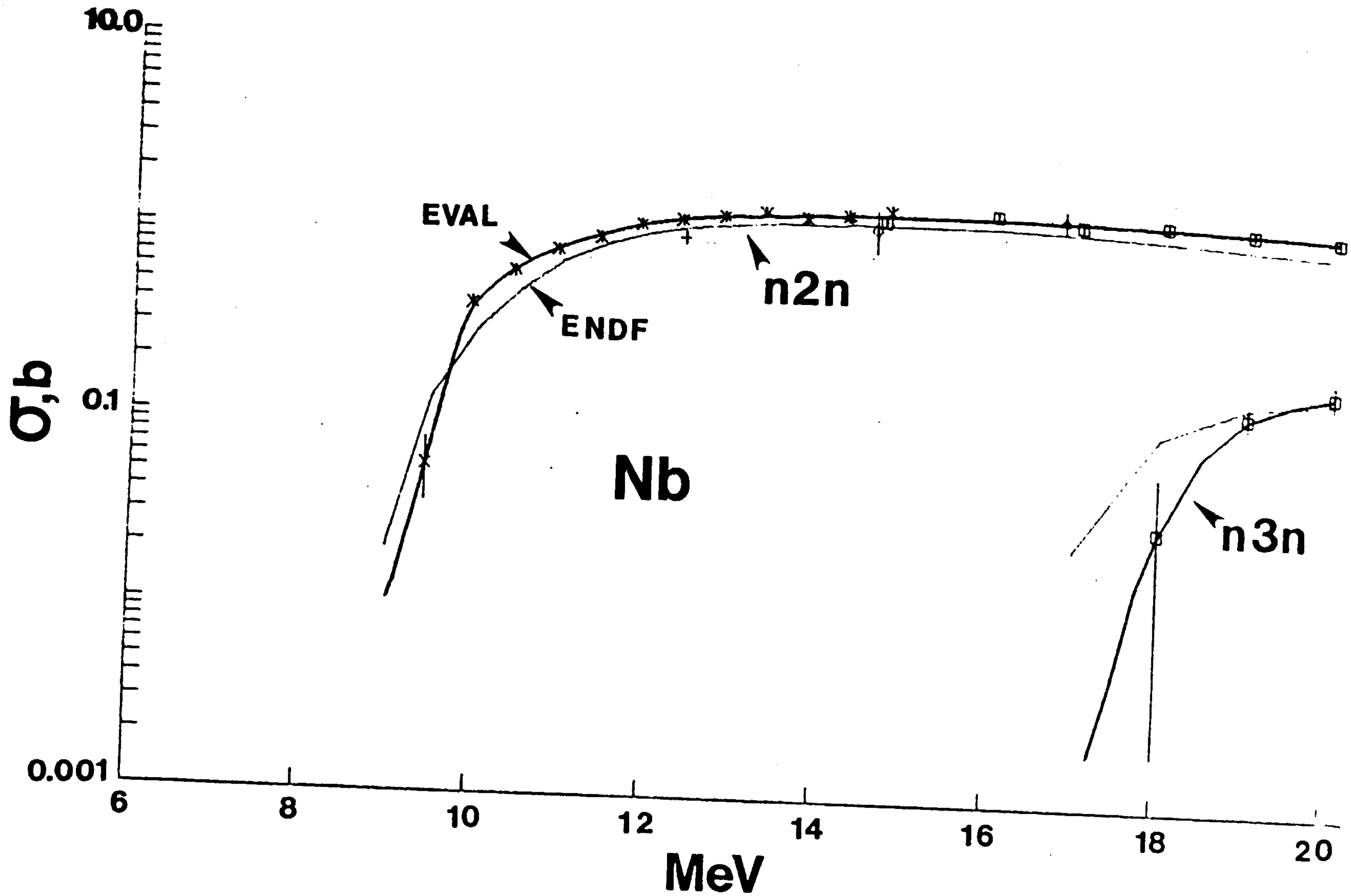

Fig 8. Comparisons of measured and evaluated (n,2n) and (n,3n) cross sections of niobium. The heavy curve notes the present evaluation, the light curve that of ENDF/B-V.

recent information and selected earlier data sets were used in the evaluation. The selected data were energy-averaged and a smooth curve was constructed through the averaged results. This curve was in good agreement with the high-resolution results of ref. 67. Therefore, the evaluation is based upon the high-resolution results of ref. 67 from 8 keV to 100 keV, and the energy-averaged behavior at higher energies. In this manner, the evaluation retains the high-resolution information which may be of use in certain applications. However, this formulation of the evaluation presents a problem as the evaluation as a whole must be explicitly internally consistent, and there is no information with equivalent or better resolution in the other reaction channels or for the total cross section. Thus the fluctuations of the low-energy portions of the capture cross section will appear as an anomaly elsewhere in the evaluation. We have chosen to place this anomaly in the elastic-scattering cross section. Generally, it takes the form of approximately 100 mb fluctuations at energies where the elastic-scattering cross section approaches 10 (i.e., approximately 1% fluctuations, which are considerably less than the elastic-scattering uncertainties in the same energy range). The uncertainties are estimated to be approximately 10% (8-100 keV) and 12% (0.1-1.0 MeV). At higher energies the data base becomes increasingly uncertain, with corresponding increases in the evaluation uncertainties. For most applications, this higher-energy region is of little concern as the cross sections become very small. However, the user is cautioned that above approximately 2.0 MeV this radiative-capture evaluation amounts to little more than a qualitative estimate.

