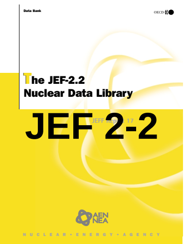


JEF-DOC- 195

CORRECTION OF INELASTIC-SCATTERING CROSS-SECTIONS OF FISSION-PRODUCT NUCLIDES IN THE JEF DATA FILE

H. Gruppelaar,
G.J.M. Janssen

Netherlands Energy Research Foundation ECN
P.O. Box 1, 1755 ZG Petten, The Netherlands

August 1987

Petten, August 1987.

ABSTRACT

In the existing nuclear data files for fission products the direct parts of the inelastic scattering cross-sections have usually been neglected. This paper reports on results of a study performed on the status of inelastic scattering cross-sections for fission-product nuclides, with regard to experimental data, theoretical predictions and evaluated data in the Joint Evaluated File (JEF-1). Based upon a combination of experimental data and calculations with a new 'regional' deformed optical-model parametrization a scheme for corrections of the inelastic scattering cross-sections of light fission fragments is suggested. Similar corrections are necessary for a number of heavy fission fragments. The main conclusion of this work is that direct effects in inelastic neutron scattering to low-lying states should be included in the evaluations of most fission-product crosssections, because these effects are already important at relatively low incident energies, relevant to applications in fast fission reactors.

CONTENTS

1. INTRODUCTION

This paper reports on the following two activities:

1. Study of the contribution of inelastic scattering of fission products in JEF-1 to the reactivity effect in fast power reactors, using available experimental data and theoretical models.
2. Study of a scheme for corrections of the inelastic scattering cross-sections of JEF-1 to improve the data file for a number of important fission products.

With respect to the reactivity effects of inelastic scattering of fission products in fast reactors and the status of evaluated and experimental data we refer to an earlier study [1] that has been reproduced in Appendix A1. A summary of the present status, partly based on Appendix A1 is given in Section 2, together with recent observations, comments and conclusions on experimental data.

Since there are reasons to believe that the available data are too high two actions were performed: a request for new inelastic scattering measurements on selected fission-product nuclei and an extensive theoretical study. The results of this last-mentioned study [2] are reproduced in Appendix A2 and are summarized in Section 3.

Based on these investigations we have developed a scheme for corrections of the JEF-1 data file and this is given in Section 4. It is noted, however, that there is still a great deal of uncertainty in our knowledge of inelastic scattering cross-sections of fission-product nuclei and that therefore the suggested improvements need validation by the (requested) experimental data. Furthermore, a scheme of modifications is designed for a fast correction of the bulk of the fission-product cross-sections. Some conclusions are presented in Section 5.

2. PRESENT STATUS OF EVALUATED AND EXPERIMENTAL DATA

2.1. Reactivity contribution of inelastic scattering

For the prediction of the reactivity effect of the lumped fission-product mixture in a large fast power reactor the capture cross-section is the most important data type. The uncertainty in the pseudo fission-product capture cross-sections is estimated to be of the order of ±5% or less. This rather low uncertainty is obtained by combining differential and integral data into the evaluations. Since there are so many individual fission products the statistical errors cancel to a great deal and the remaining uncertainty is essentially due to systematic errors in the integral fission-product data.

It is quite difficult to improve the quality of the lumped capture data much further, although significant improvements are still possible in the evaluated capture cross-sections for individual isotopes. Therefore, it is of interest to concentrate on improvements of other cross-sections contributing to the reactivity effect in fast reactors.

It is estimated that the contribution of inelastic scattering to the total reactivity effect of fission products in a large breeder may be as large as 15 to 20% (the elastic-scattering contribution is much smaller). In order to obtain a minor contribution of inelastic scattering to the uncertainty of the total reactivity effect the target accuracy of the lumped inelastic-scattering reactivity effect is therefore set equal to ± 15%. This accuracy is in general not reached for individual nuclides and most likely also not for the lumped effect.

Since many fission-product nuclides contribute to the total reactivity effect most of the statistical uncertainty in the lumped inelastic reactivity effect cancels and the remaining uncertainty must be due mainly to systematic errors. Therefore, it is quite important to search for possible systematic errors in the inelastic-scattering cross-sections and to estimate their possible impact on the pseudo fission-product cross-sections. This is one of the objectives of the present study. A very rough guess of the uncertainty in the lumped reactivity contribution due to inelastic scattering is ± 30%.

In addition, it is mentioned that the knowledge of inelastic scattering cross-sections is also very important in the analysis of central reactivity-worth measurements of samples of individual fission-product nuclei in fast assemblies such as the Dutch STEK reactor. In particular for samples consisting of even-mass fission products, the reactivity effects are small due to the low capture contribution and due to a relatively high scattering contribution of opposite sign. These corrections may be as large as 50% or more. From a comparison of STEK-500 reactivity worth measurements with activation and transmutation measurements performed in fast reactor assemblies such as RONA-3, ZONA-1, CFRMF and PHENIX it was found [3] that for most even-mass nuclides the inelastic-scattering corrections seem to be too low. Actually this observation was the first motivation to study the effects of inelastic scattering in more detail.

Finally, it is mentioned that the inelastic scattering of fission products in a fast reactor also affects the neutron flux spectrum. One of the consequences of this spectrum shift could be a change in the sodium-void effect as a function of burn-up. The contribution of inelastic scattering to the sodium-void effect is relatively small; the dominating effect comes from elastic scattering [4].

2.2. Status of existing evaluations

At the time the fission-product cross-section evaluations were performed there were only very few experimental data of discrete inelastic scattering available. Moreover, the main objective of the evaluations was to obtain the best possible radiative capture cross-sections, rather than to achieve excellent general-purpose evaluations. The present status of the fission-product evaluations in JEF-1 and of all other recent data files is that for almost all nuclides the inelastic scattering cross-sections are based on pure model calculations.

The model calculations in the current data files have been performed with the optical model and the width-fluctuation corrected Hauser-Feshbach model. Generally no direct components have been included. Thus, a spherical optical model has been used in almost all cases and in general no direct components from DWBA (Distorted-Wave Born Approximation) or CC (Coupled Channels calculations) have been added. Furthermore, precompound effects have systematically been neglected.

In [1] (Appendix A1) a survey is given of a number of possible systematic effects in inelastic scattering cross-section evaluations. A summary of these effects is given below, together with some comments.

Missing levels

If the low-energy level scheme of the target is incomplete because of gaps, the inelastic scattering cross-sections to discrete states are underestimated; this effect should not be overlooked, although the most important levels for (n,n') have been detected in scattering measurements with various particles.

Width-fluctuation correction

These corrections have been applied in the calculations, though not always according to the most modern parametrizations; systematical uncertainties of ±5 to ±10% due to different parametrizations are possible; it is not excluded that most continuum emission cross-sections are underestimated because neglect of width-fluctuation effects in the continuum.

Optical-model choice

The use of global spherical optical models in the calculations may lead to systematic errors in certain mass ranges if not enough data are used in the fitting procedure; as an example the inelastic scattering cross-sections averaged over a fast reactor spectrum are about 25% lower in ENDF/B-V than in the CEA/ENEA evaluation at A < 145.

Neglect of direct-collective excitations

The effects of direct-collective excitations have in general not been included explicitly in the current data files; this results in large underestimation of inelastic scattering cross-sections for the excitation of collective states.

Neglect of precompound effects

These effects are quite important at energies well above 5 MeV; for fast-reactor applications there is no urgent need to revise the present evaluations.

Neglect of (n,2n) cross-sections

In many fission-product evaluations these data are based upon crude approximations; although these cross-sections should be included a high precision is not required for the calculation of the reactivity effect in fast reactors.

From the above mentioned possible systematic effects we have concluded in Appendix A1 [1] that the first priority for further investigations is to study the impact of direct-collective excitations to fission-product cross-sections. A second point of concern is the optical-model parametrization. However, these points are closely related, since the failure of the global spherical optical model is mainly due to these collective excitations.

2.3. Some notes about the neglect of direct effects

First of all we mention here that collective effects are expected to be important for the major fission products, because the mass-distribution of the fission products shows two maxima at about the same masses where the deformation parameters are large, see Appendix A1 [1]. Although the deformation parameters (β_2) are known for quite some time, little information was known until recently on experimental (n,n') cross-sections, in particular at energies just above threshold. Before 1975 the only experimental information on deformation effects in inelastic neutron scattering on fission-product nuclei came from work performed at Bruyères-le-Châtel on even-mass Nd isotopes. However, this study was made at 4 to 7 MeV and no information on the cross-sections near threshold was available. Probably the evaluators assumed that direct effects were only important at high energies or that the compound-nucleus part of the cross-section was very much larger than the direct component at low energies. This is true to a certain extent, but recent evidence shows that the combination of a global spherical optical model and the neglect of direct excitations may lead to predictions that are up to a factor 2 too low in comparison with the data, see Appendix A1 [1].

2.4. Status of experimental data

A review of experimental data on inelastic scattering cross-sections to discrete levels in fission-product nuclei has been given in Appendix A1 [1]. The first indications for large inelastic enhancements at low incident energies came from (n,n'γ) work performed at 2 to 3 MeV for Nd and Sm isotopes in 1976 and 1977 (see Refs. in Appendix A1). In 1977 Govor et al. [5] published results of a systematic study of integral (n,n'γ) data measured with reactor neutrons (effective energies between 0 and 1.5 MeV) for targets with masses 28 ≤ A ≤ 152. Their results showed large enhancements for collective states compared to results of statistical-model calculations, in particular for Ru, Pd and Sm isotopes. The most important paper for the present work is that of Konobeevskii and Popov [6], issued in 1981 with results of (n,n'γ) data for even-mass isotopes of Mo, Ru, Pd (and other elements). We refer to the figures in Appendix A1 for a comparison of experimental and evaluated data, showing serious underpredictions of the current data files.

One may question the validity of these measurements. In particular for some Ru and Pd isotopes the maximum value of the inelastic-scattering cross-section to the first excited 2^+ state was measured as about 1.5 b. This value is quite high. A 'rule of thumb' is that inelastic-scattering cross-sections to discrete states are usually less than 1 b [7]. Verification of these measurements seems therefore quite important. There is an important argument in favour of the inelastic gamma-ray measurements of Konobeevskii and Popov and that is that they are in agreement with neutron measurements by Smith et al. [8] for the even-mass Mo isotopes. In fact the Sovjet data have been normalized to the Argonne data for Mo-98 at E = 1.25 MeV (1.00 ± 0.07 b). It is difficult to imagine that the Ru and Pd data of Konobeevskii and Popov are wrong while there is agreement for the Mo data. Moreover, if the Mo-98 inelastic cross-sections have already a maximum cross-section of 1 b, it is likely that the Ru-102 cross-section with a higher deformation parameter and an excited state at lower energy has indeed a cross-section well above 1 b.

One could also try to extract information of inelastic-scattering cross-sections from the difference of the total and the elastic-scattering cross-sections. At low incident energies this difference is equal to the inelastic scattering cross-section for excitation of the first excited state. At about 0.8 MeV the total cross-section is about 7 b and the elastic-scattering cross-section about 1 b with, however, an uncertainty of about ±50%. This means that a maximum inelastic scattering cross-section of 1.5 b is not excluded.

In addition to the above-mentioned experimental data base there are some elemental data, measured at Argonne for Y, Zr, Nb, Mo, Rh, Pd, Ag, Cd, In, Sn and Sb at energies from about 0.5 to 4.0 MeV (unfortunately data for Ru are lacking) [9]. It is difficult to extract from these measurements information on the inelastic-scattering cross-sections for individual levels of the isotopes. However, it is clear that the elemental total inelastic-scattering cross-section for natural Pd measured at Argonne is about a factor of 1.7 times higher (at 1.0 MeV) than the evaluated value given in ENDF/B-V [10]. This enhancement is less than that following from the Sovjet data for Pd-106, -108 and -110 (factor of about 2.0), but in the total inelastic-scattering measurement there is a large fraction (about 40%) of Pd-105. Assuming that there is no enhancement in the inelastic-scattering cross-section for Pd-105, the Argonne data also indicate a factor of about 2 enhancement for the even-mass isotopes. This assumption is based upon the fact that more than 10 levels contribute to the inelastic-scattering cross-section of Pd-105 at about 1 MeV, rather than only one (collective) state for the even-mass Pd isotopes. Collective effects in Pd-105 are smeared out over a larger energy range and may be less important for the total inelastic-scattering cross-section at about 1 MeV. Thus, the Argonne elemental Pd measurement certainly confirms that the evaluated data for (n,n') are much too low. Furthermore, the Argonne measurements on natural Pd are not a-priori in disagreement with the Sovjet data for the individual isotopes.

From the above-mentioned facts and arguments we conclude that in particular for the even-mass isotopes of Ru, Pd, Nd and Sm the evaluated inelastic-scattering cross-sections are much too low at low incident energies. The available experimental data of Konobeevskii and Popov for many light fission fragments are quite high, but there is no indication that these data are systematically in error. There is a ± 7% error due to the normalization; the uncertainty indicated in the figures ranges form about ±10 to ±15%. From an independent measurement on natural Pd these data are confirmed to within about 15%. For the heavier fission fragments there are no data near threshold, but there is some information on direct effects at higher incident energies, which can be used in theoretical models to extrapolate to lower energies. In general the data base is very poor and new measurements should be encouraged. For that reason a request for new data has been made at the Central Bureau of Nuclear Measurements of the EC, see Section 3.5.

3. THEORETICAL STUDIES

3.1. Analysis of Konobeevskii and Popov

In the paper of Konobeevskii and Popov [6] it is shown that if global spherical models are used in combination with the width-fluctuation corrected Hauser-Feshbach model, no agreement can be obtained with experimental inelastic scattering cross-sections at low energies for Mo, Ru and Pd isotopes. Therefore these authors have used the coupled-channels method (CC) to calculate the direct part of the cross-section, taking into account the vibrational states. Various coupling schemes were studied including one-phonon states (2^+ and 3^-) and two-phonon quadrupole states (0^+, 2^+ and 4^+). The statistical part of the cross-section was calculated with Hauser-Feshbach theory, generalized by Hofmann et al. (HTRW) [11] for the presence of direct reactions. We note that this approach is not used very often, since usually the statistical part is calculated without taking into account direct effects.

A good parametrization of the above-mentioned optical model is of course essential. Konobeevskii and Popov have used a standard potential with fixed geometry parameters, spin-orbit potential depth and isospin-dependence of real potential, but variable real and imaginary depths (V and W, respectively). Also the value of the deformation parameter β_2 was allowed to vary (reduction up to 70% of the deformation parameter extracted from Coulomb-excitation measurements). Furthermore, various coupling schemes were studied.

The main conclusion of Konobeevskii and Popov was that in order to fit their inelastic-scattering data it is necessary to have quite low values of W, equal to about 2 MeV. Larger values of W correspond somewhat better to the experimental values of s- and p-wave strength functions and to experimental values of total cross-sections, but spoil the description of inelastic scattering cross-sections. Some improvement is obtained if a smaller value of β_2 is used (70% of the electromagnetic value).

The results of Konobeevskii and Popov are that at an energy of 300 keV above threshold the contribution of the direct cross-section amounts 20 to 30% in the case of the Ru and Pd nuclei, 15 to 20% for Mo and Cd, and less than or equal to 10% for Sn. There is also a significant direct contribution for the second 2^+ state (30% at 150 keV above threshold).

Evaluation of the work of Konobeevskii and Popov

The theoretical analysis of Konobeevskii and Popov is very valuable for the explanation of the direct effects in inelastic neutron scattering at low incident energies. The CC method combined with statistical-model calculations is the best way to perform the analysis. The treatment of the statistical part of the cross-sections according to the HTRW-method for cross-sections with direct components is not used very often, but seems to be better than what is normally used (although there is not much experimental validation of this method). Some critical notes can be made with respect to their parametrization: this is tailored to fit the measured inelastic scattering cross-sections and may give less satisfactory results for the other cross-sections (admitted by the authors). Therefore the parametrization of Konobeevskii and Popov cannot be used as a check on their experimental data nor for the prediction of other cross-sections (as is required for evaluation purposes).

We also do not understand why a decrease in β or a more complicated coupling scheme leads to higher direct components of the inelastic-scattering cross-section of the first-excited state (table III of [6]). Furthermore, we have seen that the use of a low value of W leads to higher direct components indeed, but also to lower statistical components if the enhancement due to entrance and exit channels is neglected. Our estimate of this enhancement factor used by Konobeevskii and Popov is about 15%. Thus, the reason for the high inelastic scattering cross-sections is partly due to the use of a low W-value and partly due to the application of the inelastic enhancement due to entrance and exit channel correlations (HTWR-theory).

3.2. Analysis of Smith et al.

Smith et al. [9] have proposed a spherical 'regional' optical model to describe elastic-scattering and total cross-sections of target nuclei with Z = 39 to 51 at low-incident energies (0.8 to 4.5 MeV). The parametrization is essentially based on Argonne measurements of elemental cross-sections, including angular distributions of elastically scattered neutrons. Also s- and p-wave strength functions were considered in the fits. Only for Mo also some isotopic data were used. Inelastic scattering data have not been used explicitly in the fit.

The optical-model parameters contain A-dependent geometry parameters and isospin terms both in V and W. In addition there is an energy-dependent term in V and a cosine-shaped mass-dependent term in W. Since no explicit direct inelastic-scattering term has to be introduced the value of the imaginary strength W is quite high and is peaked at the mass range where large vibrational effects have been reported: near A ≈ 105. In other words: deformation effects have been included implicitly in the spherical optical-model potential by increasing W (quite opposite to the analysis of Konobeevski and Popov).

Evaluation of the work of Smith et al.

With this phenomenological spherical potential impressive fits are obtained over a large mass range of the total and (differential) elastic scattering cross-sections and of s- and p-wave strength functions. The question is how well the inelastic scattering cross-sections are predicted by this parametrization. Since the total inelastic-scattering cross-section is almost equal to the difference between total and elastic scattering cross-sections, this quantity should be predicted rather well. However, at high energies the excitation function of the first excited 2^+ state, containing a direct component, can never be reproduced from a pure statistical-model calculation. At low energies, where the total inelastic scattering cross-section is equal to the excitation function of the first excited state a good prediction is possible. However, since in this case we deal with the difference between two large numbers there is a large uncertainty which could be as high as 50% (see Section 2.4).

From our own statistical-model calculations with the potential of Smith et al. it is found that the calculated inelastic scattering cross-sections at low incident energies are indeed relatively high (compared to results from a global potential [6]). However, they are not as high as the measured data of Konobeevskii and Popov and also not as high as the measured elemental inelastic scattering cross-sections for natural Pd [9,10].

3.3. Present work

From the work reviewed in Sections 3.1. and 3.2. we conclude that improvements are needed in the theoretical description of inelastic scattering cross-section. Basically we agree with the method employed by Konobeevskii and Popov [6] to use the coupled-channel method in addition to the statistical model. However, we prefer not to include their experimental (n,n'γ) data into the fit, since we are interested in an independent prediction of inelastic scattering cross-sections. We also prefer not to use the HTRW-theory [11] in its version where the compound inelastic-scattering cross-section is enhanced by direct effects. The reason (apart from the absence of a computer code to perform these calculations) is that we would like to be conservative in the estimate of the inelastic scattering cross-section by adopting the standard practice of adding direct and compound effects incoherently (there is a large number of cases in other mass ranges where such calculations have been performed with success). Thus, a deformed optical model is used to calculate the total, shape-elastic, direct-inelastic, compound-formation cross-sections and transmission coefficients by means of the coupled-channels method, whereas the width-fluctuation corrected Hauser-Feshbach model is used to compute the compound cross-sections, taking care that the compound formation cross-section is consistent with that calculated by the coupled-channels calculation.

