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THE USE OF HAUSER-FESHBACH THEORY FOR PREDICTING INELASTIC SCATTERING OF NEUTRONS BY NUCLEI

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ABSTRACT

Cross sections for inelastic scattering of neutrons by nuclei are investigated using the Hauser-Feshbach theory. With transmission coefficients calculated from the optical model using a potential equivalent to the non-local potential of Perey and Buck, it is shown that it is possible to predict inelastic scattering cross sections with satisfactory results, provided corrections due to level width fluctuations are taken into account.

CONTENTS

1. INTRODUCTION

The Hauser-Feshbach theory of inelastic scattering (Hauser and Feshbach 1952) with transmission coefficients obtained from the optical model has, in the past, been fairly successful in fitting experimental data. Investigations by Auerbach and Moore (Auerbach and Moore 1964, 1967) who fitted elastic and inelastic scattering data by adjusting the optical model parameters, have shown that it is possible to find optical potentials which reproduce both the elastic and inelastic scattering cross sections. However, sets of optical model parameters for different nuclei differ in apparently unrelated ways so that no reliable estimate can be made of the inelastic scattering cross sections of nuclei for which little or no experimental data is available. Furthermore such fitting procedures are restricted to the range of incident neutron energies for which cross sections have been measured. Using the optical potentials obtained by such procedures, inelastic cross sections calculated for energies outside this range cannot be considered very reliable.

Attempts to predict inelastic cross sections using various 'general' optical potentials, such as the non-local potential of Perey and Buck (1962), have not been very successful. This has led to the belief (Towle and Gilboy 1963, Auerbach and Moore 1967) that the Hauser-Feshbach theory cannot be used to predict absolute inelastic scattering cross sections.

The work in this paper shows that this belief is unfounded and that it is possible, using the non-local potential of Perey and Buck, to predict with reasonable accuracy the inelastic scattering cross sections, provided level fluctuation effects (Lane and Lynn 1957, Moldauer 1961 and 1964) are taken into account. Certain inadequacies of the statistical theory are discussed.

2. THEORY

The cross section for inelastic scattering of neutrons with incident energy E_n, when the target undergoes the transition from its initial state i with spin I_o and parity π_o (taken to be the ground state) to a final state f with spin I_f, parity π_f, and excitation energy ϵ_f, is given, according to the Hauser-Feshbach theory (Hauser and Feshbach 1952) as

$$\sigma_{if} = \frac{\pi}{2(2I_o+1)} \sum_{\ell,j} T_{\ell}^{j}(E_n) \sum_{J} \frac{2J+1}{D_{\ell J}} \sum_{\ell',j'} T_{\ell'}^{j'}(E_f) \quad . \qquad .....(1)$$

with

$$D_{\ell J} = \sum_{p,\ell'',j''} T_{\ell''}^{j''}(E_p) \quad . \qquad .....(2)$$

The summation over p is to be taken over all accessible levels $\epsilon_p < E_n$. $T_{\ell}^{j}(E)$ are the transmission coefficients of a neutron with energy E, orbital angular momentum

ℓ and total angular momentum j, and

$$E_f = E_n - \epsilon_f$$
$$E_p = E_n - \epsilon_p \quad .$$

The angular momentum quantum numbers ℓ, ℓ', ℓ'', j, j', j" and J must satisfy

$$j = \ell \pm 1/2 \quad \text{(similarly for } j' \text{ and } j''\text{)}$$
$$|I_o - j| \leq J \leq (I_o + j)$$
$$|J - I_f| \leq j' \leq (J + I_f)$$
$$|J - I_p| \leq j' \leq (J + I_p)$$
$$(-1)^{\ell}\, \pi_o = (-1)^{\ell'}\, \pi_f$$
$$(-1)^{\ell}\, \pi_o = (-1)^{\ell''}\, \pi_p \quad .$$

When the energy of the incident neutron is increased, a point is reached where it is possible to excite the final nucleus to energies where full information about the level structure is not available. It is therefore assumed that in these regions of excitation energy the levels can be represented by a continuum with a density $\rho(I,\pi,\epsilon)$ for levels with spin I, parity π and excitation energy ϵ.