The present evaluation is very descriptive of the experimental data, as illustrated in Fig. 9. This comparison is improved if it is limited to the recent values used in the evaluation. The present evaluation is in good agreement with the energy-averaged capture cross sections of ENDF/B-V (0.1-20.0 MeV), as illustrated in Fig. 10. This is not surprising as essentially the same data base was used in both evaluations. The energy-averaged capture cross sections were calculated, using the model of ref. 3, with results that are in very good agreement with the evaluation, as illustrated in Fig. 11. The good agreement between the calculation and the evaluation supports the energy-dependent shape of the latter.

IX. Charged-Particle Emission Cross Sections

More than 35 of these processes are energetically available in the bombardment of niobium with neutrons of less than 20 MeV. The cross sections for many of the reactions are essentially unknown, but must be very small. As a consequence, they are of no significance in the neutronic analysis for

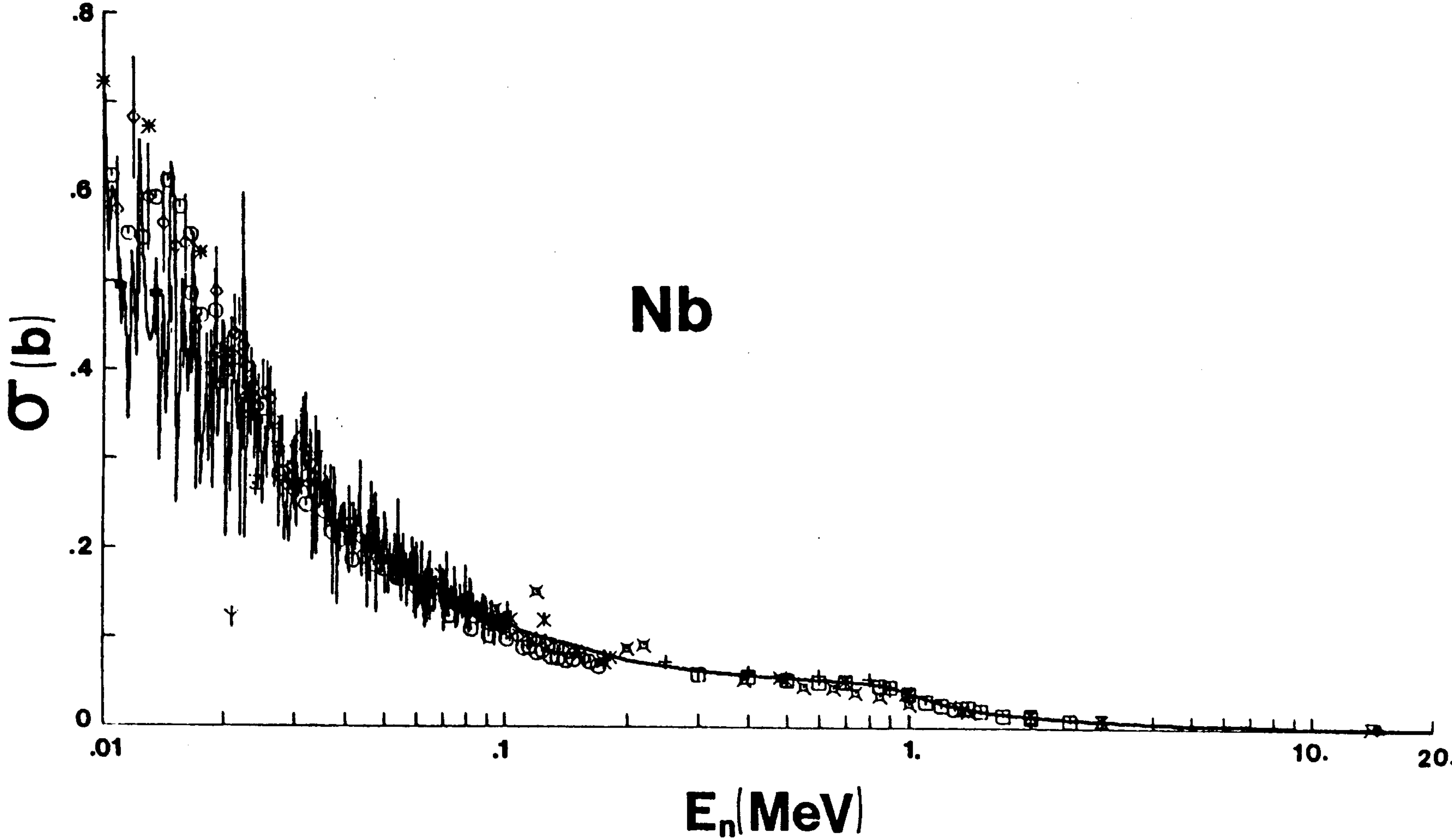

Fig 9. Comparison of the present evaluated radiative-capture cross section (curve) with the experimental data base (various symbols, see refs. 67-82).