Evidently, the most difficult problem is to find a correct optical-model parametrization. The best approach would be to repeat the analysis of Smith et al. [9] using their experimental data set, but adopting a deformed optical-model potential. This is a very time-consuming exercise. It was thought to be more practical to use their regional optical-model parametrization as a starting point to deduce a new regional deformed optical-model parametrization. This procedure was followed in Appendix A2 [2] by reducing W and correcting for V. A further simplification was, since the quality of the fit by Smith et al. is quite good for the total and elastic scattering cross-sections and the s- and p-wave strength functions, to use the calculated values as "experimental data", rather than the original - less accessible - data.

With regard to the deformation parameters we have adopted the β-values of the (p,p') work of Cereda et al. [14] without any modifications. We have applied the values used in their coupled-channels analysis for the first-order vibrational model (0^+, 2^+, 3^-).

One of the results of the analysis described in Appendix A2 is a new regional deformed optical-model parametrization for use in coupled-channels and statistical-model calculations. This model parametrization describes the total and elastic scattering-scattering cross-sections and the s- and p-wave strength functions to about the same accuracy as the regional spherical optical-model parametrization of Smith et al. The advantage of the new parametrization is that collective effects are now explicitly accounted for. The differences with the calculated data of Smith et al. are mainly in the inelastic scattering cross-sections that have another shape (due to the direct component) and another magnitude.

The absolute values of the calculated inelastic scattering cross-sections are higher than those calculated with the spherical potential of Smith et al. and also higher than those of the current (JEF-1) evaluations. However, the new results are still below the measured data of Konobeevskii and Popov by about 15 to 20%. This difference is close to the error bars of ± 10 to ± 15% given in the figures of Ref. [6]. Note that the normalization error in the measurements is ± 7% [6].

It is difficult to judge the predictive value of our calculations. Since no experimental inelastic-scattering cross-section data were included in the fit, the results depend mainly on the data base of experimental total and elastic-scattering cross-sections. This gives an independent determination of the inelastic-scattering cross-sections. However, as was shown in Section 2.4, the uncertainty of such a prediction is at low energies quite high (difference of two large numbers). Still, our result shows that relatively high inelastic scattering cross-sections are possible and that it is not justified to neglect direct effects in the calculations.

Some critical notes

The energy range of the parametrization given in Appendix A2 is relatively small: from about 0.5 to 5.0 MeV. In this range no energy dependence for V and W has been introduced. The value for V in our parametrization is different from that of other potentials. In further work a more extended energy range with E-dependent V and W should be used, consistent with those of other potentials at high energies.

A further point of concern is that the elastic angular distributions calculated with our potential are less satisfactory. Probably further adjustment of the optical-model parameters is necessary to obtain optimal agreement. In our approach only the values of V and W were varied without changing the geometry parameters. For the purpose of the present study the exact prediction of angular distributions is of minor importance.

A rather simple first-order coupling scheme was used. For the prediction of inelastic scattering to other collective states a more complicated coupling scheme is needed. This may also slightly affect the inelastic scattering cross-sections to the first excited 2^+ state. The values of the deformation parameters were taken directly from (p,p') work. A small correction should be made to correct for the different radii used in (n,n') and (p,p'): the deformation length $\delta = \beta R$, where R is the radius of the real part of the potential should be approximately constant.

With respect to the statistical-model calculations we have not used the generalized transmission coefficients of the CC-calculations, but rather those from the spherical optical model of Smith et al. This is not a serious error since we have renormalized the compound cross-sections to agree with the compound-formation cross-section of the CC calculation.

We also did not apply the most modern statistical-model theories to account for the enhancement due to competition with direct cross-sections, i.e. we did not account for the correlations in the entrance and exit channels due to direct effects. These enhancements (at the cost of mainly the elastic-scattering cross-section) can be evaluated with the HTWR-approach [11] or with Moldauer's theory [12]. There is as yet little experience in the application of these theories. Sheldon and Chan [13] have reported some calculations on (n,n') cross-sections for Th-232 and U-238. In almost all cases appreciable enhancements were found in their application of HTRW-theory. However, in many cases the enhanced cross-sections were much larger than the measured data. Our preliminary conclusion from their work is that enhancements were needed, but that the use of HTWR-theory easily leads to overpredictions. Nevertheless more study is needed in this direction and our calculations may yield too low inelastic-scattering cross-sections. From comparison of our calculations with those of Konobeevskii and Popov who also used HTRW theory, we find an enhancement factor of about 1.15 in the compound inelastic scattering cross-sections. Such an increase if applied to the results of our calculations would lead to perfect agreement with the measured data.

Finally we recall that the omission of inelastic-scattering data in our fitting procedure was done on purpose, because we did not a-priori trust the experimental (n,n'γ) data. If validated experimental data on inelastic scattering are available they should of course be included in the fit. The easiest way to do this is to use experimental data at energies where the direct component dominates, i.e. at 4 to 7 MeV.

3.4. DWBA calculations

In Appendix A2 [2] we have also made some comments on DWBA calculations. First of all it is recalled that due to the large value of the deformation parameter β the DWBA method should not be applied. This is certainly true and is demonstrated in Fig. 9 of Appendix A2. We have also experienced that the results of DWBA calculations with high values of β depend very much upon the potential adopted.

Actually, three potentials are involved in a DWBA calculation: for the entrance channel, for the exit channel and for the interaction. For the entrance channel it seems logical to use the spherical optical-model parametrization that fits the total and (shape) elastic-scattering cross-sections. In our case this means that the regional spherical-optical model parametrization of Smith et al. [9] should be adopted for the potential of the entrance channel. If the same parametrization is used for the exit channel and for the interaction, the curve labelled 'DWBA direct' indicated in Fig. 9 of Appendix A2 is obtained for the direct part of the inelastic scattering cross-section of Ru-102 (excitation of the first 2^+ state). This curve is much too low compared to the results of the CC calculations.

On the other hand, if the potentials for the exit channel and for the collective form factors are taken from our CC parametrization, a rather good result is obtained (see curve labelled 'ADWA direct' in Fig. 9 of Appendix A2) although the shapes of the CC and ADWA curves are different at higher energies. This so-called asymmetric DWBA method has been applied by several authors [15-18] and seems to give better results, although there is not much theoretical justification.

We conclude that the DWBA method may give good results, but that one should be very careful in applying it if β is large. In such cases CC calculations are needed to check the validity. In general the ADWA method gives the best results.

For the combination of DWBA (or ADWA) results with those of a statistical-model calculation the total direct inelastic scattering cross-section has to be subtracted from the compound-formation cross-section and the compound cross-sections have to be redistributed accordingly. In this way the total and shape-elastic cross-sections are conserved but the compound-elastic component is decreased. This procedure is entirely analogous to the one we have used in Appendix A2 to combine the CC calculations with the statistical-model calculations. Thus, it is possible that the total inelastic-scattering cross-section is increased at low energies; at high energies the compound elastic cross-section vanishes and addition of DWBA or ADWA components merely leads to a redistribution of the total inelastic scattering cross-section over the various inelastic channels.

A more simple method of combining results of DWBA or ADWA calculations with those of statistical-model calculations is to add the direct components to the inelastic-scattering cross-sections and to subtract the total direct cross-section from the elastic scattering cross-section. This method conserves the total and e.g. the radiative capture cross-sections, but decreases the elastic scattering cross-section. Therefore, it should not be used if β is large or if the elastic-scattering cross-sections have been fitted to experimental data.

One may wonder why there is still a need for DWBA or ADWA calculations, in particular since a modern CC code running on a supercomputer is quite fast (in our work the very fast HETEROCLITE code [19] was used). There are some practical reasons:

1. The coupling scheme is not always known, whereas quite often there are effective β values known from (p,p') analysis with a DWBA method.
2. It is still cheaper to run DWBA or ADWA than CC if the coupling scheme is complex (with modern super computers CC calculations can be quite fas).
3. Often the CC method is not integrated in the code package used to perform evaluations (integration of CC in the evaluation code system should be recommended).

Therefore in the actual evaluation it may be practical to apply the asymmetric DWA method for moderately-coupled states, whereas for the low-lying strongly-coupled states the CC method should be applied if possible [18].

3.5. Request for experimental data

From the above-mentioned experimental and theoretical arguments it seems clear that the measured (n,n'γ) data by Konobeevskii and Popov [6] are probably correct, or at least that there are no reasons to doubt that the inelastic-scattering cross-sections at low incident energies are quite high for excitation of the first-excited states in the even-mass Ru and Pd isotopes. What is required is an independent check of their measurements for one or two Ru or Pd isotopes. Therefore a request has been forwarded to the Central Bureau of Nuclear Measurements (CBNM) of the European Community in order to perform such measurements at energies in the range from threshold up to about 5 MeV. Of particular interest are the data at the maximum of the excitation curve, near 1 MeV and data at 4 to 5 MeV, where the direct component dominates.

In a discussion at CBNM (Geel, Belgium) with Dr. H. Liskien it was found that with respect to the enriched target material the isotopes of Pd-106 and Pd-108 were good candidates. The measurements could best be performed with the Van de Graaff generator, using a variable mono-energetic neutron source. Both outgoing neutrons and emitted gamma-rays could be detected by means of a time-of-flight technique and Ge(Li) detection, respectively. These two independent techniques could in principle be combined by means of coincident event detection. This last-mentioned possibility may be necessary for Pd-106 from which the inelastic γ-rays have an energy of 511.86 keV, which is very close to the 511 keV of annihilation radiation. Because the angular distribution of emitted neutrons is not isotropic, measurements should be made at various angles. Also the angular distribution of the emitted γ rays are anisotropic, but their distribution probably can be estimated by assuming pure E2 radiation.

There is experience at CBNM with inelastic neutron measurements from the Li-7(n,n') reaction at incident energies from about 1.1 to 2.3 MeV. It is difficult to extend this energy range. There is no explicit experience with (n,n'γ) measurements at CBNM.

The experimental facilities at CBNM allow an independent determination of the inelastic-scattering cross-sections with two techniques at energies between 1.1 to 2.3 MeV. Unfortunately, a measurement at higher incident energies, where the direct component dominates, is not possible with the above-mentioned set-up. From our study of the angular distribution of the emitted neutrons it is clear that at the low incident energies up to about 2.5 MeV there is not much forward-backward peaking, see Figs. 10 and 11 of Appendix A2 for the direct and compound parts, respectively. Thus we will not obtain specific information about the direct component. Nevertheless, the total excitation curve will be measured and this is what is needed in the fission-product evaluations.

It is expected that some first results might be available at the end of next year.

4. SCHEME FOR CORRECTIONS OF THE JEF DATA FILE

4.1. New evaluations

For new JEF-2 evaluations in the fission-product mass range we recommend to use the CC-method combinated with statistical-model calculations, if possible by taking into account correlations between entrance and exit channels (when a code becomes available for this purpose). Our regional optical-model parametrization for CC calculations (Appendix A2) could be used as a starting point for evaluations of light fission-fragment cross sections, cf. Sect. 3.3. At higher energies where there are more states with sometimes complicated coupling schemes one may have to resort to ADWA calculations for moderately coupled states as described in Sect. 3.4.

At ECN we plan to modify the forthcoming new evaluation for Ru-102 according to these lines. Some additional work is needed to extend the regional deformed optical-model potential from about 5 MeV to 20 MeV and to insert an output option into the CC code to produce ENDF-format.

4.2. Existing evaluations

For the update of the bulk of fission-product evaluations in JEF-1 it is at present not practical to perform large-scale CC calculations (cf. Sect. 3.4). Instead we recommend to perform only a number of CC calculations for those nuclei with states having high deformation parameters and to adopt the DWBA method (Sect. 3.4) for the bulk of the calculations. If possible the asymmetric version of DWA should be used (ADWA) and adjustments should be made to agree with the results of CC-calculations or with the experimental data (e.g. by tuning the β-parameters).

Although we did not find serious reasons to doubt the measurements of Konobeevskii et al. [6] it is probably wise to be conservative as long as no experimental verification has been made (Sect. 3.5). Therefore, it is recommended to take into account a (lower) error margin of -10 to -15% on the data of Konobeevskii and Popov and certainly not to exceed the measured data.

The developed regional deformed optical-model parametrization (Appendix A2) could be used for the light fission fragments. For the heavier fragments the parametrizations given by McEllistrem et al. [20] and by Houat et al. [21] or by Shamu et al. [22] could be tried. These CC parametrizations for Sm and Nd are based upon experimental data at relatively high energies, but may work also at lower energies (possibly some modifications are needed). For the deformation parameters results of (n,n') or (p,p') measurements can generally be adopted.

It is suggested to use the fast HETEROCLITE code [19] for the CC calculations and the DWARF code system [23] for the DWBA/ADWA calculations. This lastmentioned code system, based upon the well-known DWUCK code contains simplified input and output options for neutron inelastic scattering. Recently, a possibility to produce output in ENDF format has been added.

We propose to add the direct components of the inelastic scattering cross-sections in the most simple way (without renormalizations) to the discrete inelastic compound cross-sections given on file 3 (MT = 51 to 90). The sum of all direct components should be added to the total inelastic-scattering cross-section (MT = 4) and subtracted from the elastic-scattering cross-section (MT = 2) if the corrections are marginal. If the corrections are large, subtraction from the elastic scattering cross-section is not justified. In such cases we propose to renormalize all major cross-sections, i.e. elastic-scattering (MT = 2), inelastic to continuum (MT = 91) and the (n,2n) cross-section (MT = 16). The total inelastic scattering cross-section should be reconstructed from the sum of all components (MT = 51 through 91). The total cross-section remains the same, like other (small) cross-sections e.g. those for (n,γ), (n,p), (n,α), etc. These additions and renormalizations can be performed with the manipulation code CRECTJ5, available from the NEA Data Bank.

With respect to the angular distributions (file 4) we note that for most fission-product evaluations at present isotropy in the center-of-mass system is assumed for the discrete-inelastic scattering cross-sections. The DWBA/ADWA calculations only give the angular distributions (in the c.m. system) of the direct component. Therefore, in order to store angular distributions a constant angular distribution equal to the compound cross-section divided by 4π has to be added. If the angular distributions are stored in the reduced Legendre-polynomial representation (with zero-order coefficient normalized to 1) this means that the non-zero-order coefficients need to be multiplied with the ratio of the direct over the total excitation cross-section. We note that the update of angular distributions is of second priority.

The nuclides that need to be updated are the even-mass nuclides with states having large deformation parameters. With first priority the even-mass isotopes of Ru, Pd, Sm and Nd need to be updated. Note that in this work we have not considered direct effects on the cross sections of odd-mass nuclides, because at low energies there are much more states in general, whereas for the even-mass nuclides it is usually the first-excited (collective) state that dominates the low-energy range.

5. CONCLUSIONS

The main conclusion from Sect. 2 is that from experimental evidence (see also Appendix A) it follows that in particular for the even-mass isotopes of Ru, Pd, Nd, and Sm the evaluated inelastic scattering cross-sections are much too low at low incident energies. The available experimental data of Konobeevskii and Popov [6] for the light fragments are quite high, but there is no indication that these data are systematically in error. It is argued that from an independent measurement on natural Pd [10] these data are confirmed to within 15%. For the heavier fragments there is some information on direct effects at relatively high energies only. More measurements are in general required.

From the theoretical analyses described in Sect. 3 (and Appendix A2) we confirm that direct effects can be quite large in low-energy inelastic scattering. In fact our own calculations show that the inelastic scattering cross-sections of light fission fragments become rather close to the very high experimental data of Konobeevskii and Popov [6]. The preferred method for theoretical analysis is the CC method in combination with the statistical model. Due to correlations between entrance and exit channels the statistical contribution is somewhat uncertain (too low predictions). There is as yet no documented code available to perform these statistical-model calculations using the most modern theory [11,12]. From our theoretical analysis a new "regional" deformed optical-model parametrization has resulted (Appendix A2). This parametrization could be used to improve all inelastic-scattering cross sections of the light fission-product nuclides. For the heavier fragments some potentials have already been suggested in literature [20-22].

In order to check our conclusions it is quite important to perform new measurements. Therefore a detailed request has been made for new data (Sect. 3.5).

A scheme for corrections of the existing JEF-1 fission-product data file has been presented in Sect. 4. This scheme is meant for a fast revision of the bulk of the fission product cross-sections and therefore approximate methods are recommended. For new evaluations the CC method in combination with modern Hauser-Feshbach theory including the effect of entrance-exit channel correlations is needed. Such an option could perhaps be added to an existing CC code.

The importance of the present work for the prediction of the reactivity effect of fission products in a fast power reactor follows from the discussion in Sect. 2.1, where the target accuracy for the lumped effect of inelastic scattering was set equal to ±15%. We estimate that this accuracy is not reached at present due to the systematical neglect of direct effects in low-energy inelastic scattering.

There is still a large amount of work to be performed. We mention: the experimental efforts needed to validate existing $(n,n'\gamma)$ data, theoretical efforts to validate the most modern statistical-model theories for the present applications, study of the ADWA method, study of direct effects in odd-mass fission-product nuclei, improvements in the parametrization of deformed "regional" models, computational improvements to improve the existing computer codes and last but not least the revision of the existing data files.

6. REFERENCES

[1] H. Gruppelaar and H.A.J. van der Kamp, Inelastic scattering cross-sections in the fission-product mass range, Specialists Mtg. on the Use of Optical Model for the Calculation of Neutron Cross-Sections below 20 MeV, Nov. 1985, Paris, NEANDC-22"U", p. 221 (1986), reproduced in Appendix A1.

[2] G.J.M. Janssen, H. Gruppelaar and J.M. Akkermans, Regional potential for coupled-channel calcualtions of neutron scattering cross-sections of light fission products, ECN-87-106, Restricted Distribution Report, Netherlands Energy Research Foundation, reproduced in Appendix A2.

[3] A.J. Janssen, H. Gruppelaar, H.A.J. van der Kamp, N. Karouby-Cohen, L. Martin-Deidier, G. Rimpault and M. Salvatores, Integral test of JEF-1 fission-product cross-sections, ECN-176 (1985), Netherlands Energy Research Foundation, see also Proc. Int. Conf. on Nuclear data for Basic and Applied Science, Santa Fe, May 1985, p. 1537, Gordon and Breach Publishers, New York (1986).

[4] R.J. Heijboer and A.J. Janssen, Status of pseudo fission-product cross-sections for fast reactors; sensitivity study for sodium void effect, Proc. Spec. Mtg. on Neutron Cross-Sections of Fission Product Nuclei, December 1979, Bologna, NEANDC(E)209"L" (1980), p. 375.

[5] L.I. Govor, A.M. Demidov and M.M. Komkov, Sov. J. Nucl. Phys. 29 (1979), p. 731.

[6] E.S. Konobeevskii and V.I. Popov, Sov. J. Nucl. Phys. 33 (1981), p. 7.

[7] A.V. Ignatyuk, Obninsk USSR, private communication 1986.

[8] A.B. Smith, P.T. Guenther and J.F. Whalen, Nucl. Phys. A244 (1975), p. 213 and ANL/NDM-7 (1974) Argonne National Laboratory.

[9] A.B. Smith, P.T. Guenther and J.F. Whalen, Nucl. Phys. A415 (1984), p. 1.

[10] A.B. Smith, A model for fission-product calculations, Proc. NEANDC Topical Conf. on Measurements and Evaluations of Nuclear Data and Decay Heat for Fission Products, JAERI-M-84-182 or NEANDC(J)100/U, p. 61.

[11] H.M. Hofmann, J. Richert, J.W. Tepel and H.A. Weidenmüller, Annals of Phys. 90 (1975), p. 744.

[12] P.A. Moldauer, Phys. Rev. C12 (1975), p. 744.

[13] E. Sheldon and D.W.S. Chan, Evaluation of (n,n') scattering cross-sections from 0.8 to 2.5 MeV for higher collective bands of Th-232 and U-238 in "standard" (CN+DI) and "unified" (Weidenmüller S-matrix) formalisms, Proc. Spec. Mtg. on Fast Neutron Scattering on Actinide Nuclei, Paris, Nov. 1981, NEANDC-158"U", (1982), p. 169.

[14] E. Cereda et al., Phys. Rev. C26 (1982), p. 1941.

[15] K.I. Kubo and P.E. Hodgson, Nucl. Phys. A366 (1981), p. 320.