The inelastic scattering cross section for final excitation between ϵ and $\epsilon + d\epsilon$ is (Hauser and Feshbach 1952, Towle and Owens 1967)

$$\sigma(E_n,E_f)d\epsilon_f = \frac{\pi}{2(2I_o+1)k^2} \sum_{\ell,j} T_\ell^j(E_n) \sum_J \frac{2J+1}{D_{\ell J}} \sum_{I_f,\pi_f} \sum_{j',\ell'} T_{\ell'}^{j'}(E_f)\, \rho(I_f,\pi_f,\epsilon_f)d\epsilon_f \quad , \qquad .....(3)$$

where

$$D_{\ell J} = \sum_{p,\ell'',j''} T_{\ell''}^{j''}(E_p) + \sum_{I_p,\pi_p} \sum_{j''\ell''} T_{\ell''}^{j''}(E_p)\ (I_p,\pi_p,\epsilon_p)d\epsilon_p \quad . \qquad .....(4)$$

The summation in Equation 4 extends over all individual levels. The lower limit ϵ_o of the integral is the energy of the highest level in the level scheme.

For cases where only a small number of levels are excited in the course of the inelastic scattering process, as is so with low incident neutron energies, analyses of the statistical theory have shown (Lane and Lynn 1957, Moldauer 1961, 1964) that the Hauser-Feshbach theory as it stands is not satisfactory. In such cases the effects due to level width fluctuations may be very important. In order to take into account the corrections due to fluctuations the expression for the inelastic scattering cross section, Equation 1, is replaced by (Moldauer et al. 1964)

$$\sigma_{if} = \frac{\pi}{2(2I_o+1)k^2} \sum_{\ell,j} T_\ell^j(E_n) \sum_J \frac{2J+1}{D_{\ell J}} \sum_{j',\ell'} S_{\ell'}^{j'} T_{\ell'}^{j'}(E_f) \quad . \qquad .....(5)$$

Using the Porter-Thomas level distribution function (Porter and Thomas 1956) the fluctuation corrections $S_{\ell'}^{j'}$ can be expressed as (Moldauer et al. 1964)

$$S_{\ell'}^{j'} = \int_0^\infty \frac{1 + 2\,\delta_{if}}{\left[1+2t\,T_\ell^j(E_n)/D_{\ell J}\right]\left[1+2t\,T_{\ell'}^{j'}(E_f)/D_{\ell J}\right] \prod_{\ell'',j'',p} \left[1+2t\,T_{\ell''}^{j''}(E_p)/D_{\ell J}\right]^{\frac{1}{2}}}\, dt \; .$$

Apart from being very complicated it is of course not useful to apply these corrections to Equation 3 as this equation can only be used when the number of competing final levels is very large, in which case the quantities $S_{\ell'}^{j'}$ are all approximately equal to unity.

3. METHOD OF CALCULATION

Calculations of the inelastic, compound elastic, and differential elastic scattering cross sections were carried out for the nuclei ^{27}Al, ^{56}Fe, ^{208}Pb and ^{238}U using the computer code COMPOST (Bertram 1969a). The transmission coefficients and the differential elastic scattering cross sections were obtained from the optical model using a potential of the form

$$\mho = \mho_L(r) - \mho_s(r)\, \underset{\sim}{\sigma}\cdot\underset{\sim}{\ell} \quad . \qquad .....(7)$$

The potential $\mho_L$ is the local equivalent of the non-local potential $\mho_{NL}$ of Perey and Buck (1962).

$$\mho_L = \exp\left\{\frac{m\alpha^2}{2\hbar^2}(E - \mho_L)\right\} = \mho_{NL} \quad , \qquad .....(8)$$

with

$$\begin{aligned} \mho_{NL} &= Vf(r) + iWg(r) \\ f(r) &= [\,1 + \exp(r-R)/d_1\,]^{-1} \\ g(r) &= 4\exp[\,(r-R)\,d_2]\,\{1 + \exp[\,(r-R)/d_2\,]\,\}^{-2} \; . \end{aligned} \qquad .....(9)$$

The spin orbit interaction was taken to be of the form

$$\mathcal{V}_s(r) = V_s \left(\frac{\hbar^2}{\mu c}\right)^2 \frac{1}{r} \left|\frac{df(r)}{dr}\right| \quad , \qquad .....(10)$$

where μ is the π-meson mass.