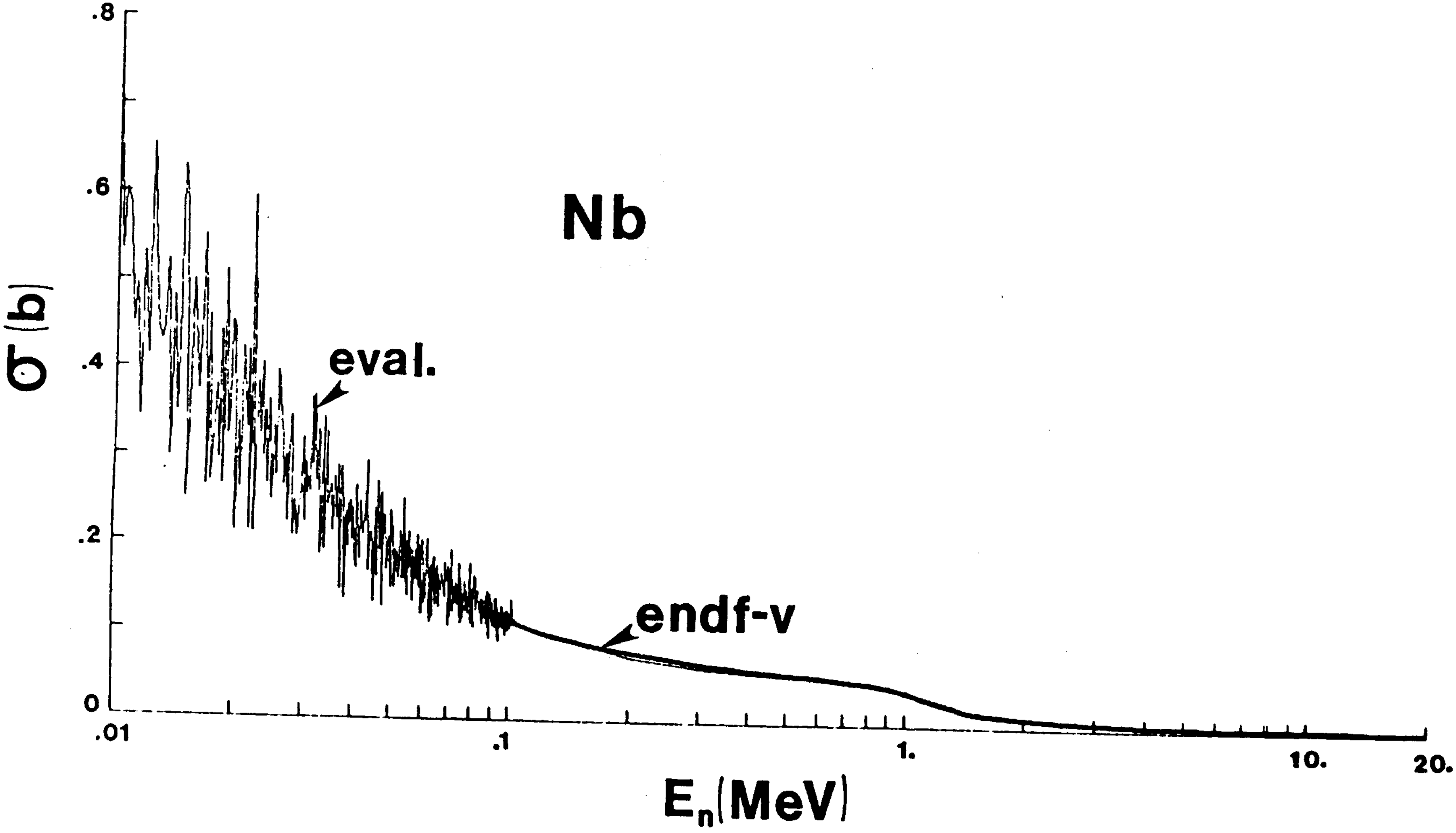

Fig 10. Comparison of the present evaluated radiative-capture cross section (light curve) with that of ENDF/B-V (heavy curve).