[16] G.R. Satchler, Direct Nuclear Reactions, Claredon Press, Oxford (1983), p. 563.

[17] P.E. Hodgson, The Neutron Optical Model in the Actinide Region, Proc. Spec. Mtg. on Fast Neutron Scattering on Actinide Nuclei, Paris, Nov. 1981, NEANDC-158"U" (1982), p. 69.

[18] T. Ohsawa, Combined Use of Coupled-Channel, DWBA and Hauser-Feshbach, Proc. of the 1986 Seminar on Nuclear Data, Japan, NEANDC(J) 123/U (1987), p. 320.

[19] Ch. Lagrange, HETEROCLITE code, private communication, Service de Physique Nucléaire, Centre d'Etudes de Bruyeres-le-Châtel, Montrouge, France (1986).

[20] M.T. McEllistrem et al., Phys. Rev. C15 (1977), p. 927.

[21] G. Houat et al., Phys. Rev. C20 (1970), p. 78.

[22] R.E. Shamu, E.M. Bernstein and J.J. Ramirez, Phys. Rev. C22 (1980), p. 1857.

[23] J.M. Akkermans, DWARF: DWBA calculations of neutron inelastic scattering for evaluation purposes, internal report, Netherlands Energy Research Foundation (1983).

APPENDIX A1.

INELASTIC SCATTERING CROSS-SECTIONS IN THE FISSION-PRODUCT MASS RANGE

H. Gruppelaar and H.A.J. van der Kamp
Netherlands Energy Research Foundation, ECN,
Petten, The Netherlands

ABSTRACT

Part of the reactivity contribution of fission products in fast reactors is due to inelastic scattering. Integral experiments in various fast facilities indicate that the inelastic scattering cross sections on the present fission-product nuclear data files are systematically too low for many even-mass nuclides. Possible reasons for this discrepancy are discussed. The neglect of direct-collective effects in the current evaluations seems to be one of the important omissions. This is confirmed by some recent differential data measured at low incident neutron energies. More experimental data are needed to study these effects. Corrections of the present nuclear-data files using DWBA or coupled-channels calculations are required for the next generation of nuclear data files.

1. INTRODUCTION

For the prediction of the reactivity effect of the lumped fission-product mixture in fast power reactors the cross sections of the fission-product files of recent evaluations such as JEF-1 and ENDF/B-V are needed. About 15% of this effect is due to inelastic scattering. Unlike the well-tested capture cross-section data, the status of the inelastic scattering data has not been reviewed in much detail. Therefore, this paper gives some discussion on this subject.

From a recent integral-data test [1,2] of JEF-1 fission-product cross sections using STEK integral data, it follows that there are systematic differences between evaluated and measured reactivity effects in the reactor cores with the hardest neutron flux spectra (STEK-500, -1000) for nuclides with even numbers of Z and A. These reactivity worths consist of a large capture component and a somewhat smaller scattering component of opposite sign. Correcting the total worths for scattering gives "capture reactivity worths" which for most even-mass nuclides are below the calculated values (in absolute values). Possible reasons for this effect could be:

(1) Systematic errors in the measured quantities or in the flux- and adjoint flux spectra of STEK.
(2) Systematic errors in the evaluated capture cross sections (too high values).
(3) Systematic errors in the evaluated inelastic-scattering cross sections

(too low values).

We assume that possibility (1) is less likely, since we see no systematic differences in the soft-spectrum cores (STEK-4000, -3000) and there are also no systematic problems for odd-mass nuclides. However, we cannot exclude that there are systematic errors in the adjoint-flux spectra. The second possibility has been checked by inspecting integral data obtained by activation or transmutation. There is no clear systematic effect visible in the C/E-values for these data given in Refs. [1,2] for the even-mass nuclides. However, we cannot exclude that possibility (2) plays a role, although in the current fission-product evaluations there has been a great deal of attention to the capture cross section. The last possibility (3) will be inspected in this paper. Since the evaluation of the capture cross section has been the main goal to obtain the present evaluated-data files, it may well be that there are some deficiencies in the inelastic-scattering cross sections on these files.

2. EVALUATION METHODS

According to our knowledge almost all evaluations in the fission-product mass range are based upon optical-model and statistical-model calculations of the Hauser-Feshbach type. In a few cases deformed optical models have been used, but for most materials a spherical optical model has been adopted. In all recent evaluations the Hauser-Feshbach theory with a width-fluctuation correction has been applied. Generally, no direct components have been included from DWBA or coupled-channels calculations. Also precompound effects have been neglected and at high energies the evaluation of (n,2n) is usually based upon simple approximations or completely neglected. The following effects could cause systematic errors:

(1) Missing levels;
(2) Width-fluctuation correction;
(3) Optical-model choice;
(4) Neglect of direct-collective excitation;
(5) Neglect of precompound effects;
(6) Neglect of (n,2n), (n,3n), (n,pn) cross sections.

2.1. Missing levels

At relatively low neutron energies the inelastic scattering cross section is represented by excitation functions describing the inelastic scattering to the first 10 to 30 levels. For this reason the level schemes of the fission-product target nuclei need to be known quite well, at least upto the first 10 to 15 levels. Missing levels may cause a too low inelastic-scattering cross section. Evaluations based upon old level schemes could therefore be systematically too low. The effect of different level schemes has been studied by Kikuchi et al. [3]. In general, many evaluations are based upon a poor level scheme with gaps and too few levels. This often leads to relatively low inelastic-scattering cross sections at low energies.

2.2. Width-fluctuation correction

In all recent evaluations the width-fluctuation correction has been applied. This correction can be quite large and may reduce the "pure" Hauser-Feshbach cross section by 50% at low-incident energies. There are a number of different approaches to calculate this correction. They have been summarized in Ref. [4]. Some recent refinements for the parametrization of the various expressions reviewed in Ref. [4] have been given in Refs. [5] and [6]. The important parameter is the "number of degrees of freedom" ν, occurring in work of Moldauer [5] or the "elastic enhancement factor" w introduced by Tepel et al. [6]. In the oldest evaluations ν=1 or w=3 has been adopted. In more recent evaluations, slightly higher values for ν or correspondingly lower values for w were adopted, depending upon the transmission coefficients. This may increase the inelastic cross section by 5 to 10% at low energies. In the RCN-2, -3 evaluations we have assumed ν=1 (w=3) for incident energies upto the threshold of the second-excited state and we have used the method of Tepel et al. in its most simple form at higher incident energies.

In the continuum the width-fluctuation factor is usually neglected. In the RCN-evaluations we approximate this by assuming an elastic enhancement factor of w=2, corresponding to the method of Tepel et al. [6]. This reduces the inelastic scattering in the continuum (above energies of E_{cut}≈2 to 3 MeV). At ENEA the method of lumped channels [4] is used, leading to a similar, but somewhat smaller reduction. The combined effect may be that the ENEA evaluations of inelastic scattering are about 5% higher than the RCN-3 evaluations (when all the other parameters are the same).

Altogether, we do not believe that in the recent evaluations the different methods of calculating the width-fluctuation factor leads to differences much larger than 5 to 10%. We note that recently there has been further progress in Hauser-Feshbach theory, see the review by Fröhner [25].

2.3. Optical-model choice

At energies above about 2 MeV the total inelastic-scattering cross section becomes quite close to the compound-formation cross section. Therefore, it directly depends on the optical-model parameters. From the work of Kikuchi et al. [3] it follows that differences of 20% to 30% are no exception. Since quite often "global" optical-model potentials have been used, systematic effects may occur. Generally the ENDF/B values are quite low for masses below A=147 [3]. This also follows from graphs in Ref. [7].

In almost all evaluations a spherical optical model was used, in spite of the large deformation effects observed for many nuclides. This is perhaps not too serious when the optical-model parameters are fitted to the total and elastic-scattering data for each individual nucleus. However, since global models have often been applied, deviations may occur.

Altogether, it seems that systematic differences could at least be partly caused by the use of global optical models in the calculations. For the nuclides given in Ref. [3] with masses below 145 the ENEA values are on the average 25% higher than the ENDF/B-IV (or -V) values (averages over fast-reactor spectrum for nuclides given in [3]). There are no clear odd-even effects.

2.4. Neglect of direct-collective excitations

To our knowledge there are no fission-product evaluations in which direct-collective inelastic excitations have been included. Until recently, it was assumed that these excitations are relatively small compared to the compound-nucleus contribution, at least at low incident energies. However, from experimental work e.g. from (n,n'γ)-measurements at low-incident energies [8-13] it became clear that these components can be quite large, not only for the stably-deformed rotational nuclei, but also for the dynamically-deformed vibrational nuclei. In a large number of cases [8-13] it was found that in paricular the cross section for excitation of the first-excited state with spin and parity 2^+ in even-even nuclei are strongly enhanced by a direct-collective component. Enhancements of a factor of 1.5 or more are no exception. In Sects. 3,4 we further discuss these cases. It seems that in future fission-product evaluations these effects should be accounted for. Theoretical treatment of these processes means the use of a deformed optical model and coupled-channels calculations. A simple approximation could perhaps be obtained by performing DWBA calculations. However, since the magnitude of direct and compound processes are comparable, interference effects are possible. These can be treated in principle with more sophisticated models such as those of Moldauer et al. [14] or Hofmann et al. [15]. Examples of such treatments are given in Refs. [10,12] and - for actinide nuclei - by Sheldon [16]. Recently, a more simple method using DWBA and experimental data has been suggested [17].

2.5. Neglect of precompound effects

In all existing fission-product evaluations the precompound effects have been neglected. These effects play a role above about 5 MeV incident energy, and therefore are of relatively small importance to reactivity effects in fission reactors. Moreover, the total inelastic scattering cross section below the threshold for (n,2n) is not very sensitive to precompound effects. It is mainly the energy distribution of the scattered neutrons that is affected ("harder" spectrum). Above the (n,2n)-threshold the cross section for inelastic scattering becomes much larger at the account of the (n,2n) cross section, see Sect. 2.6. For the reactivity effect in fast reactors, the effects of including precompound processes are probably quite small.

2.6. Neglect of (n,2n), (n,3n), (n,pn) cross sections

For fission-product nuclides the thresholds for the above-mentioned reactions are quite high in energy. Therefore, it is not necessary to evaluate their cross sections with great accuracy. However, neglecting the (n,2n)-reaction as has been done in a number of evaluations seems a too crude approximation. For nuclides with low (n,2n)-thresholds this neglect would mean that the reactivity worth due to the first energy group of the ABBN-scheme (6.5 to 10.5 MeV) is about 50% too low. We conclude that (n,2n) cross sections should be included on evaluated data files for fission products.

3. DIRECT-COLLECTIVE EXCITATIONS

In the fission-product mass-range most of the nuclides with $A<145$ are spherical, whereas the nuclides with higher masses are deformed. Therefore, the level scheme of the lighter fission fragments may show vibrational states, and the heavier fragments rotational bands. A measure for collective effects is the parameter β_2, the quadrupole deformation parameter that can be derived from the reduced electromagnetic transition probability (BE2) from the ground to the first-excited 2^+ state of even-even nuclides [19]. A parametrization of these parameters for $A>140$ has recently been given by Jänecke [20]. From these references we expect the following for the important fission products (see Table I):

(1) large to very large effects for the heavy-mass isotopes of Mo, Ru and Pd (vibrational character);
(2) very large effects for the heavy-mass isotopes of Nd, Sm, Gd (vibrational effects for low-mass isotopes of Nd, Sm; rotational effects for heavier

masses).

For the isotopes of Nd and Sm it is well-known that deformation effects need to be considered in the evaluation of total, elastic and inelastic-scattering cross sections [20-22]. However, direct effects in inelastic scattering have been neglected in the current evaluations, because it was assumed that these effects are relatively small at low-incident neutron energies. From a measurement of Andreev et al. [8] of ^{144}Nd(n,n'γ) cross sections, it became clear that direct effects are quite important already at E=2.75 MeV (the measured cross section for the first-excited state was about twice as large as the calculated cross section based upon the statistical model). Similar findings were reported by Coope et al. [9] for inelastic scattering on ^{148}, ^{150}, ^{152}Sm at E=2.47 MeV.

After these preliminary indications that direct effects may also be quite important at low neutron energies, Govor et al. [11] made a comparison of experimental and calculated integral cross sections ("populations") of levels of even-even nuclei with 28<A<152 excited in inelastic scattering of fast reactor neutrons (effective energy: 0.6-1.5 MeV). This work showed that the experimental data were 1.5 to 2.0 times greater than calculated with the statistical model for excitation of the first 2^+-states of isotopes with large dynamic deformations and high anharmonicity of vibrations and a similar excess of 1.5 to 3.0 times for most 4^+ and 6^+ levels of nuclei with 90<A<130 [11]. The greatest enhancements were found for ^{108}, ^{110}Pd, ^{152}Sm (restricting ourselves to important fission products).

At about the same time differential measurements were reported of (n,n'γ) on Ge and Se isotopes from threshold up to about 1.5 MeV. Again, the measured data were much larger than expected on the basis of the statistical model [10], in agreement with the findings of Govor et al. [11]. More recently this was also confirmed by Konobeevskii and Popov [12] for Mo, Ru, Pd isotopes. No significant effects were seen for the Cd and Sn isotopes (low β).

Altogether, there seems considerable evidence that direct effects should be included to calculate inelastic scattering cross sections already at low incident energies. The theoretical treatment of these processes in the quoted Russian papers [10,12] is based upon the HTRW-approach [15]. A similar method has been developed by Moldauer [14] and has been applied by Sheldon [16]. In both approaches the initial step in the calculations is the evaluation of the S-matrix using the coupled-channels method for obtaining the direct part of the cross section. The fluctuating part cannot simply be derived from the width-fluctuation corrected Hauser-Feshbach expression that is strictly valid only in the absence of direct components. In fact, the calculation is much more involved [16]. The approximation of using the H.F. formula with WFC is not justified when the number of open channels that are strongly coupled by direct reactions is small. In other cases the direct and H.F. parts could be added incoherently. We note that in this approximation the "generalized" transmission coefficients should be used to calculate the H.F. parts. A further approximation is to calculate the direct part from the DWBA model, which is allowed only when the coupling of states is relatively small, i.e. for small values for β_2. Still, this model may provide a first estimate of the effects (see next section: Ru isotopes). It could also be used in combination with adjustments to experimental data as suggested by Hodgson [17].

4. TEST OF JEF-1 CROSS SECTIONS

In the following we describe a first check of the JEF-1 fission-product file on possible direct effects in low-energy inelastic scattering to the first 2^+ states in even-even nuclei.

4.1. Zr isotopes

Not yet fully checked, but effects are expected to be smaller than for the Mo isotopes. From work at Argonne [23] we see that the statistical model is quite capable to reproduce the measured data. See, however, Ref. [9], Fig. 10, ^{94}Zr.

4.2. Mo isotopes

The available measurements for low-energy neutron scattering [12,24] on ^{96}, ^{98}, ^{100}Mo have been plotted in Fig. 1, together with various recent evaluations. We conclude that all evaluations, but in particular the ENDF/B-V evaluations are systematically too low. Enhancement factors of 1.2 to 2.0 are needed. Please note that the Argonne data [23] are consistent with the Russian measurements [12].

4.3. Ru isotopes

Fig. 2 displays the experimental [12] and evaluated data for ^{102}Ru and ^{104}Ru. The evaluations need to be increased by almost a factor of 2.0, in agreement with the large values of β_2 for these nuclides (0.264 and 0.288 respectively). A DWBA calculation with β=0.264 has been performed for ^{102}Ru. Indeed, the result is much better (Fig. 2). We note that the remaining difference could very well be ascribed to width-fluctuation effects: using the Tepel correction [6] one finds excellent agreement. The increase in scattering effect due to direct effects of the 2^+ and 4^+ states is estimated to be 16% in the STEK-cores. However, the evaluation seems also much too low in the continuum range [3]. Altogether we expect an increase of about 36% in the inelastic-scattering contribution of the reactivity worth in STEK. This improves the C/E-ratio of the capture reactivity effect by about 27%. We conclude that for the Ru isotopes revisions in the inelastic-scattering cross section are very much wanted and that these effects may help to reduce the discrepancy between measured and calculated reactivity worths.

4.4. Pd isotopes

For ^{106}, ^{108}, ^{110}Pd the experimental [12] and evaluated cross sections for excitation of the first 2^+ state are given in Fig. 3. Again, large enhancement factors are observed, in agreement with the large values for β_2 (0.25-0.29). It is clear that revisions are needed.

4.5. Cd, Sn, Te isotopes

For these nuclides the values of β_2 are much smaller. From the work of Konobeevskii et al. [12] it is seen that the usual statistical model gives reasonable good predictions, except for ^{122}Te and ^{124}Te that have still large β-values (0.18, 0.17 respectively). However, these are unimportant fission products. We have not checked the evaluations for these nuclides.

4.6. Xe, Ba, Ce isotopes

The β_2 values for these isotopes are quite small (<0.15) for the lighter Xe isotopes, which are unimportant fission products. We don't expect large enhancements of the inelastic-scattering cross sections. This has been checked by Govor et al. [11] for the isotopes of Ba and Ce.

4.7. Nd isotopes

For these nuclides the β_2-values rise from 0.10 (^{142}Nd) to 0.28 (^{150}Nd) as a function of neutron mass. We refer here to Refs. [21,22] for results at relatively high incident neutron energies and to Ref. [8] for (n,n'γ)-measurements on ^{144}Nd at 2.75 MeV, where large enhancements were found for excitation of the lowest 2^+ and 4^+ states. There are no data known to us near threshold energies. In Ref. [9] it was shown that the low-lying 2^+, 4^+ and 3^- states in ^{146}Nd are strongly excited at 2.47 MeV, with compensating effects for the excitation of other states.

4.8. Sm isotopes

For these transitional nuclides the excitation to the first 2^+ state can be described by the vibrational model for the lowest masses and by the rotational model for the highest masses [20,22]. At 2.47 MeV large effects have been observed in the (n,n'γ)-reaction on ^{148}, ^{150}, ^{152}Sm [9]. No data are known to us near threshold energies. We note that for ^{154}Sm the first 2^+-state has a very low excitation energy of 82 keV. It is therefore difficult to separate it from elastic scattering in experiments. See also Ref. [11].

4.9. Gd, Dy, Er isotopes

Very large deformations have been observed for these nuclides. Their effects on inelastic scattering cross sections remain to be investigated.

5. CONCLUSION

We have made a first attempt to check the evaluations of inelastic-scattering cross section of fission-product data files. This study was motivated by the systematic effects observed in reactivity worths measured in STEK (Sect. 1). Possible systematic effects in the evaluation methods were investigated in Sect. 2. Special attention was given to the neglect of direct-collective excitations at relatively low neutron incident energies (Sect. 3). A preliminary comparison between experimental and evaluated data has been presented in Sect. 4. It was found that in particular for the Ru, Pd, Nd and Sm isotopes the evaluated cross sections need to be increased with direct components for excitation of the first 2^+ (and higher collective) states. This comparison is still fragmentary and needs to be completed. There are indications (Sect. 4.3 and [1,2]) that the observed deficiencies may help to reduce the discrepancies between measured and calculated reactivity worths. Further evaluation work is needed to check these indications. Another, perhaps more important question, deals with the accuracy of the lumped inelastic-scattering cross sections of pseudo fission-products and the reactivity effect due to inelastic scattering in a fast power reactor [2] that may give a contribution of about 15%. We hope to consider these points in a follow-up study.
Finally it is mentioned that more experimental inelastic-scattering data are needed, in particular for cross sections at the lowest incident energies.

We thank Dr. A.J. Janssen for his evaluation of reactivity-worth measurements.

REFERENCES

[1] A.J. Janssen, H. Gruppelaar, N. Karouby-Cohen, L. Martin-Deidier, G. Rimpault and M. Salvatores, Integral test of JEF-1 fission-product cross sections, ECN-176 (1985).

[2] Ibid, Int. Conf. on Nuclear Data for Basic and Applied Science, Santa Fe, May 1985.

[3] Y. Kikuchi et al., Neutron cross sections of 28 fission-product nuclides adopted in JENDL-1, JAERI-1268 (1981).