The parameters, which remained fixed throughout our calculations, were those obtained by Perey and Buck (1962) from the scattering of 7 MeV and 14.5 MeV neutrons by lead:

$$V = 71 \text{ MeV}$$

$$W = 15 \text{ MeV}$$

$$V_s = 7 \text{ MeV}$$

$$R = 1.22A^{1/3}$$

$$d_1 = 0.65 \text{ F}$$

$$d_2 = 0.47 \text{ F}$$

$$\alpha = 0.85 \text{ F} \quad .$$

The elastic scattering angular distributions were obtained by adding the compound elastic cross section, as calculated from the Hauser-Feshbach theory, to the shape elastic cross section. The angular distribution of the compound nucleus contribution to the elastic scattering was assumed to be isotropic.

The calculations of the inelastic scattering cross sections, when the incident neutron energies were sufficiently high, were performed assuming a density $\rho(I,\pi,\epsilon)$ of levels of the form

$$\rho = K \frac{(2I+1)\ \exp(2\sqrt{aU})}{1.796\ aAU^2} \quad , \qquad .....(11)$$

where $U = \epsilon - P(Z) - P(N)$,

$a = (0.00917\,\delta + 0.142)A$,

$\delta = S(Z) + S(N)$,

$P(Z), P(N)$ are the pairing energies ,

and $S(Z), S(N)$ are the shell corrections.

This is the form given by Gilbert and Cameron (1965), but without the spin cut-off factor. The normalisation constant K which does not appear in the formula of Gilbert and Cameron was found (Towle and Owens 1967) to be necessary in order to obtain the correct magnitude of the cross sections for the individual levels.

4. RESULTS

4.1 Aluminium

The inelastic scattering cross sections, calculated for neutron energies from 1.5 MeV to 5 MeV using the level scheme (Table 1) of Towle and Owens (1967), are compared with the experimental data of Towle and Gilboy (1962) and Tsukada et al. (1962) in Figure 1.

Only for the (0.842 + 1.013) MeV and the 2.212 MeV levels is sufficient experimental data available. For the higher levels experimental results consist of only one point, except for the measurements by Tsukada et al. for the (2.73 + 2.98 + 3.00) MeV levels. These however, do not agree with the results of Towle and Gilboy. The cross sections for the (0.842 + 1.013) MeV and the 2.21 MeV levels, calculated without fluctuation corrections, show disagreement with experiment when the incident energy is less than about 3 MeV. For energies greater than this, agreement is quite good. This is to be expected when fluctuation corrections are ignored.

With the level scheme used (Table 1), cross sections with fluctuation corrections can be calculated only for incident energies up to 4.5 MeV. As can be seen from Figure 1, when fluctuations are included the calculated cross sections are in very good agreement with experiment, although because of the lack of data, the results for the higher levels cannot be considered too meaningful.

For elastic scattering at 4 MeV (Figure 2c) the agreement between theory and experiment is only fair and becomes worse at lower energies (Figure 2a and b). The compound elastic contributions calculated with fluctuations are too large, and relatively better agreement is obtained when fluctuation corrections are not included. Total cross sections of ^{27}Al (Stehn et al. 1964) show resonances below approximately 3.5 MeV, which probably account for the disagreement between theory and experiment at these energies.

4.2 Iron

Calculations of inelastic scattering cross sections of ^{56}Fe for 7 MeV incident neutrons were done by Towle and Owens (1967). Using the parameters of Perey and Buck and a level density formula not much different from the one we have used, their results were in good agreement with their experimental measurements.

Our predicted cross sections without fluctuation corrections, calculated for neutron energies from 1 MeV to 5 MeV using the level scheme (Table 2) of Towle and Owens, are in good agreement with experiment for all levels except the 0.845 MeV level (Figure 3). For this level the calculated cross sections are too large at low energies and too small at high energies. The latter is probably caused by the onset of direct reaction mechanisms at approximately 4 MeV (see for example Towle and Owens 1967). When fluctuations are taken into account the theoretical results are in good agreement with experiment, even for the 0.845 MeV level near threshold.