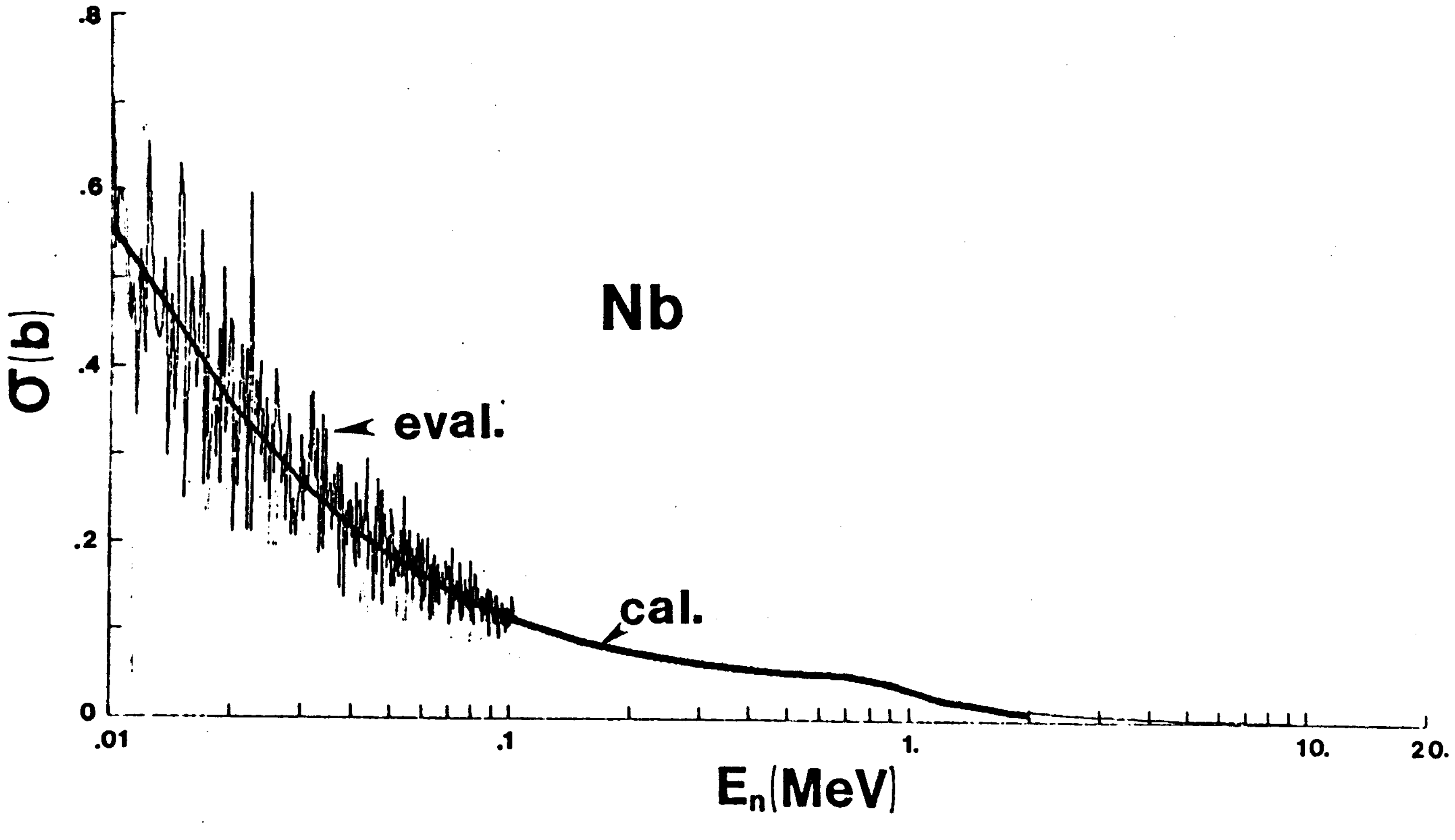

Fig 11. Comparison of the present evaluated radiative-capture cross section (light curve) with the result of model calculations (heavy curve).

which this File is intended. In special applications, the resulting residual activities may be of importance even though the respective cross sections are very small. For such special purposes, the user is encouraged to consult an activation file, such as that maintained at LLNL (4). At present the general purpose ENDF formats do not make provision for charged-particle energy deposition and thus such parameters as KERMA cannot be deduced from the general-purpose file. Again, it is suggested that the user desiring such information consult a special-purpose file (4). In the present evaluation, we exclude all charged-particle-emission processes in which two or more charged-particles are emitted, as the double barrier transmission implies very small cross sections. Also, all processes where three or more light particles are emitted (excluding the (n,3n) process) are ignored since the cross sections are very small. With these selection criteria, the available reactions are:

Reaction	Q-value (MeV) (a)
(n,p)	+0.690
(n;n',p)	-6.042
(n,alpha)	+4.918
(n;n',alpha)	-1.938
(n,d)	-3.817
(n;n',d)	-12.452
(n,t)	-6.195
(n;n',t)	-13.395
(n,He-3)	-7.720
(n;n',He-3)	-15.660

a. Q-values taken from ref. 4.