[4] H. Gruppelaar and G. Reffo, Some properties of the width fluctuation factor, Nucl. Science and Eng. 62 (1977), p. 756.

[5] P.A. Moldauer, Statistics and the average cross section, Nucl. Phys. A344 (1980), p. 185.

[6] J.W. Tepel, H.M. Hofmann and M. Herman, Improved formulas for compound nucleus cross sections, Proc. Int. Conf. on Nuclear cross sections for Technology, Knoxville (1979), NBS-SP594 (1980), p. 762.

[7] A. Montaguti, G.C. Panini and M. Vaccari, Multi-group sections for 63 fission-product nuclei from different nuclear data files, RT/FI(78)16, (1978).

[8] E.A. Andreev, V.K. Basenko and S.P. Sit'ko, Excitation of ^{144}Nd by dd neutrons, Sov. J. Nucl. Phys., 23 (1976) 6.

[9] D.F. Coope et al., Strong collective excitations in low-energy neutron scattering from transitional nuclei, Phys. Rev. C16 (1977) 2223.

[10] V.P. Efrosinin, R.M. Musaelyan and V.I. Popov, Intermediate structure in the inelastic scattering of low-energy neutrons at A-70-80, Sov. J. Nucl. Phys. 29 (1979) p. 326.

[11] L.I. Govor, A.M. Demidov and M.M. Komkov, Cross sections for the excitation of levels in the (n,n'γ) reaction in spherical even-even nuclei with 28<A<152, Sov. J. Nucl. Phys. 29 (1979), p. 731.

[12] E.S. Konobeevskii and V.I. Popov, Excitation of collective states in inelastic scattering of low-energy neutrons in the 3p-resonance region, Sov. J. Nucl. Phys. 33 (1981), p. 7.

[13] V.M. Bychkov et al., The contribution of direct and statistical reaction mechanisms during fast neutron scattering at low-lying levels of light and medium nuclei, Fiz. Ehlem. Chastits At. Yadra 14 (1983), p. 2, translated by IAEA, Vienna, INDC(CCP)-217/LI (1983).

[14] P.A. Moldauer, Direct effects on compound cross sections, Phys. Rev. C12 (1975), p. 744.

[15] H.M. Hofmann, J. Richert, J.W. Tepel and H.A. Weidenmüller, Direct reactions and Hauser-Feshbach theory, Annals of Physics 90 (1975), p. 403.

[16] E. Sheldon, Level excitation data for faste neutron scattering on actinide nuclei calculated with the unified statistical S-matrix formalism, Proc. Int. Conf. on Nuclear data for Science and Technology, Antwerp, 1982, Reidel, Dordrecht (1983), p. 518.

[17] P.E. Hodgson, The neutron optical model in the actinide region, Prof. of Specialists' Mtg on Fast neutron scattering on actinide nuclei, NEANDC-158"U", (1981), p. 69 and private communication.

[18] P.H. Stelson and L. Grodzinds, Nuclear transition probability B(E_2) for $0^+_{g.s.} \rightarrow 2^+_{first}$ transitions and deformation parameter β_2, Nuclear Data A1 (1965), p. 21.

[19] J. Jänecke, Simple parametrization of nuclear deformation parameters, Phys. Lett. 103B (1981), p. 1.

[20] M.T. McEllistrem et al., Deformation effects in neutron scattering from the Sm isotopes, Phys. Rev. C15 (1977), p. 927.

[21] G. Houat et al., Optical potential and nuclear deformation for even Nd isotopes from fast neutron scattering, Phys. Rev. C20 (1970), p. 78.
[22] R.E. Shamu, E.M. Bernstein and J.J. Ramirez, Effects of deformation on neutron total cross sections of even-A, Nd and Sm isotopes, Phys. Rev. C22 (1980), p. 1857.
[23] A.B. Smith and P.T. Guenther, Fast-neutron scattering cross sections of elemental zirconium, ANL/NDM-69 (1982).
[24] A.B. Smith, P.T. Guenther and J.F. Whalen, Nucl. Phys. A244 (1975), p. 213 and ANL/NDM-7 (1974).
[25] F.H. Fröhner, Int. Conf. on Nuclear Data for Basic and Applied Science, Santa Fe, May 1985.

Table I Deformation parameters in even-even fission-product nuclei*

Isotopes	β_2 range	Character	Comment
Zr	<0.1	vib.	small effect
Mo	0.11-0.25	vib.	large effect for large A
Ru	0.23-0.29	vib.	very large effects
Pd	0.22-0.25	vib.	large effects
Cd	0.19-0.20	vib.	medium-large effects
Sn	0.11-0.13	vib.	small effects
Te	0.13-0.18	vib.	medium large effects
Xe	0.12-0.19	vib.	small effect for large A
Ba	0.12-0.18	vib.	small effect for large A
Ce	0.10-0.12	vib.	small effects
Nd	0.10-0.28**	vib.	very large effects for large A
Sm	0.19-0.35**	vib.+rot	very large effects for large A
Gd	0.17-0.36	vib.	very large effects for large A
Dy	0.30-0.35	vib.	very large effects
Er	0.32-0.34	vib.	very large effects

* Exp. data from compilation [19]
** Smaller values were found from inelastic scattering studies [20-22]

GR85/940-dvh.1

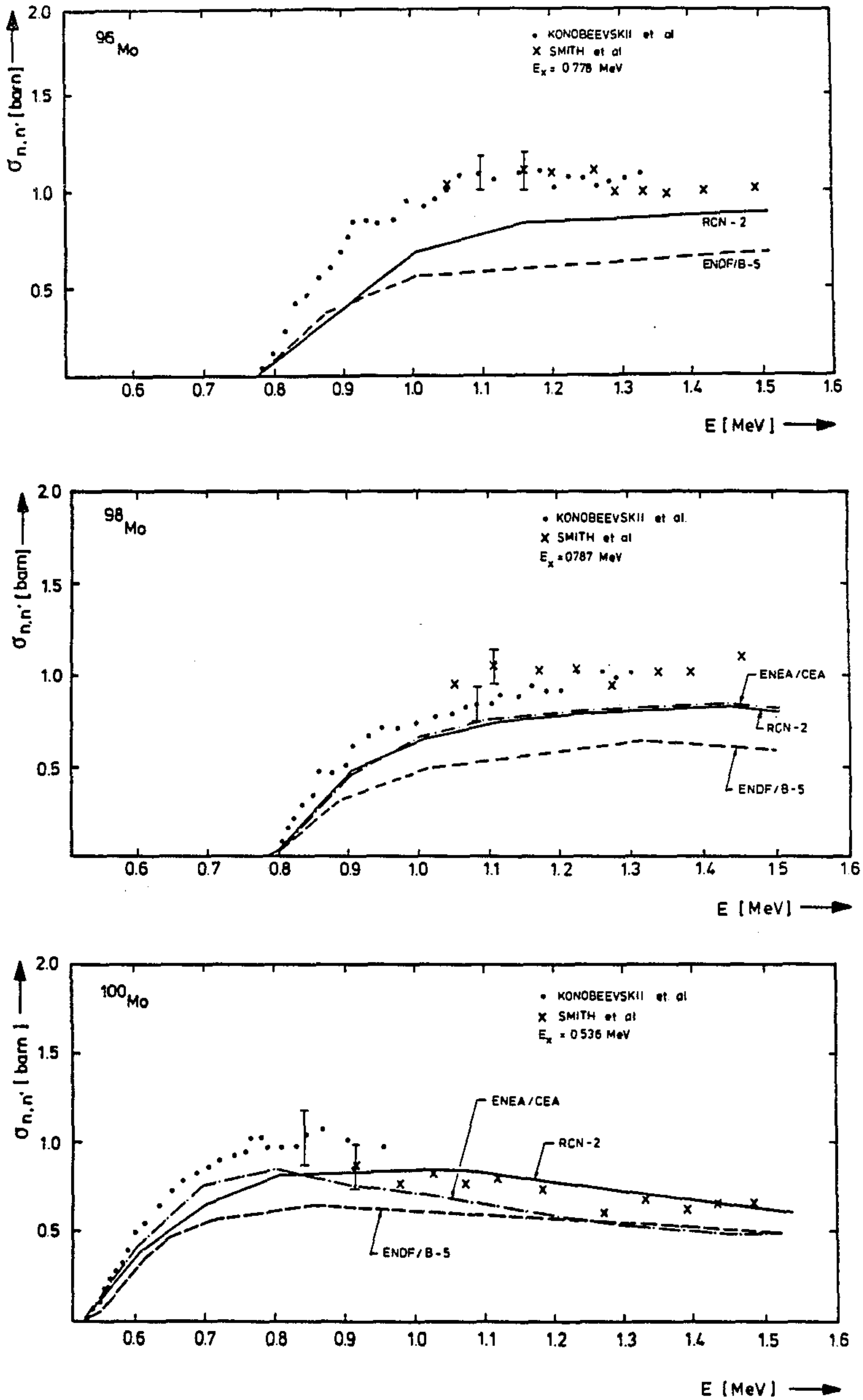


Fig. 1. Comparison of experimental and calculated inelastic scattering cross sections for Mo-isotopes.

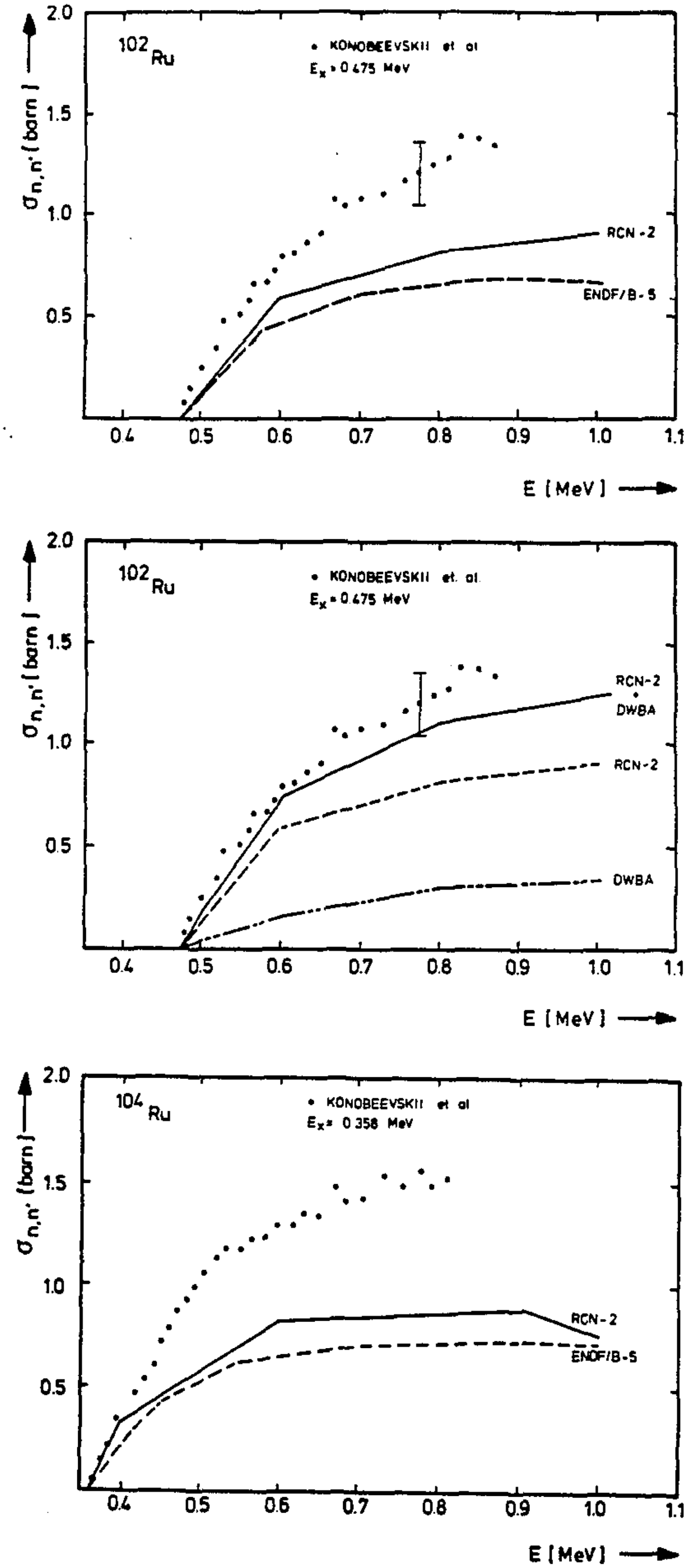
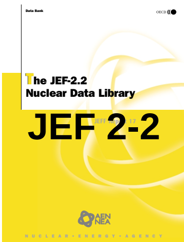


Fig. 2 Comparison of experimental and calculated inelastic scattering cross sections for Ru-isotopes.

14140252



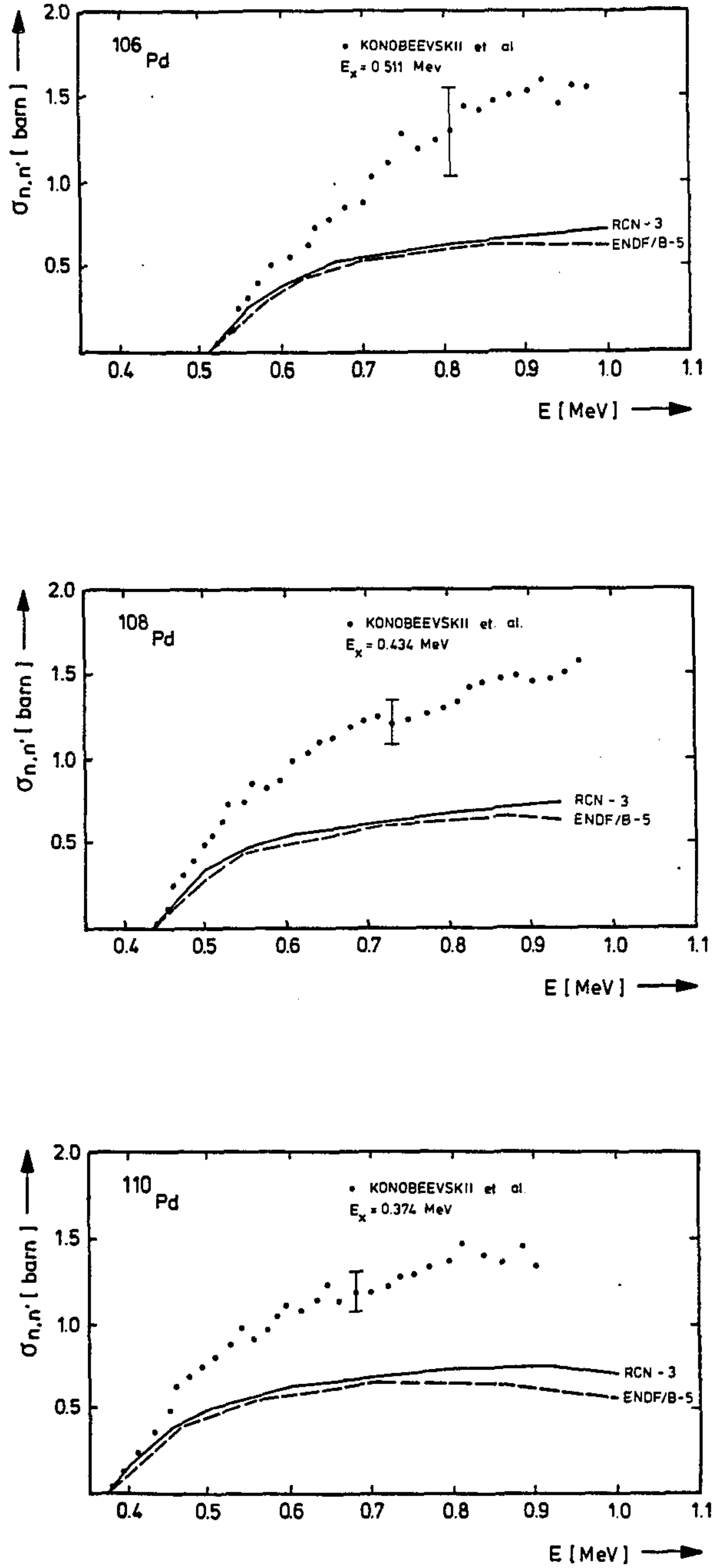


Fig. 3. Comparison of experimental and calculated inelastic scattering cross sections for Pd-isotopes.

14140256

APPENDIX A2.

Regional potential for coupled-channel calculations of neutron scattering cross-sections of light fission products

G.J.M. Janssen
H. Gruppelaar
J.M. Akkermans

ABSTRACT

For the calculation of the direct part of the inelastic cross-sections at low incident energies a regional deformed optical model parametrization is proposed. This parametrization is derived from the regional spherical optical model of Smith et al., valid for light fission product fragments at energies from 0.5 to 5 MeV, by adjusting the real and imaginary parts of their potential. The direct inelastic cross-sections calculated with this potential give a substantial contribution to the total inelastic cross-sections even at low energies.

1. INTRODUCTION

The simplest way to calculate the direct-inelastic scattering cross-sections is to use the distorted wave Born approximation (DWBA). However, the DWBA is no longer sufficient if the deformation parameter β (quadrupole) becomes large ($\beta > 0.2$) and if the interacting level has a low excitation energy. In such cases coupled-channel (CC) calculations are recommended.

Present spherical potential parameter sets have been obtained by a fit of the experimental values of the total and elastic scattering cross-sections and the s- and p-wave strength functions. If the same optical model parameters are used in CC calculations both a smaller shape-elastic and a smaller direct-inelastic cross-section may result.

From the above it is clear that the potential must be adapted to give a good agreement between CC results and experiment. Generally it is assumed that the parameter W must be decreased as the absorption of the strongly coupled level is now explicitly taken into account [1]. Since the elastic channel also changes V must be corrected as well. However, this is supposed to be a much smaller correction.

In the present paper this situation will be investigated for light fission products such as ^{102}Ru and ^{106}Pd where β is about 0.25 and the first vibrational 2^+ level is only about 0.5 MeV above the ground state. There are strong indications that the statistical model calculations based upon a spherical optical model (SOM) are insufficient for these systems as the calculated inelastic cross-sections are much smaller than inferred from experiment [2]. The potential obtained for these systems is shown to be also satisfactory for ^{92}Mo where β is much smaller and the first excited state occurs at a much higher energy.

2. METHOD

In this work the fast program HETEROCLITE especially adapted to run on a CRAY-computer [3] has been used to carry out the CC calculations. This program treats the full one-phonon vibrational coupling exactly. Evidently, a calculation with deformation parameter β = 0 will give the same results for the total, the shape-elastic and the compound-formation cross-sections as would be obtained from a SOM calculation with the same parameters. For a correctly fitted SOM potential these should agree with the experimental data. In this work the total and shape-elastic cross-sections and the s- and p-wave strength functions obtained in a β = 0 calculation with the regional SOM potential determined by Smith et al. [4] (Table 1) have been used as 'experimental' data in a fit to obtain a CC potential. It is noted that the regional spherical optical model potential of Smith et al. reproduces the experimental data for σ_t and $\sigma_{el}(\theta)$ rather well. Still, in some cases the real experimental data show some deviations e.g. for ^{92}Mo. It is noted that the parametrization of Smith et al. is mainly based upon elemental data in the A≈85-125 region.

The incident energies considered are 0.8, 2.5 and 4.0 MeV (laboratory coordinates). The level scheme data and β values of the nuclei studied in this paper are listed in Table 2.