For elastic scattering at 2 and 4 MeV, (Figure 4) there is good agreement between theory and experiment although again, as for ^{27}Al, the compound nucleus contributions are too large when fluctuations are included. For 1 MeV incident neutrons the results are not so good; however this is probably due to the resonant nature of the cross sections below 2 MeV (Gilboy and Towle 1964).

4.3 Lead

The theoretical cross sections without fluctuation corrections (Figure 5) do not at all agree with the experimental results of Towle and Gilboy (1963) whose level scheme (Table 3) we used in our calculations. For the 2.615 MeV and 3.475 MeV levels the calculations are out by as much as a factor of 2. The theoretical results are greatly improved when fluctuation corrections are taken into account. The results for the 2.615 MeV level at incident energies greater than 3.5 MeV are in good agreement with experiment. However, from threshold up to 3.5 MeV the theoretical cross section still increases too rapidly with increasing energy. The calculated cross sections for the 3.198 MeV and 3.475 MeV levels appear to become too large at energies greater than about 4.2 MeV. This is probably due to the omission of levels between 4.0 and 4.3 MeV in the level scheme (Towle and Gilboy 1963). These levels, the spins of which are not known, could very well affect the cross sections for the 3.198 MeV and 3.475 MeV.

The results for elastic scattering (Figure 6) are quite good although at 2.2 and 3.2 MeV there are discrepancies at large scattering angles. At 2.2 MeV incident energy (Figure 6a) the compound nucleus contributions calculated with and without fluctuations are identical as there are no other channels competing. At 4.1 MeV the theoretical cross sections are in very good agreement with experiment when the contributions due to compound elastic scattering are calculated using fluctuations.

4.4 Uranium

Experimental data on inelastic scattering cross sections of ^{238}U is extensive for neutron energies up to 1.6 MeV. For our calculations we have used the level scheme (Table 4) of Barnard et al. (1966). However, the spins and parities of the levels above 838 keV are not certain. The measurements of Smith (1963) are rather problematic when referred to this level scheme. The energy of the 1^- level given by Smith as 630 ± 20 keV does not agree with the result of Barnard et al. who gives 681 keV. In view of the inconsistency here it is difficult to interpret the measurements of Smith for the 1000 ± 30 keV and the 1050 ± 30 keV levels. We have assumed them to correspond to the (0.968 + 1.006) MeV levels and the (1.047 + 1.076) MeV levels respectively. This may not be correct and could account for the differences between the measurements of Smith and those of Barnard et al.

The theoretical cross sections agree very well with experiment (Figure 7) except for the 45 keV and 681 keV levels. When fluctuations are ignored the results for the 45 keV levels are particularly bad; the calculated cross section rises to 3 barns at 0.25 MeV. Even when fluctuations are taken into account there are still large discrepancies between theory and experiment below 0.5 MeV incident energies, although above 0.5 MeV the results are much improved.

The results for elastic scattering (Figure 8) are not good. When fluctuations are included, the compound elastic contribution tends to be too large. The fits are only improved slightly when fluctuations are omitted.

5. DISCUSSION

The non-local potential of Perey and Buck, or any potential equivalent to it, has been fairly successful in predicting differential elastic, absorption and total cross sections. An example is the analysis by Wilmore (1964) who investigated eight nuclei in the mass range A > 28 for incident neutron energies between 1 and 14 MeV. The optical model can of course only describe average properties of the nuclear many-body system, especially when spherically symmetric potentials are used. In view of this, our results are quite good, although for particular nuclei better results can be obtained by varying the parameter of the optical potentials (Auerbach and Moore 1964, 1967). However, such procedures are rather limited in their usefulness and their results provide little information as to the accuracy of the statistical theory used.