IX-1. (n,p) and (n;n',p)+(n;p,n') Cross Sections

There is essentially no direct experimental evidence for these three cross sections as the residual products do not lend themselves to activity measurements. The total proton-production cross section at 15 MeV has been measured by Grimes et al. (83) to be 51$\pm$8 mb. There have been several calculational-cross-section estimates, illustrated by the work of refs. 84 and 85. These calculational estimates are not particularly consistent, with differences of more than an order of magnitude at 20 MeV. Contributing to such calculational discrepancies may be the influence of the precompound process which has been shown to be significant (85). The present evaluation accepts the recent calculations of Young as indicative of the energy-dependent cross-section shapes and as defining the relative magnitudes of the three cross sections. These calculated results were normalized by a factor of 1.23 to give agreement with the observed total hydrogen production cross section at 15 MeV (83). The neutron emission is assumed to be isotropic and represented by a maxwellian distribution having a constant "temperature" T=0.8 MeV and a SQRT(E) energy dependence. The latter assumptions are only qualitative but are of little concern in neutronic applications of the File. The sum of the cross sections is known to 15-20% at 15 MeV. The uncertainties are much larger at other energies, and the relative ratios of the cross sections are uncertain by at least 20% throughout the energy range of the evaluation. The present evaluated (n,p) cross section is qualitatively consistent with the ENDF/B-V values. ENDF/B-V contains no (n;n',p) or (n;p,n') information.

IX-2. (n,alpha) and (n;n',alpha)+(n;alpha,n') Cross Sections

The (n,alpha) cross section is reasonably defined by experiments to approximately 20 MeV (86-89). The experimental uncertainties range from 5-20% and the measured values are generally consistent to within their respective uncertainties. In addition, the cross section for the production of helium at approximately 15 MeV has been reported by Grimes et al. (83) and Haight (90). There have been a number of efforts to calculated the (n,alpha) cross section (notably by Young (85), by Gardner (91), and by Strohmaier (60), using a variety of statistical models with and without precompound contributions). These calculated results are consistent to within approximately 10% at 14-15 MeV but deviate from one another by much larger amounts at both higher and lower energies. The present evaluation is based upon the relatively good experimental data base above approximately 5 MeV. The lower-energy approach to threshold follows the calculations of Strohmaier (60) as the latter seem to be consistent with the lower-energy experimental values. There are a number of measurements of the cross section for the production of the Y-90m isomer and these too seem to be relatively consistent with the calculations of ref. 60. There is only one set of experimental values above 16 MeV (88) and they lie between the calculated results. However, the latter are very divergent at 20 MeV (differing by as much as a factor of two). The evaluation follows the experimental results at these higher energies.

Very little is experimentally known of the (n;n',alpha)+(n;alpha,n')) cross sections. The above (n,alpha) cross section and the measured total helium production imply a (n;n',alpha) cross section of section of approximately 5.5 mb at 15 MeV, in agreement with the calculated results of ref. 85. Therefore, the calculations of ref. 85 were used for the present (n;n',alpha) evaluation. They differ from the calculations of ref. 91 in both shape and magnitude, but the latter are not consistent with the above (n,alpha) evaluation or with the observed helium production at 15 MeV. Neutron emission from the (n;n',alpha) process was assumed to be isotropic with a maxwellian spectrum having a "temperature" T=0.8 MeV at 8.0 MeV and a SQRT(E) energy dependence of T. These neutron-emission approximations are of little note in most applications as the cross sections are relatively small.

The (n,alpha) cross-section uncertainty is approximately 10-15% in the 13-16 MeV energy range and increases at both higher and lower energies. The (n;n',alpha) uncertainties are approximately twice as large. The present (n,alpha) evaluation is in good agreement with that of ENDF/B-V near 14 MeV. This is not surprising as both use essentially the same data base. The present (n;n',alpha) evaluation is approximately 30% larger than that of ENDF/B-V at 14 MeV. This change is a reflection of the availability of new helium-production data.

IX-3. (n,d) and (n;n',d)+(n;d,n') Cross Sections

Experimental knowledge of these two processes appears confined to a single gas-production measurement at 15 MeV (83), where the cross section is reported to be 8$\pm$3 mb. Due to the high threshold, the (n;n',d) process must make a small contribution to this value. The evaluation employs a simple barrier penetration calculation to estimate the shape of the (n,d) cross section and the normalization is to the measured gas-production value. A similar approach was used for the (n;n',d) cross section with normalization to 5 mb at 20 MeV, in analogy to the (n,p) and (n;n',p) processes. The neutron emission was assumed to isotropic with a maxwellian spectrum having a constant "temperature" T=0.6 MeV. The evaluation is an approximation with uncertainties of 30+%. The experimental information is very limited and, as evident elsewhere in this evaluation, model calculations tend to give conflicting results without substantive experimental data for comparison. Thus the large uncertainties probably cannot be reduced until better experimental information becomes available. None of these reactions is given in ENDF/B-V.

IX-4. (n,t) and (n;n',t)+(n;t,n') Cross Sections

Experimental knowledge of these reactions is confined to a pair of measurements at 14.6 MeV (92) and a broad-spectrum-averaged measurement with a mean energy of 14-16 MeV (93). There is a similiar broad-spectrum measurement at a mean energy of approximately 23 MeV (93). Both of the broad-spectrum results pertain to total tritium production. This is a minimal experimental data base but it does indicate small cross sections (below 1 mb) up to 20 MeV. The evaluation is based upon relative energy-dependent calculations by M. Blann (94), normalized to the fragmentary experimental information. The uncertainties are large (e.g., 30+%) but probably of little concern in neutronic calculations due to the small cross sections. The neutron emission was assumed to be isotropic with a maxwellian spectrum having a constant "temperature" of T=0.6 MeV. There are no comparable ENDF/B-V files.