.. RESULTS

3.1. Determination of a regional CC potential

3.1.1. ^{102}Ru, E_{inc} = 0.8 MeV

In Table 3 the results from the CC and SOM calculations based upon the optical model parameters of Smith et al. are shown (potential I). From these results it is clear that the coupling effects are quite large at these low incident energies. At 0.8 MeV (0.3 MeV above threshold) the CC shape-elastic scattering cross-section is 20% smaller than calculated with the spherical optical model using Smith's regional potential. The compound formation cross-section is also smaller, resulting in a total cross-section that is 1.1 barn lower than obtained in the SOM calculation. The direct-inelastic cross-section for scattering to the first excited state is only 40% of the DWBA value. For comparison some other potentials have been used in CC calculations on ^{102}Ru, with about the same results for σ_t and σ_{se} (potentials II and IV). The inelastic scattering cross-section, however, appears to be quite sensitive to the choice of potential parameters. The potential from Ref. [6] seems to have been tailored to obtain a high inelastic scattering cross-section (low value of imaginary otential).

has been suggested [5,8] that the anomalous cosine dependence in th's W (Table 1) is a result of effectively incorporating the coupling ts, and that this should be removed in a CC calculation, decreasing this procedure, however, the total and shape-elastic cross-sections ly slightly increased. From Fig. 1 it can be seen that with V at a value and E_{inc} = 0.8 MeV, the shape-elastic value of the SOM can eproduced if W is decreased to about 2 MeV, but that the correct the total cross-section can never be obtained. This problem is the low incident energies; at 4.0 MeV the CC results can be ecreasing W by just a few MeV (Fig. 2). The absorption is low incident energies and therefore more sensitive to the nannels.

ts show the necessity of a more extensive search on the r small E_{inc}. For several values of W, V was varied over a large interval, 40-70 MeV. If the value for W is small the total and shape-elastic cross-sections are oscillating functions of V (Fig. 3). Again it is clear that for a correct fit of these cross-sections W needs to be smaller than 4 MeV, but V also must be decreased by a few MeV. A least-squares fit of these cross-sections and the s- and p-wave strength functions yields V = 45.0 MeV and W = 3.5 MeV. From Fig. 3 it can be seen that the value for V is quite sharply determined at 4 MeV.

3.1.2. ^{102}Ru, E_{inc} = 2.5 MeV, 4.0 MeV

The above potential was tested for other incident energies up to about 4 MeV. No energy dependence was assumed in the relatively small range 0.8 MeV < E_{inc} < 4.0 MeV.

From Fig. 2 it can be seen that at higher incident energies the total and shape-elastic cross-sections are only slowly varying functions of W. As a fucntion of V the total and shape-elastic cross-sections are still oscillating functions, but not as strongly as at 0.8 MeV (Figs. 4 and 5). It was mentioned above that a good representation of the data is possible by just decreasing the SOM value for W, but the potential obtained above for the lower energy can be used as well. In a fit optimizing the total and the shape-elastic cross-sections for all three incident energies the values V = 45.0 MeV and W = 3.0 MeV are obtained. A survey of the calculated cross-sections is given in Table 4.

At E_{inc} = 0.8, 2.5 and 4.0 MeV the differential cross-sections (scattering to the ground state) have been plotted (Fig. 6) for a slightly different CC potential (see 3.1.3). Considerable discrepancies with the values obtained in the SOM calculation (squares) are found. The deviations are only large at large scattering angles, where the differential cross-section is small. This means that the CC potential may still need further refinements although the absolute values of the cross-sections are nicely reproduced.

The differences between the angle-integrated CC and SOM cross-sections are 3-4%. All are well within the error bounds of the measured total cross-sections for natural Ru [9].

3.1.3. Results for ^{106}Pd

^{106}Pd is very similar to ^{102}Ru; the level scheme, the deformation and the asymmetry (N-Z)/A parameters are almost the same. If we assume the same dependence for this latter parameter in the present CC potential as was used by Smith et al., we have to correct the ^{102}Ru values (V = 45.0 MeV and W = 3.0 MeV) into V = 45.15 MeV and W = 3.13 MeV. These values give a reasonable representation of the data, although a slightly better fit can be obtained (V = 44.0 MeV, W = 3.5 MeV). The calculated cross-sections are listed in Table 5.

The CC results give a fair representation of the SOM results, the discrepancies are slightly larger when compared to experiment, especially for the first potential (I in Table 5).

3.1.4. Results for ^{92}Mo

This nucleus differs considerably from the others: the lowest excited state is at about 1.5 MeV, and the deformation parameter is small (β = 0.065), so large coupling effects are not expected. This is confirmed by a comparison of the results from calculations for $\beta = 0$ with those for $\beta = 0.065$. Therefore it is expected that the regional potential as obtained by Smith et al. will do quite well also in these coupled-channel calculations. The same holds, however, for the CC potential obtained above, if Smith's asymmetry dependence is applied. A still better agreement is obtained if the values that can be extrapolated from the best ^{106}Pd potential are used (Table 6). The results from the present CC calculations do not agree very well with SOM calculations using Smith's regional potential, but the agreement with experiment is good.

3.1.5. Adopted regional potential for CC calculations

The potential eventually adopted for the CC calculations of the direct-inelastic cross-section is:

$$U(r) = Vf_v(r) - 4iW \frac{df_w(r)}{dr} + 2\,V_{so} \frac{1}{r} \frac{df_v(r)}{dr} \vec{L} \cdot \vec{\sigma}$$

with:

$f_i = (1 + e^{x_i})^{-1}$,

$x_i = (r - r_i A^{1/3}) a_i$,

$V = 48.12 - 30.0\ (N-Z)/A$ MeV,

$r_v = 1.131 + 0.00107\ A$ fm,

$a_v = 1.203 - 0.00511\ A$ fm,

$W = 6.93 - 25.0\ (N-Z)/A$ MeV,

$r_w = 2.028 - 0.00683\ A$ fm,

$a_w = -0.1061 + 0.005551\ A$ fm,

$V_{so} = 6.0$ MeV.

Note that this CC potential has no anomalous A dependence. V_{so} and the geometry parameters have been taken over from Smith et al. They may need readjustment to fit correctly the angular distribution of the differential cross-sections.

3.2. Inelastic scattering cross-section

The calculated direct-inelastic cross-sections for scattering to the 2^+ level in ^{102}Ru and ^{106}Pd are listed in Tables 7a and 7b, respectively. The value obtained at E_{inc} = 0.8 MeV for ^{102}Ru is larger than most of the values found in DWBA or CC calculations with a SOM potential (Table 3). The experimental values for the inelastic scattering cross-sections are still higher. At this energy there are large compound-formation contributions which are obtained from statistical model calculations with the width-fluctuation corrected Hauser-Feshbach model.

These calculations have been performed with transmission coefficients taken from the spherical optical model of Smith et al. However, the compound-elastic, compound-inelastic and radiative capture cross-sections were renormalized such that their sum agrees with the compound-formation cross-section calculated with the CC model. This simple method was used because our present statistical model code cannot read the generalized transmission coefficients computed by HETEROCLITE. The width-fluctuation correction was calculated by means of the most recent parametrization of Hofmann et al. [12]. It was checked that for these nuclides this model agrees very well with the alternative parametrization of Moldauer [13]. The final results are given in Figs. 7 and 8 and in Tables 7a and 7b. It is seen that the total inelastic scattering cross-sections for excitation of the first 2^+ state is still below the measured data, although close to the lower error bounds.

A comparison between direct inelastic-scattering cross sections calculated with DWBA and CC is given in Fig. 9. For the DWBA calculation the SOM potential of Smith et al. was used. It is seen that the CC calculation yields a much higher cross section. Furthermore, the shape of the CC curves is quite different from that of DWBA. [It is noted that in the DWBA calculation the SOM potential was used for the entrance and exit channels and also for the calculation of the collective form factors. If the SOM potentials are replaced by the CC potentials very high DWBA cross-sections are obtained. Fairly good results are obtained if the asymmetric distorted-wave approximation (ADWA) is applied: the SOM potential for the entrance channel and the CC potential for the exit channel (and the form factors). This is also illustrated in Fig. 9. We note that the ADWA method [14,15] is not very well founded and the agreement with the present CC calculations seems to be rather accidental.]

Also shown in Fig. 9 is the effect of neglecting the 3^- state at 2.044 MeV. The cross section to the 2^+ state is only slightly increased.

The angular distributions of the CC component at various incident energies are shown in Fig. 10. Only at relatively high energies there is a clear forward peaking. The compound angular distribution, symmetric around 90°, has not been added. However, this component is rather flat.

4. DISCUSSION

4.1. Optical model parameters

In this paper a regional CC potential has been derived from a regional SOM potential by adjusting V and W only. The regional SOM parameters have been fitted by Smith et al. to an extensive set of experimental data. Therefore we assumed that the SOM values for σ_t, σ_{se} and the s- and p-wave strength functions can be used as 'experimental' data in a search for CC potential parameters. Actually, σ_{el} should be used instead of σ_{se}, but since the HETEROCLITE code does not compute σ_{el}, the shape-elastic part was used. This procedure is questionable at low-incident energies but justifiable at 4 MeV, since at high energies the compound-elastic scattering is small.

It can also be questioned whether a good deformed optical model potential can be found from a SOM potential by adjusting V and W only. In several papers (e.g. Ref. [1,16]) it was shown that a similar procedure, restricted to a decrease of W, can be a good starting point to find a CC potential, but this does not mean that the method has general validity. In the cases of ^{102}Ru and ^{106}Pd the coupling effects are very large, affecting both σ_t and σ_{se}. The fact that this leads to large corrections in V, together with the strongly oscillating behaviour of σ_t and σ_{se} as a function of V, makes the present potential seem rather ad hoc.

Comparison with other potentials in the literature, shows that our adopted value for W is quite close to other values found for this parameter, both in SOM and deformed optical models. The SOM parameter set optimized by Lagrange for ^{93}Nb contains an imaginary potential depth equal to $W = (3.4 + 0.37E)$ MeV [17]. Rapaport et al. found $W = (4.28 + 0.4E - 12.8(N-Z)/A)$ MeV [7]. For ^{238}U where there is also a very low-lying collective state the deformed optical-model W parameter is $(2.7 + 0.4E)$ MeV [18]. In this respect the imaginary potential in Smith's potential must be considered as exceptionally large, a feature enhanced by the anomalous cosine mass dependence.

On the other hand our V value is much smaller than the one found in other studies, e.g. for ^{93}Nb $(49.5 - 0.28E)$ MeV [17]. However, in the latter case no deformation effects were included. The fact that our V value is relatively low does not result from our choice to fit σ_{se} instead of σ_{el} since the optimization of the fitted value of σ_t at low energies also requires a small V. From Fig. 3 can be seen that the reduction in V is almost independent of W. A much larger value of V (~ 60 MeV) may also fit the total and shape-elastic cross-sections but then the strength functions are not predicted well.

It should be noted that, if we take into account the positive E-dependence found in most SOM potentials for W and a negative E-dependence for V, we expect a 'normal' relation between the CC and SOM potentials at higher energies, i.e. only a slightly decreased W when coupling effects are included. Of course this is consistent with the observation that for high incident energies the coupling effects are small.

The fact that the angular distribution of the elastic scattering is worsened, is somewhat disturbing. Probably, also some of the other (geometry) parameters need readjustment. However, we are not very much interested in a detailed prediction of the angular distribution as long as the main experimental features are reproduced. Our first goal is the prediction of the (angle-integrated) inelastic cross-sections of which no experimental data were included in the (SOM and CC) fits.

It is difficult to estimate the quality and validity of the present potential. In any case it reproduces the values of σ_t, σ_{se} and the s- and p-wave strength functions well for the light fission products considered, both for cases with strong and weak coupling. To find such a potential was the main purpose of our study. In view of the large changes with respect to the regional SOM parameters that had to be made, a global potential may be a better starting point to obtain a regional CC potential than the regional SOM potential of Smith et al. in which apparently large coupling effects are effectively included.

Finally we mention here that one of the implicit assumptions of this work is that the SOM potential of Smith et al., which is based mainly upon elemental data, can be used to predict isotopic cross-sections.

4.2. Inelastic scattering cross-sections

In the present work the statistical and direct parts of the inelastic cross-section were added incoherently. This method is justified if one of the two components is predominant, e.g. at very high energies. At lower energies interference effects are possible which have been neglected in the present approach. Since in ^{102}Ru and ^{106}Pd the direct and indirect inelastic cross-sections at low energies are of the same order of magnitude, this may lead to an additional uncertainty in the total inelastic scattering cross-sections. From calculations by Sheldon and Chan [19] for ^{232}Th and ^{238}U it follows that the so-called unified S matrix approach based upon the latest work of Moldauer [20] (or Hofmann et al. [12]) in general leads to higher cross-sections.

Next, we want to discuss the quite large values of $\sigma_{nn'}^{direct}$ at low incident energies. These must be due to the relatively large β value and the relatively low excitation energy of the first excited state. It is hard to specify to which extent the large value for the direct inelastic cross-section is related to the specific choice of the adopted optical model parameters. Comparison of our CC data with the CC data obtained with other parametrizations (Table 3) shows that our result for E_{inc} = 0.8 MeV is mid-way between the value obtained with the (unmodified) SOM potential of Rapaport et al. [7] and the potential of Konobeevskii and Popov [6]. However, these parametrizations are not in good agreement with other quantities, like σ_t, σ_{el} and the s- and p-wave strength functions.

Finally, we note that the inelastic scattering cross-section to the first excited 2^+ state, calculated with the statistical model using the SOM potential (Tables 7a,b,$\sigma_{nn'}^{stat}$) is lower than that calculated with the CC potential ($\sigma_{nn'}^{total}$). Still, also the SOM potential correctly predicts σ_t, σ_{el} and the s- and p-wave strenght functions. The difference between σ_t and σ_{el} is at low incident energy about equal to $\sigma_{nn'}$. Since this is a difference between two large numbers the uncertainty in $\sigma_{nn'}$ is large. Therefore it is possible that the CC potential gives much larger inelastic scattering cross sections while still σ_t and σ_{el} are correct within their error margins.

5. CONCLUSIONS

In light fission-product nuclei like ^{102}Ru and ^{106}Pd direct scattering to the first excited (2^+) state requires a correct treatment of the full coupling between the ground state and excited state channels. A DWBA calculation is no longer sufficient here. This effect is most pronounced at small incident energies (< 1 MeV).

By readjustment of the V and W parameters of the SOM parametrization of Smith et al. a regional CC potential has been found which fits correctly σ_t, σ_{se} and the s- and p-wave strength functions in the energy range of 0.5-4.0 MeV for these nuclei and for the almost spherical nucleus ^{92}Mo. V and particularly W are greatly reduced with respect to the SOM values. The reduction of W is explained by the fact that the large absorption effect due to scattering to the 2^+ state is now explicitly accounted for. The reduction in V leads to a value smaller than obtained so far in other parametrizations. The present potential is valid only for energies in the range 0.5-4.0 MeV, for higher energies modifications are required. This can be done by making V and W energy-dependent, in such a way that at higher energies agreement with other parameterizations is obtained.

The calculation of the direct-inelastic cross-sections shows that the direct component of the cross-sections at low energies is non-negligible, e.g. in ^{102}Ru at 300-500 keV above threshold it is 20-25% of the total scattering to the 2^+ state. When the direct contributions are incoherently added to the compound contributions the total (n,n') scattering cross sections at low energies are consistent with experiment, taking into account error margins of 15 to 20%. The experimental data are still systematically somewhat higher. As yet it is not clear whether coherent addition of direct and statistical components according to modern Hauser-Feshbach theory [12,20] may significantly enhance the calculated values.

ACKNOWLEDGEMENT

This work has been supported by the NEA Data Bank in the framework of the Joint Evaluated File project. The authors would like to thank Dr. Ch. Lagrange (CEA, Bruyères-le-Châtel, France) for providing them with the HETEROCLITE code. Thanks are also due to Drs. H.A.J. van der Kamp for some additional calculations and to Dr. J.F.A. van Hienen (ECN, Petten) for helpful discussions.

6. REFERENCES

[1] Perey, F.; Satchler, G.R.: Phys. Rev. Lett. 5 (1984), 212.

[2] Gruppelaar, H.; Kamp, H.A.J. van der: Inelastic scattering cross-sections in the fission product mass range, Specialists Mtg. on the Use of Optical Model for the Calculation of Neutron Cross Sections below 20 MeV, Nov. 1985, Paris, NEANDC-222"U", p. 221 (1986) .

[3] HETEROCLITE code written by Ch. Lagrange, Service de Physique Nucléaire, Centre d'Etudes de Bruyères-le-Châtel, Montrouge, France.

[4] Smith, A.B.; Guenther, P.T.; Whalen, J.F.: Nucl. Phys. A415 (1984), 11.

[5] Cereda, E.; Pignanelli, M.; Micheletti, S.; Geramb, H. von; Hahakeh, M.; DeLeo, R.; D'Erasmo, G.; Pantaleo, A.: Phys. Rev. C26 (1982), 1941.

[6] Konobeevskii, E.S.; Popov, V.I.: Sov. J. Nucl. Phys. 33 (1984), 7.

[7] Rapaport, J.; Kulnarni, V.; Finlay, R.W.: Nucl. Phys. A330 (1979), 15.

[8] Cereda, E.; Pignanelli, M.; Micheletti, S.; Geramb, H. von; Hahakeh, M.; DeLeo, R.; D'Erasmo, G.; Pantaleo, A.: Nucl. Phys. A396 (1983), 281.

[9] Divadeenam, M.: Thesis, Duke University, 1968 (numerical data available from NEA Data Bank, Saclay) and also:
Foster, D.G.; Glasgow, D.W.: Phys. Rev. C3 (1971), 576.

[10] Smith, A.B.; Guenther, P.T.; Whalen, J.F.: Argonne National Laboratory Report, ANL/NDM-71 (1982).

[11] Lambropoulos, P.; Guenther, P.T.; Smith, A.B.; Whalen, J.F.: Nucl. Phys. A201 (1973), 1.

[12] Hofmann, H.M.; Richert, J.; Tepel, J.W.; Weidenmüller, H.A.: Ann. Phys. 90 (1975), 403 and also:
Hofmann, H.M.; Mertelmeier, T.; Herman, M.; Tepel, J.W.: Z. Physik A297 (1980), 153.

[13] Moldauer, P.A.: Nucl. Phys. A344 (1980), 185.

[14] Satchler, G.A.: "Direct Nuclear Reactions", Clarendon Press, Oxford (1983).

[15] P.E. Hodgson, The neutron optical model in the actinide region, Proc. Spec. Mtg. on "Fast Neutron Scattering on Actinide Nuclei", OECD, Paris, 1982, NEANDC-158"U", p. 69; P.E. Hodgson and A.M. Kobos, The inelastic scattering of neutrons by ^{238}U, to be published; K.I. Kubo and P.E. Hodgson, Nucl. Phys. A366 (1981), 320.

[16] Madland, D.G.; Young, P.G.: Proc. Int. Conf. on Neutron Physics and Nuclear Data for Reactors and Other Applied Purposes, Harwell, published by OECD (1978) p. 349.

[17] Lagrange, Ch.: Contribution to the 3rd Soviet Nat. Conf. on Neutron Physics, Kiev (1975).

[18] Lagrange, Ch.: Proc. of the NEANDC Topical Discussion on "Critique of Nuclear Models and their Validity in the Evaluation of Nuclear Data", JAERI-M5984, T. Fuketa, ed., Tokyo (1975).

[19] Sheldon, E.; Chan, D.W.S.: Proc. of a Specialists' Meeting on "Fast Neutron Scattering on Actinide Nuclei", Paris, OECD (1982), NEANDC-158"U" (1982), p. 169.

[20] Moldauer, P.A.: Phys. Rev. C12 (1975), p. 744.

Table 1. Regional spherical optical model parameters a),e) determined by Smith et al. [4]

real potential b)			
strength	V	$= 52.58-0.3E-30.0(N-Z)/A$	(MeV)
radius c)	r_V	$= 1.131+0.00107A$	(fm)
diffuseness	a_V	$= 1.203-0.00511A$	(fm)
imaginary potential d)			
strength	W	$= 11.70-25.0(N-Z)/A-1.8\cos(2\pi(A-90)/29)$	(MeV)
radius c)	r_W	$= 2.028-0.00683A$	(fm)
diffuseness	a_W	$= -0.1061+0.005551A$	(fm)

a) With 6 MeV spin-orbit potential of Thomas form and real-potential geometry.

b) Saxon-Woods form.

c) All radii in form $R = r_i A^{1/3}$.

d) Saxon-derivative form.

e) Applicable only to the mass-energy range $A \approx 85 - 125$ and $E_n < 5$ MeV.