An interesting feature of our results for ^{208}Pu and ^{238}U is the difference between theory and experiment near the inelastic scattering threshold. Although a more extensive investigation of the heavy nuclei is needed, it appears that such discrepancies exist for most heavy nuclei. Similar discrepancies for heavy nuclei have been found in (n,2n) reactions (Bertram 1969b). When the (n,2n) excitation functions given by the statistical theory were compared with experiment, they were also found to increase too rapidly with energy. This seems to suggest that the differences between theory and experiment near the inelastic scattering threshold are not so much due to a failure of the Perey and Buck (1962) optical potential at low neutron energies, but are caused by a breakdown of the statistical theory itself, at least the form of it that we have used.

If these discrepancies were caused by the incorrect low energy behaviour of the potentials then we would expect similar discrepancies to occur in the inelastic scattering cross sections for all levels near their respective thresholds and not just for the first excited state. It may be noted that from Equation 5 it does not necessarily follow that the sum of inelastic scattering cross sections and the compound elastic scattering cross section is equal to the optical model absorption cross section. In this respect the Hauser-Feshbach theory with fluctuations is not self-consistent. A rigorous analysis of the statistical theory by Moldauer (1961, 1964) has shown that the use of the optical model transmission coefficients in the Hauser-Feshbach theory is only an approximation and that one should instead use modified transmission coefficients. However, modified transmission coefficients have the effect of increasing the inelastic scattering cross sections. Calculations for ^{56}Fe by Barnard et al. (1968) have shown that these corrections can increase cross sections by up to 15 per cent.

These corrections can be expected to be much more important for compound elastic scattering due to the appearance of a resonance interference term (Moldauer 1964). The omission of this term from Equation 5 is the main cause of the result that the sum of the inelastic and compound elastic scattering cross sections does not equal the absorption cross section and it explains why the compound elastic scattering cross sections calculated with fluctuation corrections are too large.

6. CONCLUSION

The results of our calculations show that, at least for those nuclei we have considered, it is possible to predict inelastic scattering cross sections with reasonable accuracy using the Hauser-Feshbach theory with fluctuation corrections and using transmission coefficients obtained from the optical model with the potential of Perey and Buck.

The Hauser-Feshbach theory with fluctuation corrections is not self-consistent; the sum of the cross sections over all outgoing channels does not equal the absorption cross section of the optical model.

The main cause of this is the omission of resonance interference effects. Without resonance interference the compound elastic scattering cross sections are much too large. A more satisfactory method for calculating the compound elastic scattering cross section is subtraction of the total inelastic scattering cross section from the absorption cross section. This at least ensures self-consistency and in most cases produces more accurate results.

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TABLE 1

ENERGY LEVELS OF ^{27}Al (AFTER TOWLE AND OWENS 1967)

Energy (MeV)	J^{π}
0	$5/2^+$
0.842	$1/2^+$
1.013	$3/2^+$
2.212	$7/2^+$
2.731	$5/2^+$
2.980	$3/2^+$
3.000	$9/2^+$
3.674	$1/2^+$
3.950	$3/2^+$
4.050	$1/2^-$
4.400	$5/2^+$
4.500	$1/2^+$

TABLE 2

ENERGY LEVELS OF ^{56}Fe (AFTER TOWLE AND OWENS 1967)

Energy (MeV)	J^{π}
0	0^+
0.846	2^+
2.084	4^+
2.654	2^+
2.939	0^+
2.957	2^+
3.119	5^-
3.122	3^+
3.368	2^+
3.388	6^+
3.445	3^+
3.450	1^+

TABLE 3

ENERGY LEVELS OF ^{208}Pb (AFTER TOWLE AND GILBOY 1963)

Energy (MeV)	J^{π}
0	0^+
2.615	3^-
3.198	5^-
3.475	4^-
3.703	5^-
3.750	(3^-)
3.961	6^-
4.30	4^+

TABLE 4

ENERGY LEVELS OF ^{238}U (AFTER BARNARD ET AL. 1965)

Energy (keV)	J^{π}
0	0^+
45	2^+
149	4^+
300	6^+
681	1^-
732	3^-
838	5^-
939	(2^+)
966	(2^+)
1006	(0^+)
1047	(2^+)
1076	(2^+)
1123	(1^+)
1150	(4^+)