IX-5. (n,He-3) and (n;n',He-3)+(n;He-3,n') Cross Sections

There is little experimental knowledge of these reactions. What evidence there is indicates that the (n,He-3) cross section is considerably less than 1 mb at approximately 14.7 MeV (e.g., i) less than 60 micro-b (86), ii) approximately 3.3 micro-b (95), and iii) 17.9±9 micro-b (96)). The cross sections for the (n;n',He-3) and (n;He-3,n') processes must be even smaller and the threshold is at approximately 16 MeV. Thus all these processes are not a concern in the neutronic calculations for which this File is designed, and are ignored.

X. Gamma-Ray Production Processes

Gamma-ray production is dealt with in two parts: the first is the gamma-rays resulting from the capture process and the second is gamma-rays resulting from all other processes.

For the capture process, the only measurements are those of ref. 97 and they are for thermal neutrons. The spectrum of photons reported in ref. 97 was used for the lowest incident neutron energy and a multiplicity was derived by forming the quotient of the energy available (the Q-value of the capture reaction) and the average energy of the measured spectrum. For greater incident neutron energies, the same spectrum was used and energy was conserved by adjusting the multiplicity of photons.

For all other reactions that produce gamma-rays, a multiple-step process was used to derive photon production cross sections and spectra. First, explicit energy distributions were developed for charged particles that are associated with charged-particle producing reactions (e.g. (n,p), (n,d), (n,n'p), etc.). Next, the sum of the average energies of secondary particles and the recoil nucleus were subtracted from the available energy for each reaction (i.e., E_n+Q). The resulting total photon energy and the cross sections for the reactions were combined using the R-parameter method of Perkins, Haight and Howerton (98). The final step was to check the total available energy for photon production from all reactions against the energy produced by the photon production cross sections and spectra. Any non-conservation of energy greater than 10% or 0.1 MeV (whichever was larger) was noted and the photon-production cross section adjusted to conserve energy. This procedure was iterated until energy was conserved within the limits described.

XI. Activation of ^{93m}Nb Dosimetry

The Nb-93(n,n')Nb-93m reaction is of prime dosimetry interest due to the low threshold and long half life for the reaction product (13.6±0.3 y (48)). These properties are useful for radiation-damage dosimetry applications in nuclear reactors (99). The study of this reaction with the relatively low neutron fluences associated with monoenergetic neutron sources is formidable. Problems stem mainly from the long half life and the low isomeric-transition energy (30.4 keV), with a predominance of internal conversion. Apparently the only formally published direct experimental result is that of Ryves and Kolkowski at 14.68 MeV (100). In addition, there are some very recent preliminary results by Uttley et al. (101), extending down to 1 MeV. The isomer activation cross section can be estimated by summing partial (n;n'gamma) cross sections for transitions that ultimately populate the 1/2- isomeric level. However, the uncertainties associated with this procedure are large and the method is preferably avoided.

Strohmaier et al. (60,102) generated an evaluation for this reaction which probably represents the best effort to date. The results are based entirely on model calculations. The calculated cross section of 34.3 mb for the 13.92-14.93 MeV range agrees well with the experimental value of 36.5±3.0 mb reported in ref. 100. Also, the calculated values of refs. 103 and 60 appear generally consistent with the results of ref. 99, considering the combined errors. It should be pointed out that there is considerable diversity in the accepted half life for Nb-93m, with one author reporting a value as large as 16 y (104).

For the present evaluation we use the results of Strohmaier et al.(60) above 700 keV neutron energy. Unfortunately, the final values for this evaluation, as presented in ref. 60 and 103, are in group form while a point representation is required for the present evaluation. We assign the group values to the group midpoint energies to obtain a point-wise evaluation that should adequately represent the cross section within the uncertainties of the Strohmaier evaluation. Below 700 keV, the information provided by Strohmaier et al. (60) yields only a crude representation of the threshold behavior. Therefore, we have generated an evaluation for this region, based upon our own model calculations, which represent the cross section in greater detail. In this region the cross section is based entirely upon neutron excitation of the first-excited level (the isomeric level) of Nb, in competition with radiative capture. The two independent evaluations were joined at approximately 700 keV.

Strohmaier et al. have provided a detailed covariance matrix for their evaluation (103). We used the portion of that matrix representing the region above 700 keV, except for the correction of an obvious error in the IRDF files (104) for the variance of the 1.16-1.41 MeV energy-group cross section (it was clearly a factor of 10 too small). For the region below 700 keV we assumed an error of approximately 25% for our model-calculated results, 100%-correlated below 700 keV but uncorrelated with the results of Strohmaier et al. (60,104).

The present evaluation was tested by calculating the spectrum-averaged cross section for the ENDF/B-V (30) standard thermal-neutron fission spectrum, with a result of 160.4 mb. This is noticeably larger than the value of 122±9 mb reported by Kobayashi and Kimura (105), but the two results are not inconsistent in view of the large uncertainties (16-50%) for the evaluated cross sections in the range below approximately 3 MeV which makes the major contribution to the fission-spectrum response.