Table 2. Vibrational energy levels, asymmetry and quadrupole deformation parameters of light fission product nuclei[a]

	^{102}Ru	^{106}Pd	^{92}Mo
$E_x(2^+)$ [b]	0.475	0.512	1.509
$E_x(3^-)$ [b]	2.044	2.070	2.849
$\beta(2^+)$	0.265	0.254	0.065
$\beta(3^-)$	0.169	0.164	0.129
N-Z/A	0.137	0.132	0.087

[a] β values from Ref. [5], energy levels from recent issues of Nuclear Data Sheets.

[b] In MeV.

Table 3. Calculated cross-section for ^{102}Ru at E_{inc} = 0.8 MeV (cross-sections given in barn)

potential[a)]	model	σ_t	σ_{se}	$\sigma_{nn'}(2^+)$	σ_{cf}
I	CC	5.66	3.31	0.04	2.31
II	CC	5.75	3.49	0.08	2.18
III	CC	5.40	3.46	0.27	1.67
IV	CC	5.81	3.48	0.15	2.18
I	SOM	6.79	4.12	-[b)]	2.67

a) The following potentials were considered:

I : Smith's regional potential (Table 1, W = 9.81 MeV);

II : Smith's regional potential without anomalous A dependency, W = 6.47 MeV);

III: Konobeevskii and Popov [6] (W = 2 MeV);

IV : Rapaport potential [7].

b) A DWBA calculation yields 0.11 b.

Table 4. Total and shape-elastic neutron scattering cross-sections for ^{102}Ru from CC and SOM calculations (in barn)

E_{inc} (MeV)	I σ_t	I σ_{se}	II σ_t	II σ_{se}	III σ_t	III σ_{se}	IV σ_t	IV σ_{se}
0.8	7.01	4.51	6.83	4.29	7.04	4.17	6.79	4.12
2.5	4.41	2.16	4.38	2.13	4.39	2.11	4.57	2.31
4.0	3.96	1.87	3.96	1.84	4.11	1.95	3.95	1.79

I : CC, V = (49.12-30(N-Z)/A) MeV, W = (6.43-25(N-Z)/A) MeV;
II : CC, V = (49.12-30(N-Z)/A) MeV, W = (6.93-25(N-Z)/A) MeV;
III: CC, V = (48.12-30(N-Z)/A) MeV, W = (6.93-25(N-Z)/A) MeV (adopted);
IV : SOM, Smith potential (Table 1).

Experimental total cross-sections for natural Ru [9] (5% error margin assumed):

- E_{inc} = 0.8 MeV : (7.10 ± 0.36) b;
- E_{inc} = 2.5 MeV : (4.45 ± 0.23) b;
- E_{inc} = 4.0 MeV : (3.82 ± 0.19) b.

Table 5. Total and shape-elastic neutron scattering cross-section for ^{106}Pd from CC and SOM calculations (in barn)

E_{inc} (MeV)	I σ_t	I σ_{se}	II σ_t	II σ_{se}	III σ_t	III σ_{se}	IV σ_t	IV σ_{se}
0.8	6.74	4.50	6.63	4.33	6.96	4.39	6.74	4.14
2.5	4.41	2.15	4.39	2.13	4.43	2.13	4.70	2.44
4.0	3.81	1.74	3.85	1.73	4.00	1.88	4.02	1.82

I : CC, V = (49.12-30(N-Z)/A) MeV, W = (6.43-25(N-Z)/A) MeV;
II : CC, V = (49.12-30(N-Z)/A) MeV, W = (6.93-25(N-Z)/A) MeV;
III: CC, V = (48.12-30(N-Z)/A) MeV, W = (6.93-25(N-Z)/A) MeV (adopted);
IV : SOM, Smith potential (Table 1).
Experimental total cross-sections for natural Pd [10] (5% error margin assumed):

- E_{inc} = 0.8 MeV : (6.90 ± 0.35) b;
- E_{inc} = 2.5 MeV : (4.68 ± 0.23) b;
- E_{inc} = 4.0 MeV : (4.15 ± 0.21) b.

Table 6. Total cross-sections for ^{92}Mo from CC and SOM calculations (in barn)

$E_{inc}^{a)}$	I	II	III	IV	V
0.8	6.84	6.28	5.79	6.98	(5.9 ± 0.3)
2.5	5.02	4.37	4.03	5.05	(4.3 ± 0.2)
4.0	4.39	4.08	3.93	4.44	(3.9 ± 0.2)

a) In MeV.

I : CC, Smith's potential;

II : CC, V = (49-30(N-Z)/A) MeV, W = (6.4-25(N-Z)/A) MeV; derived for ^{102}Ru;

III: CC, V = (48-30(N-Z)/A) MeV, W = (6.9-25(N-Z)/A) MeV (adopted); derived for ^{106}Pd;

IV : SOM, Smith's potential;

V : Experimental values [11], 5% error margin.

Table 7a. Inelastic scattering cross-sections for ^{102}Ru (barn)

$E_{inc}^{a)}$	$\sigma_{nn'}^{stat.}$	$\sigma_{nn'}^{renorm.\ comp.}$, b)	$\sigma_{nn'}^{direct}$, c)	$\sigma_{nn'}^{total}$
0.4798	0.0	0.0	0.0	0.0
0.5	0.166	0.201	0.009	0.210
0.6	0.585	0.661	0.082	0.743
0.8	0.883	0.885	0.207	1.092
1.0	0.963	0.896	0.267	1.163
1.2	0.840	0.748	0.292	1.040
1.5	0.734	0.634	0.306	0.940
1.8	0.570	0.485	0.323	0.808
2.0	0.498	0.422	0.341	0.763
2.5	0.304	0.248	0.401	0.649
3.0	0.186	0.152	0.456	0.608
4.0	0.063	0.048	0.477	0.525

a) In MeV.

b) $\sigma_{nn'}^{renorm.\ comp.} = \sigma_{nn'}^{stat.} \cdot \dfrac{\sigma_{cf}^{CC}}{\sigma_{cf}^{stat.}}$

c) CC calculation.

Table 7b. Inelastic scattering cross-sections for ^{106}Pd (barn)

$E_{inc}^{a)}$	$\sigma_{nn'}^{stat.}$	$\sigma_{nn'}^{renorm.\ comp.,\ b)}$	$\sigma_{nn'}^{direct,\ c)}$	$\sigma_{nn'}^{total}$
0.5168	0.0	0.0	0.0	0.0
0.6	0.438	0.450	0.051	0.501
0.8	0.791	0.728	0.180	0.908
1.0	0.922	0.803	0.242	1.045
1.2	0.884	0.751	0.266	1.017
1.5	0.746	0.651	0.281	0.933
1.8	0.597	0.497	0.302	0.799
2.0	0.526	0.437	0.323	0.760
2.5	0.321	0.264	0.386	0.650
3.0	0.198	0.158	0.428	0.586
4.0	0.062	0.056	0.425	0.481

a) In MeV.

b) $\sigma_{nn'}^{renorm.\ comp.} = \sigma_{nn'}^{stat.} \cdot \dfrac{\sigma_{cf}^{CC}}{\sigma_{cf}^{stat.}}$

c) CC calculation.

FIGURE CAPTIONS

Fig. 1. CC σ_t and σ_{se} as a function of W. E_{inc} = 0.8 MeV and V = 48.0 MeV. SOM results with W = 9.81 MeV.

Fig. 2. CC σ_t and σ_{se} as a function of W. E_{inc} = 4.0 MeV and V = 47.3 MeV. SOM results with W = 9.81 MeV.

Fig. 3. σ_t and σ_{se} as a function of V. E_{inc} = 0.8 MeV.

Fig. 4. σ_t and σ_{se} as a function of V. E_{inc} = 2.5 MeV.

Fig. 5. σ_t and σ_{se} as a function of V. E_{inc} = 4.0 MeV.

Fig. 6. Differential σ_{se}. CC versus SOM. E_{inc} = 4.0 MeV.

Fig. 7. Inelastic scattering cross-sections for ^{102}Ru.

Fig. 8. Inelastic scattering cross-sections for ^{106}Pd.

Fig. 9. Direct inelastic-scattering cross sections for ^{102}Ru (comparison with DWBA and ADWA calculations).

Fig. 10. Angular distributions of direct inelastic scattering cross sections for ^{102}Ru.

Fig. 11. Angular distributions of compound inelastic scattering cross sections for ^{102}Ru.

Fig. 1.CC σ_t and σ_{se}
as a function of W.
E_{lab}=0.8 MeV V=48.0 MeV
SOM results with W=9.81 MeV

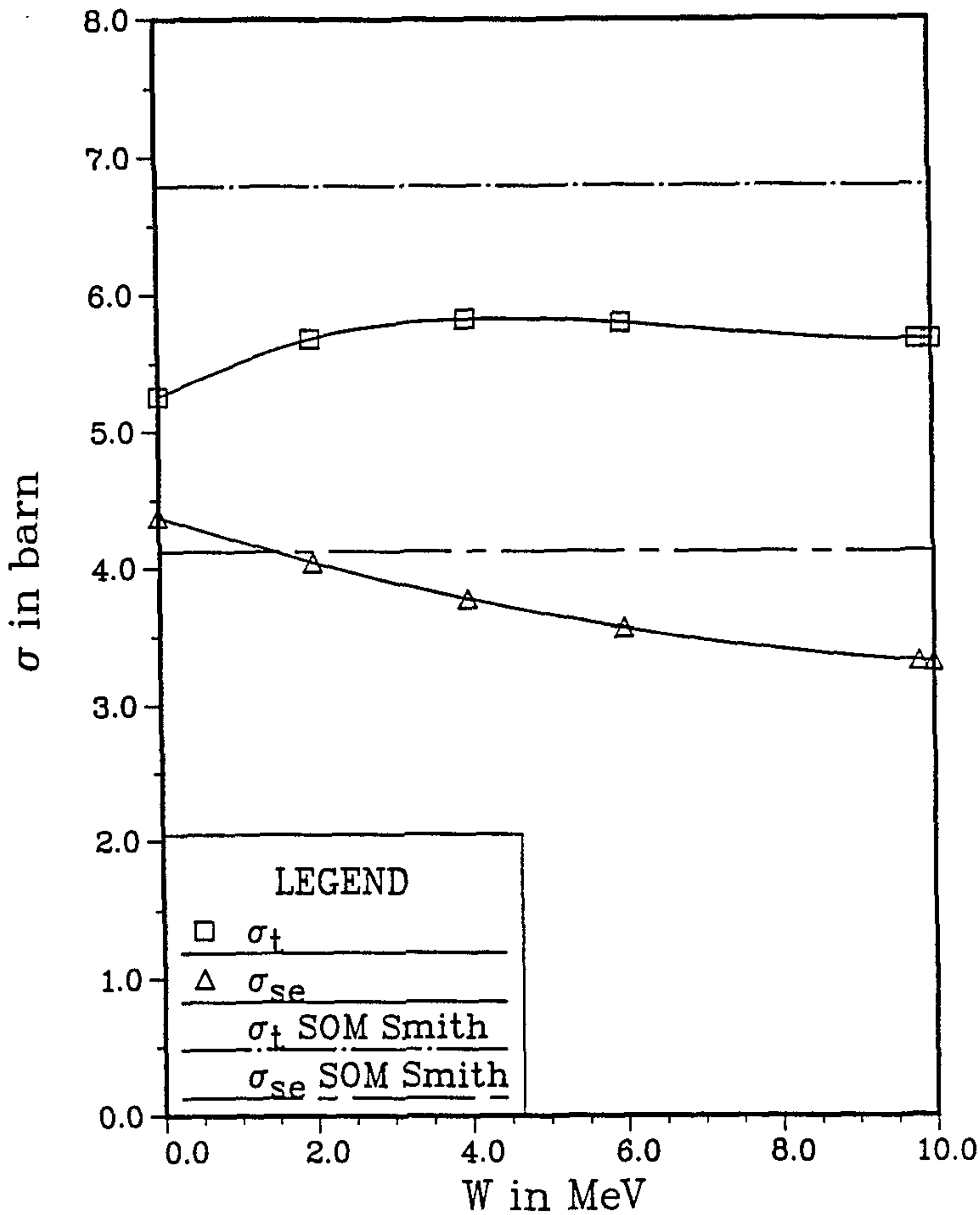
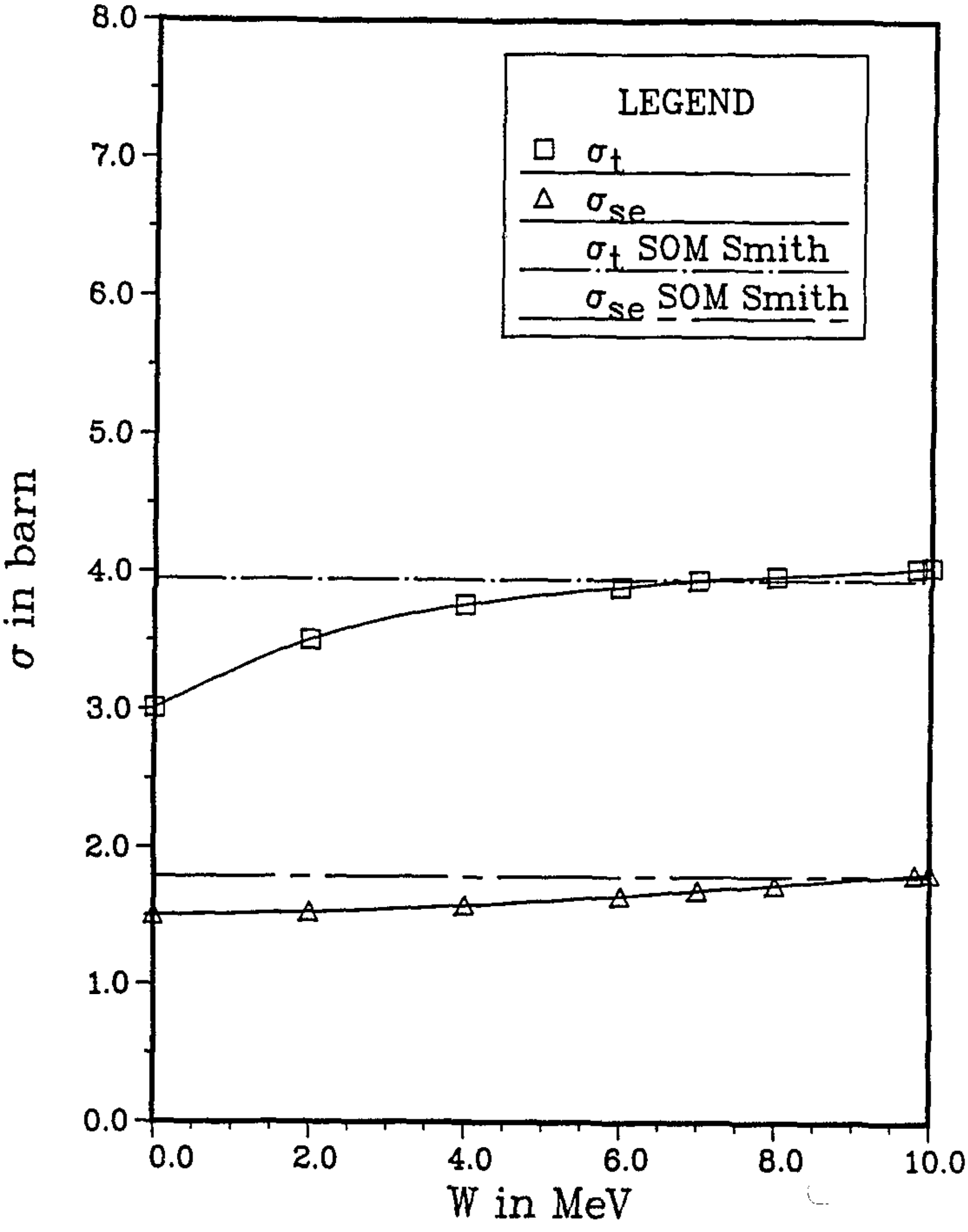


Fig. 2.CC σ_t and σ_{se}
as a function of W.
E_{lab}=4.0 MeV V=47.3 MeV
SOM results with W=9.81 MeV