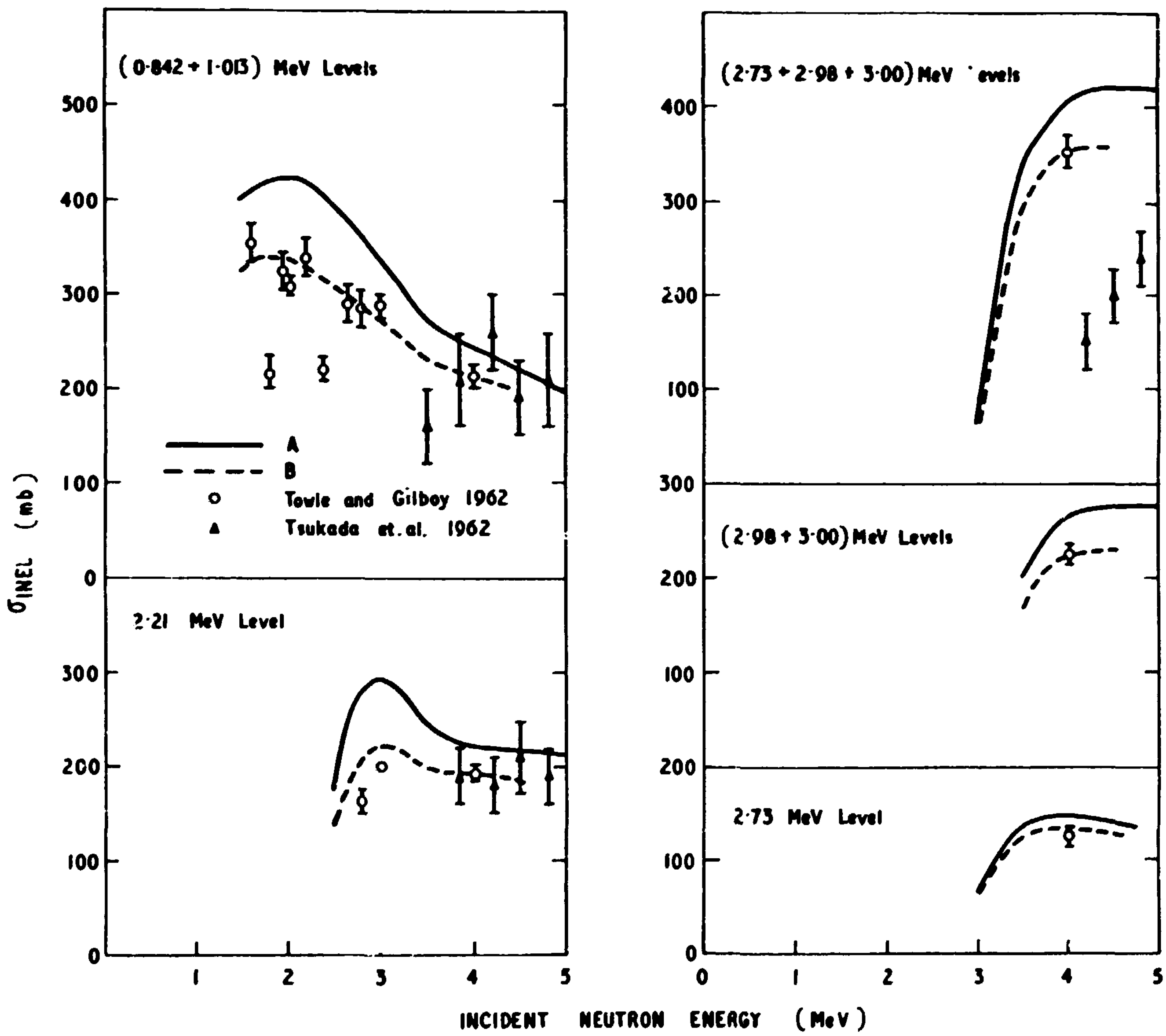

FIGURE 1. INELASTIC SCATTERING CROSS SECTIONS OF ^{27}Al PREDICTED USING THE PARAMETERS OF PEREY AND BUCK (1962) AND HAUSER FESHBACH THEORY WITHOUT FLUCTUATIONS (CURVE A) AND WITH FLUCTUATIONS (CURVE B)