A format for incorporating the above dosimetry cross section, together with its uncertainties, into the general ENDF file is presently a matter of debate within CSEWG. Therefore, this portion of the present evaluation cannot be formally incorporated in the numerical files. As an alternative, the cross sections and their associated uncertainty file are given in the 1-451 comment section. When the requisite formats are established, the numerical values can be properly inserted with the main body of the File.

XII. Integral Tests

The only integral experiment of relevance to this evaluation is a pulsed-sphere experiment (106) done at LLNL in 1978. In this experiment D-T neutrons were produced at the center of a four cm. radius sphere of niobium by allowing a 250 keV beam of deuterons to impinge upon a tritiated target through an entrance channel. The neutrons thus produced ranged in energy from 13.2 to 16.8 MeV. The neutrons escaping from the sphere were detected at a distance of 9.54 meters using a stilbene detector with its bias such that, using time-of-flight techniques, the time spectrum of neutrons from source energy to 1 MeV was measured at an angle of 26° to the deuteron beam.

The experimental configuration was described as input to the TART Monte Carlo (107) neutron transport code and the time spectrum of the neutrons escaping from the sphere was calculated. Comparison of the calculated and experimental results showed generally excellent agreement of the integrals of the spectra over two important regions as illustrated in Fig. 12. For the transmitted neutrons and those that were elastically scattered, (from time 0 to time 200 nsec.) the ratio of calculation to experiment was 0.993. For neutrons with energies between the least elastically scattered neutron energy and one MeV, (from time 200 nsec. to 680 nsec.) the corresponding ratio was 1.018. The compensation of the integrals in the two time ranges resulted in an overall agreement, in the integral sense, of 1.001. This does not imply that such spectacularly good agreement between calculation and experiment was true at all secondary neutron energies. There is clearly a deficiency of calculated neutrons from 250 to 300 nsec. (corresponding to secondary neutron energies of 7.5 to 5.7 MeV) that is as much as a factor of two at isolated times. This deficiency is the most marked and is compensated for by other smaller ranges where the calculation is greated than experiment. It is important, however, that the integral of the experiment and that of the calculation agree so well from source energy to one MeV. It means that, for that range of secondary neutron energies, the cross sections at $\approx$14 MeV are reasonably close to reality.

XIII. Outstanding Problems

In the course of an evaluation data deficiencies became apparent. It is the objective of this section to set forth some of these deficiencies for the guidance of future work.

Resonance properties are sufficiently known for fusion-energy neutronic design. However, if another application (e.g., a very high temperature fast reactor) places stringent demands on such matters as the doppler effect, more detailed attention should be given to the resonance region, extending up to 30 keV. There should be consistent measurements and interpretations of neutron scattering and capture processes.