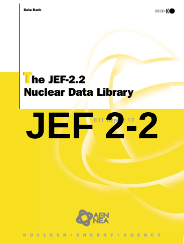


Fig. 3.
σ_t and σ_{se}
as a function of V
$E_{lab} = 0.8$ MeV

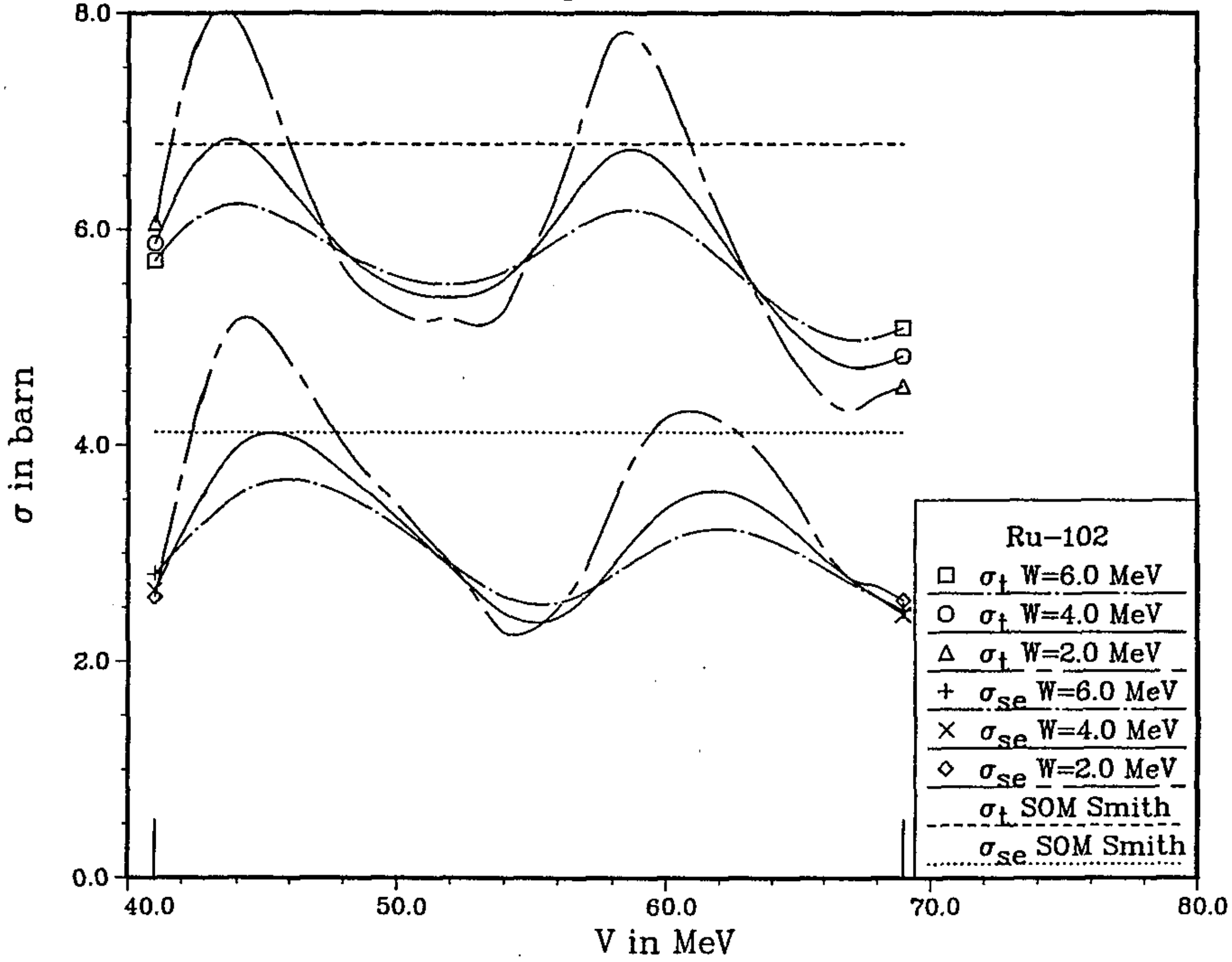
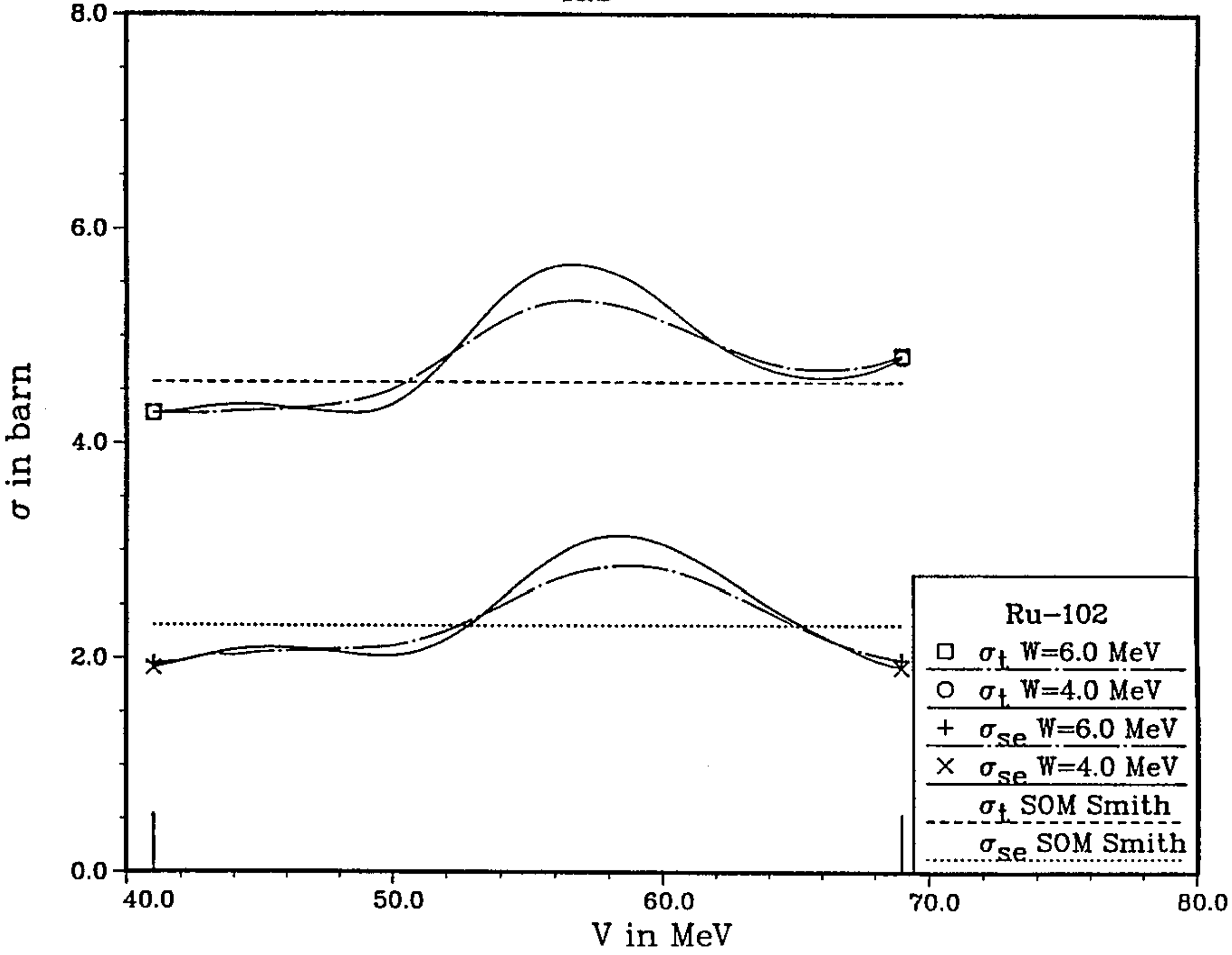


Fig. 4.
σ_t and σ_{se}
as a function of V
$E_{lab} = 2.5$ MeV



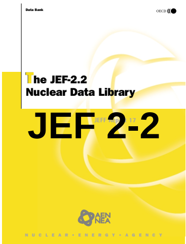


Fig. 5.
σ_t and σ_{se}
as a function of V
E_{lab} = 4.0 MeV

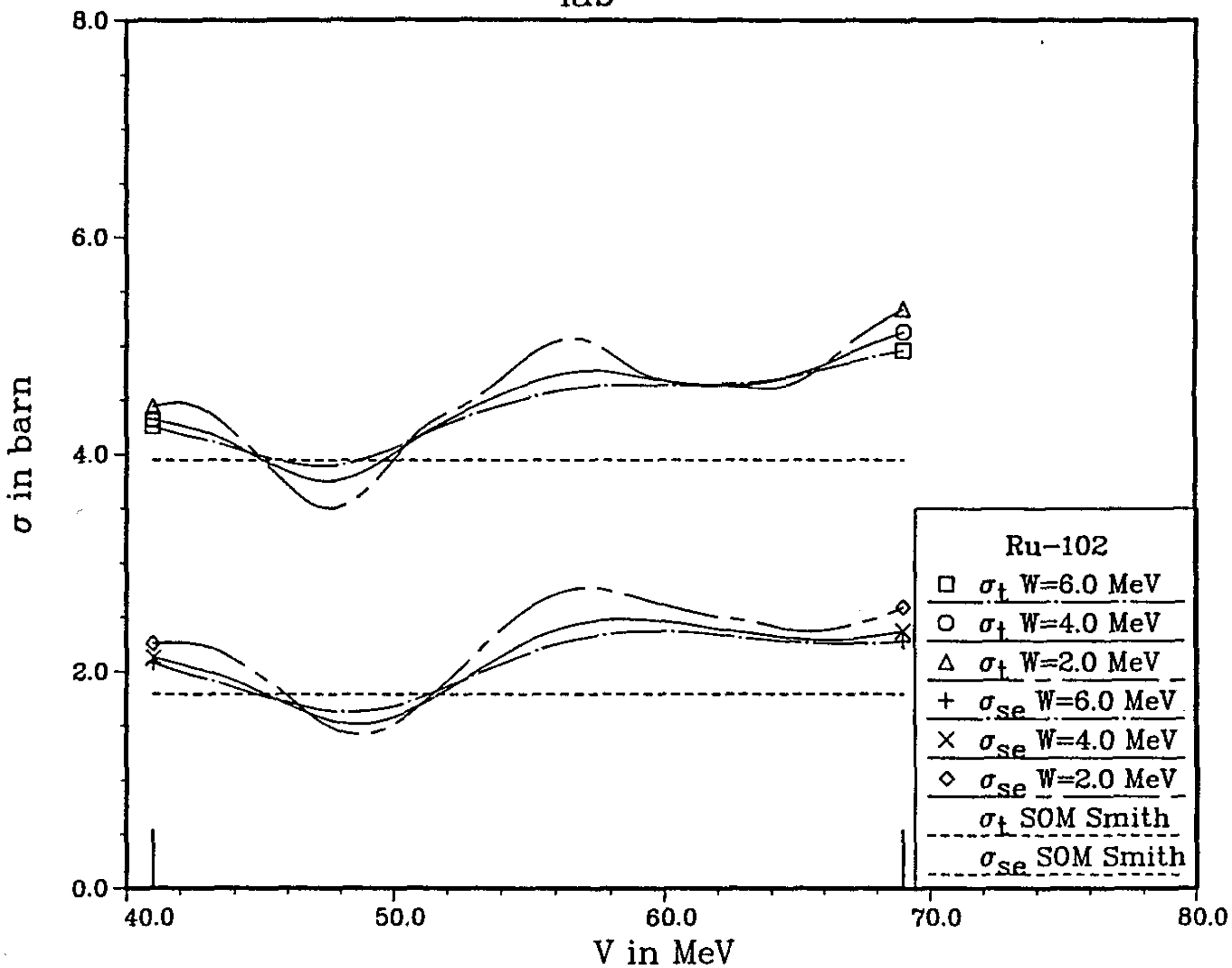
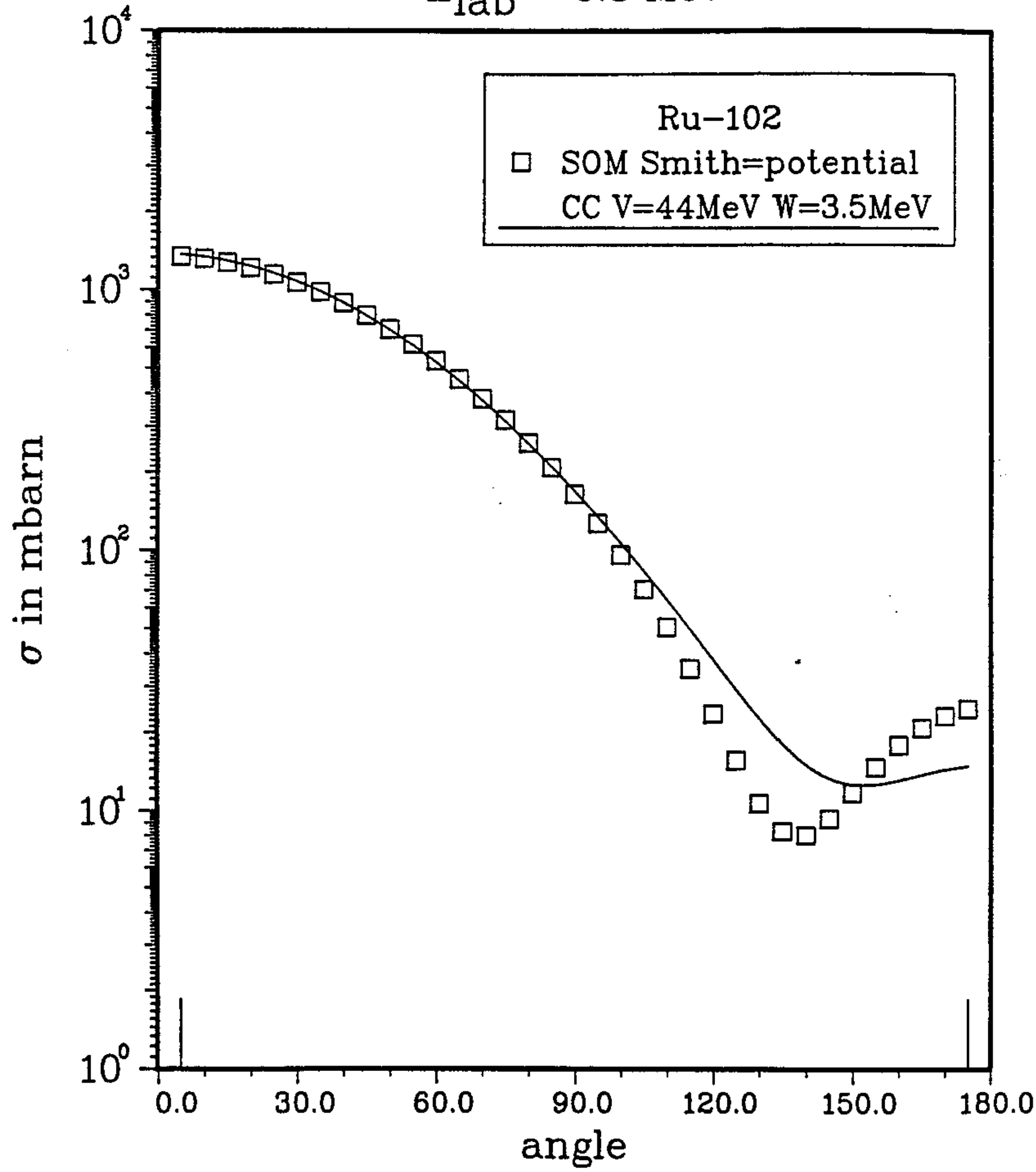


Fig. 6a.
differential σ_{se}
SOM versus CC
$E_{lab} = 0.8$ MeV



14140284

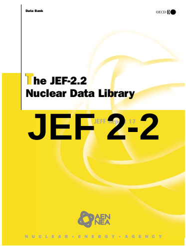


Fig. 6b.
differential σ_{se}
SOM versus CC
$E_{lab} = 2.5$ MeV

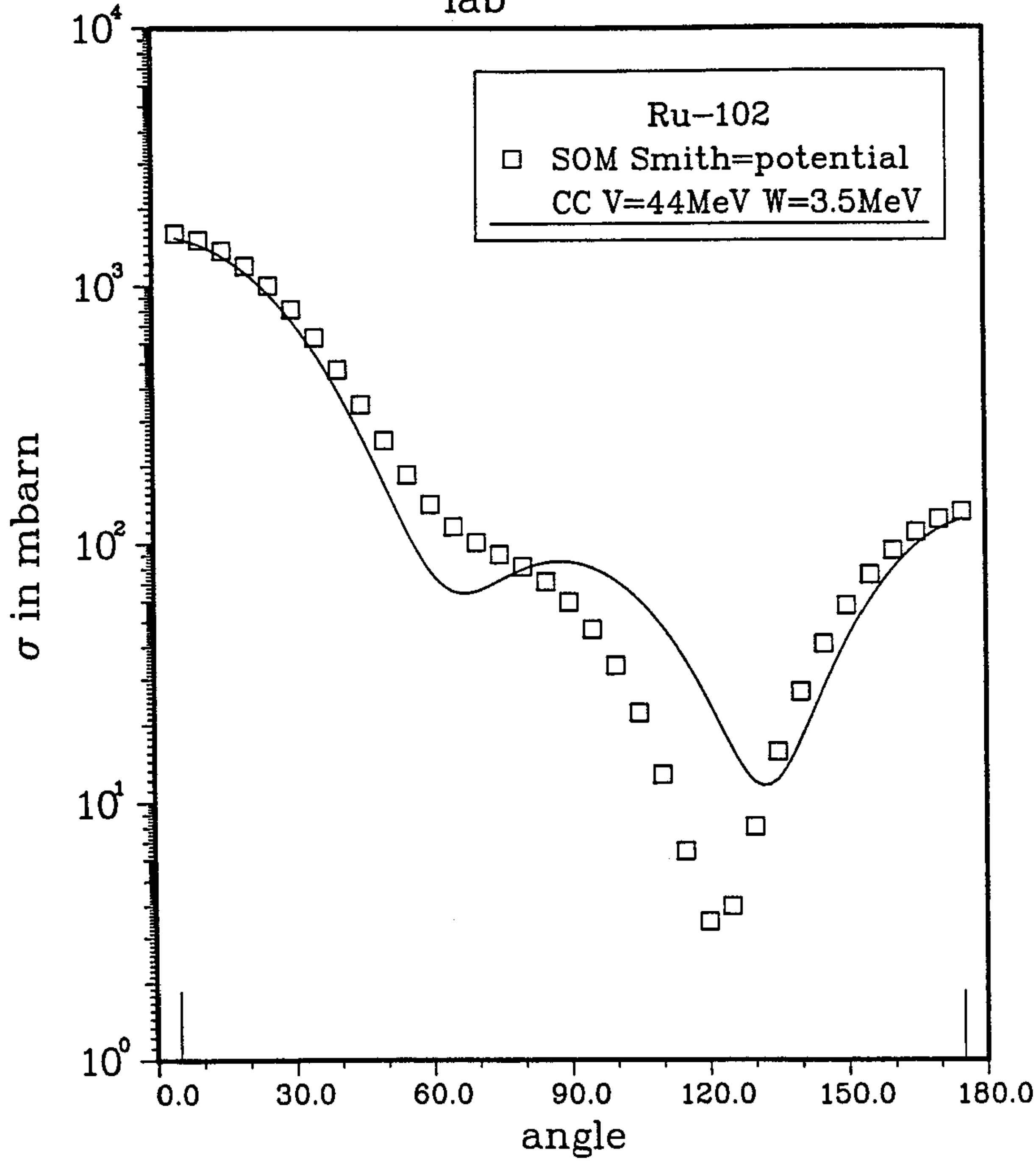
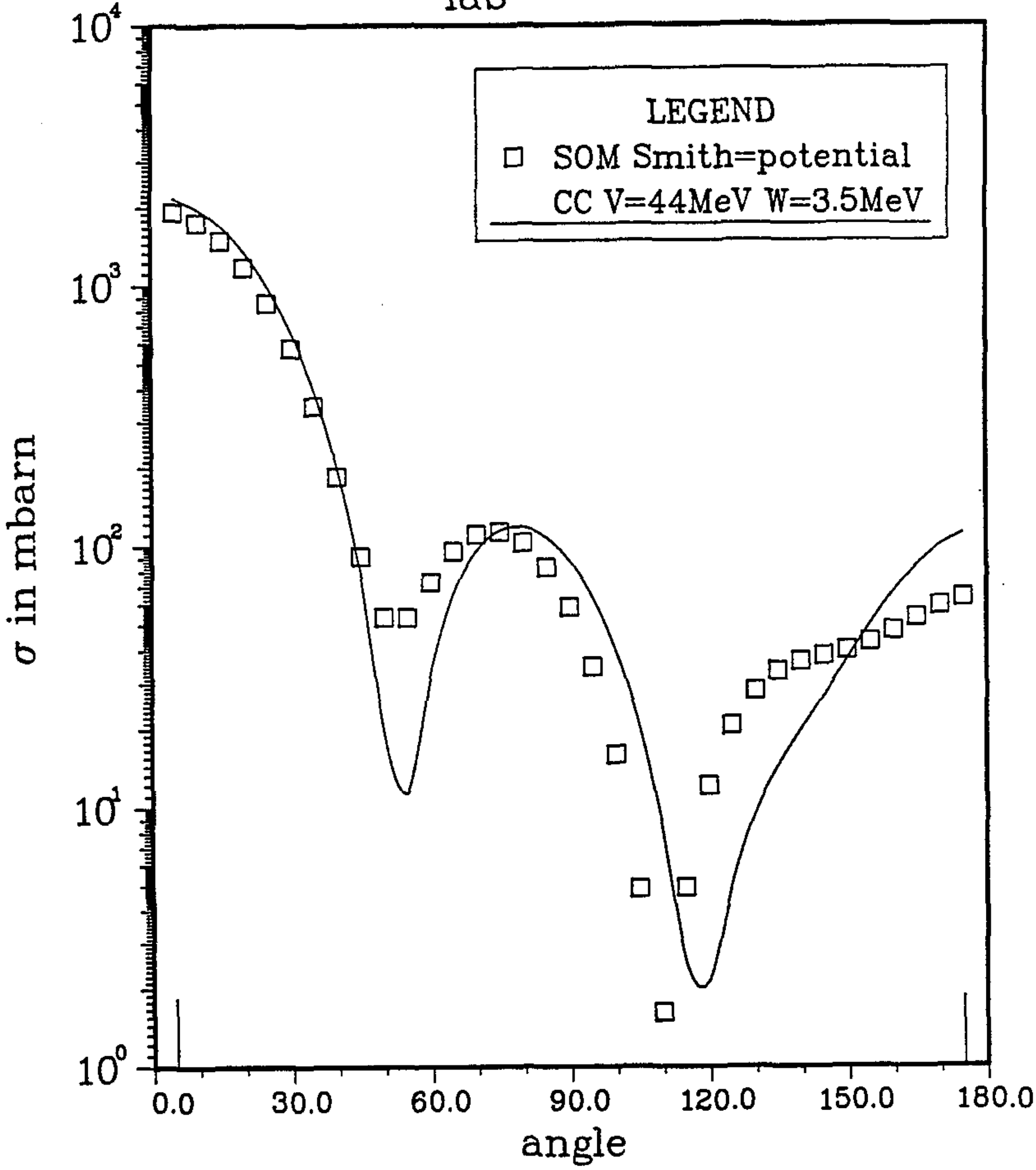