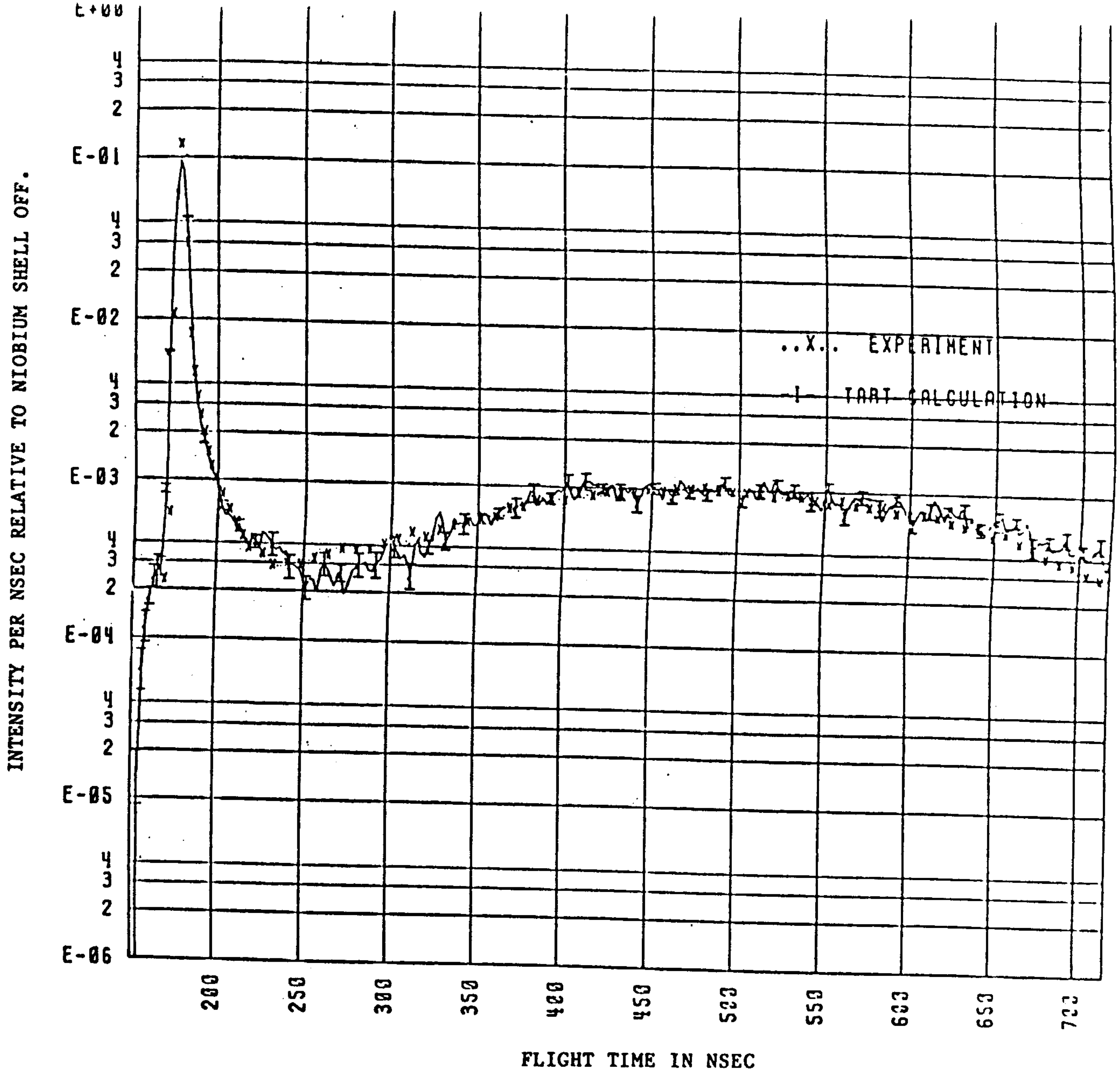

Fig 12. Illustrative comparison of measured and calculated neutron velocity spectra resulting from an approximately 14 MeV neutron source at the center of a one mean-free-path-thick niobium shell. The prominent peak is the uncollided and 14 MeV elastically scattered neutron source energy and the emitted distribution extends to 1.0 MeV (650 nsec on the scale).

The energy-averaged neutron total cross sections are very nearly of a "standard quality" and thus warrant no further attention.

Energy-averaged elastic-scattering is sufficiently known to 10 MeV. The measurements should be extended from 10-20 MeV at intervals of about 1.0 MeV and with an accuracy objective of 3-5%. Such measurements are a key to improved inelastic-scattering cross sections in this higher-energy region. The measurements will be difficult and must give careful attention to the very-forward scattering angles.

Discrete inelastic-neutron scattering remains of basic physical interest, but is probably well enough known for present applications.

Attention to continuum inelastic-neutron scattering is very much warranted. Particular consideration should be given to the region 4-9 MeV (i.e. up to the (n,2n) threshold) in steps of approximately 1.0 MeV. The objectives should be: i) the emitted-neutron spectrum shape with relatively-broad resolution, ii) its dependence on incident energy, and iii) an assessment of possible structure. An improved measurement of the emission spectrum near 14 MeV would also be useful. All of the measurements should be of such an angular scope as to reasonably define the anisotropy. The requisite measurements are feasible.

The (n,2n) cross section is probably well enough known for the present. The (n,3n) cross section is uncertain but that is of little application concern as the threshold is very high.

Radiative capture-cross sections are probably sufficiently known for present purposes.

In the future there may be stringent requirements for charged-particle emission processes leading to specific activities. These are very specialized needs that will have to be defined and addressed as they arise. However, it is clear that attention should be given to the energy dependence of these cross sections away from 14 MeV if the present evaluation is to be significantly improved in this area.

Many of the charged-particle processes of interest do not lead to residual activities, thus the use of new experimental approaches is sought.

Improved gamma-ray production results of a quality that permits a realistic assessment of energy deposition are warranted. More qualitative results are of little value.

Specification of energy deposition and KERMA information is not possible with the currently accepted general ENDF formats. The formats and the the physical information should be addressed.

The Nb-93(n,n')Nb-93m activity is far from well enough known for dosimetry purposes, and particularly so in the important region toward threshold. Until that situation is improved by detailed measurements, the reaction will be of little practical dosimetry use. A more general concern is the inability to incorporate dosimetry cross sections of this type and their associated uncertainties in the general ENDF file.

Theoretical calculations were of modest assistance in the present evaluation. Differences between calculated results and measured values can be very large. Better correlation of the calculations with experimental "benchmark" values is clearly warranted. Also, the physical reasons for the very large differences between calculated results should be ascertained. Generally, the calculations are most effective when used for interpolation between measured values.

XIV. Summary

A comprehensive evaluated neutronic file has been derived, making use of extensive new experimental data and better physical understanding to considerably improve the quality of the evaluated data base and to quantify the evaluation uncertainties. This file should be particularly suitable for fusion-neutronic calculations. Many aspects of the file appear to be of a quality that will meet long-term needs. There remain some problem areas and perhaps more will arise with changing applications. Many of these problem areas are such that they can be successfully addressed using established technologies and such actions are suggested. Certain aspects of the File need augmenting, and that will require attention to the ENDF format system as well as to the physical content.

Acknowledgments

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