Fig. 6c
differential σ_{se}
SOM versus CC
E_{lab} = 4.0 MeV



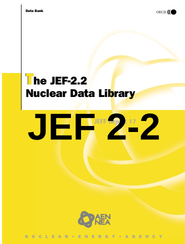


Fig. 7.
Inelastic scattering cross sections
for Ru–102

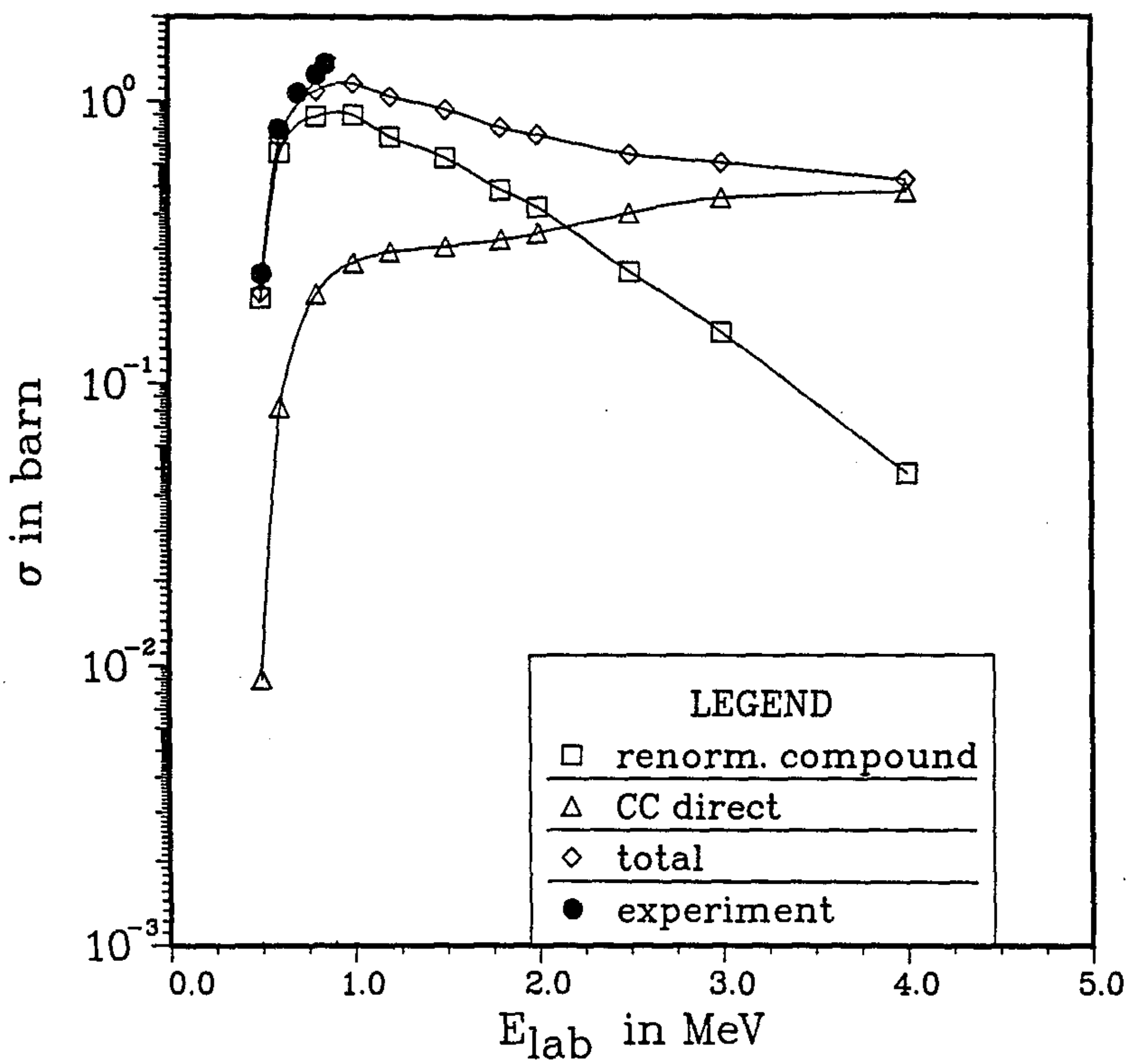
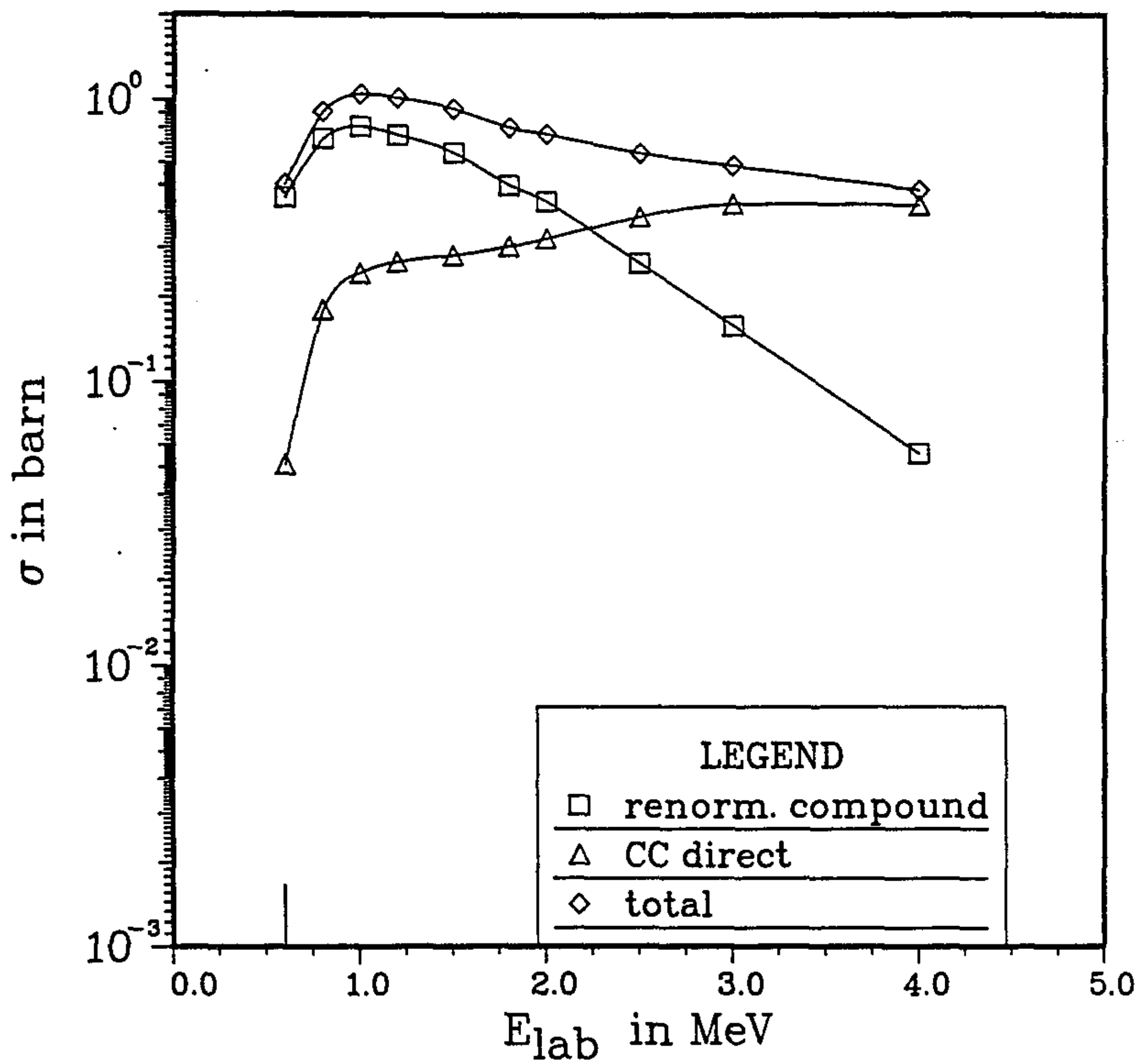


Fig. 8.
Inelastic scattering cross sections
for Pd–106



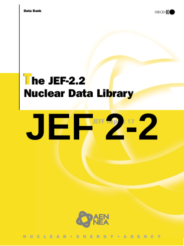


Fig. 9.
Inelastic scattering cross sections
for Ru–102

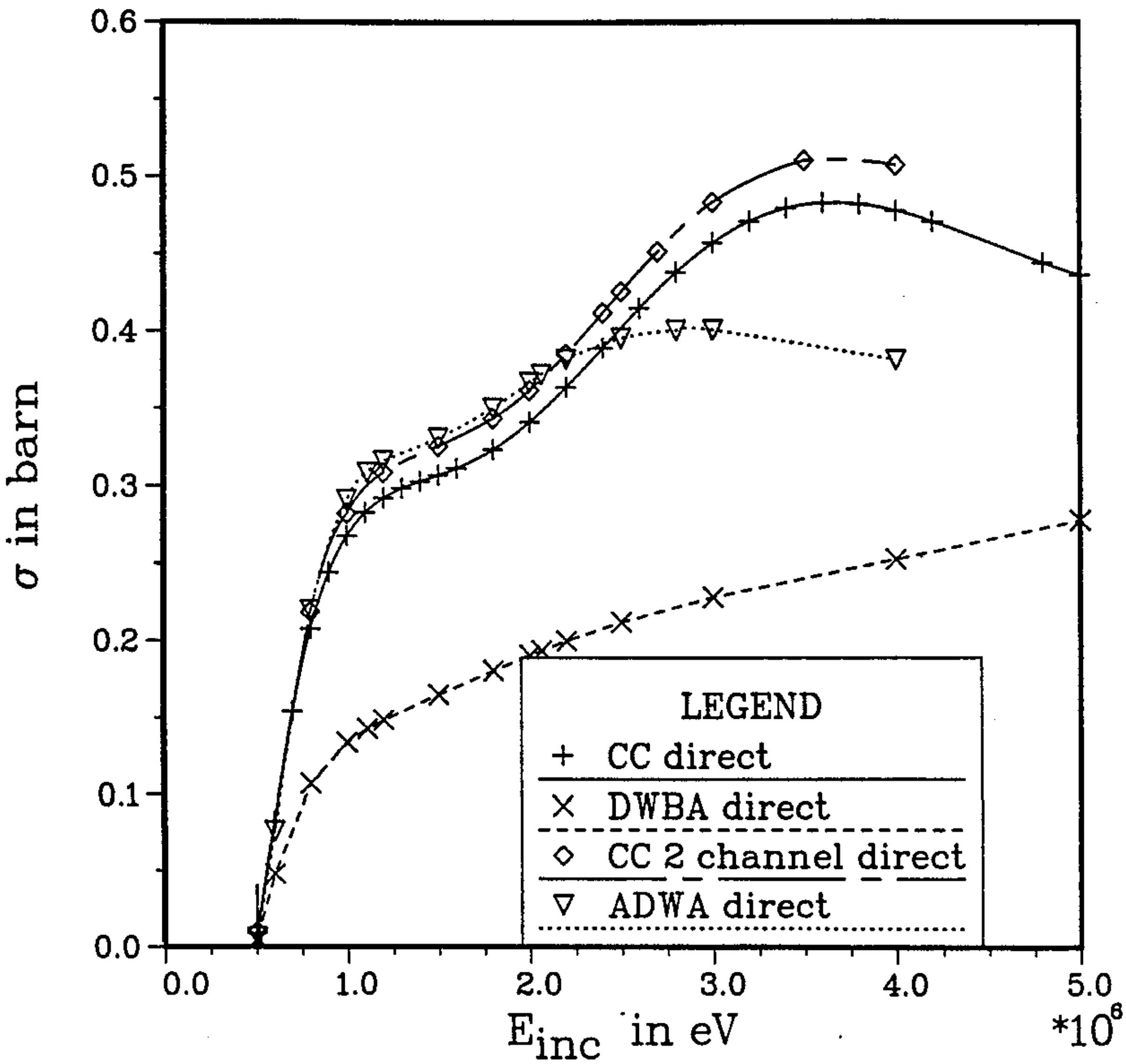
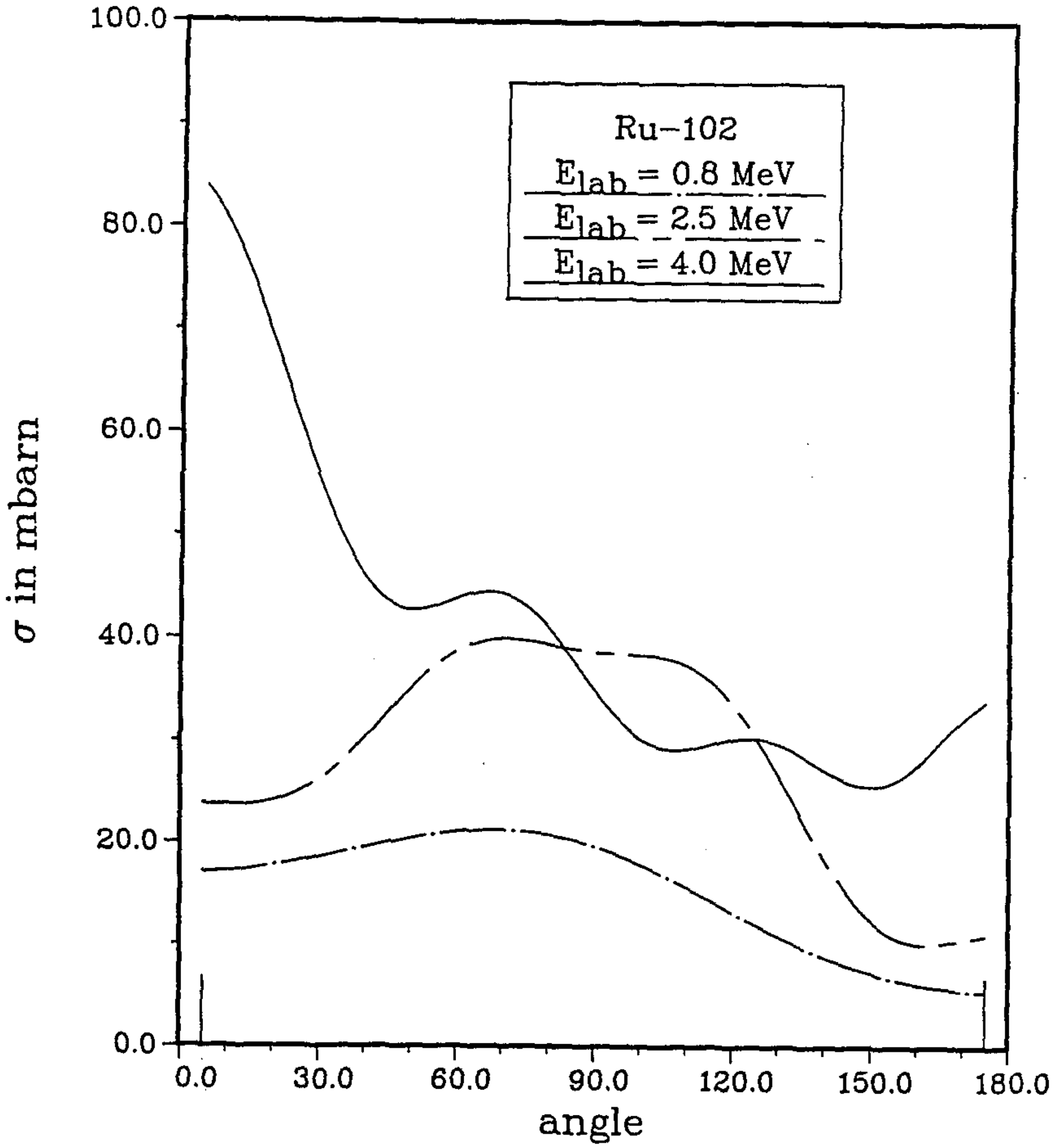


Fig. 10.
differential $\sigma_{nn'}$
V=44 MeV W=3.5MeV



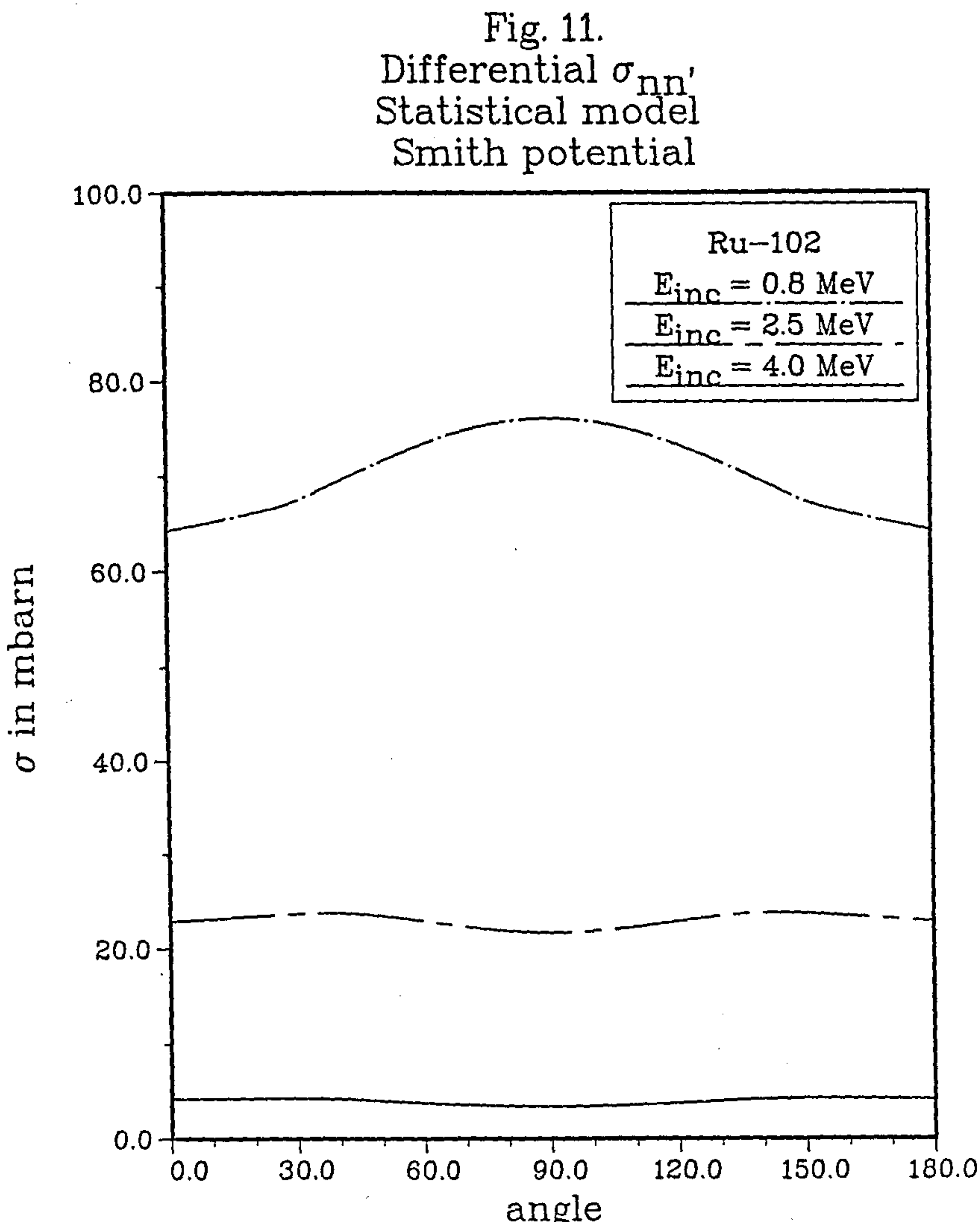


Fig. 11.
Differential $\sigma_{nn'}$
Statistical model
Smith potential
Ru–102
E_{inc} = 0.8 MeV
E_{inc} = 2.5 MeV
E_{inc} = 4.0 MeV
100.0
80.0
60.0
40.0
20.0
0.0
σ in mbarn
0.0
30.0
60.0
90.0
120.0
150.0
180.0
angle

1414029