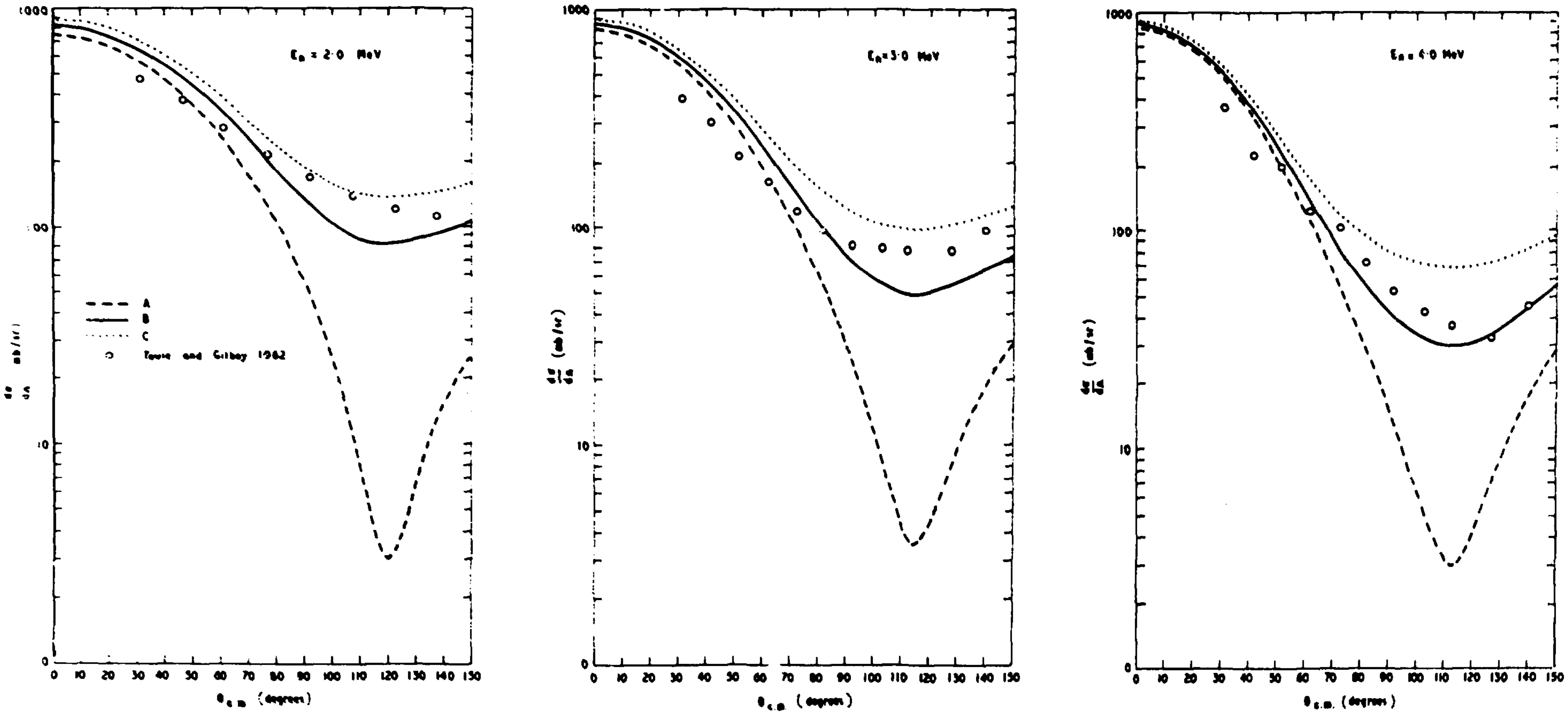

FIGURE 2. DIFFERENTIAL ELASTIC SCATTERING CROSS SECTIONS OF ^{27}Al FOR VARIOUS INCIDENT NEUTRON ENERGIES, CALCULATED USING (i) THE OPTICAL MODEL WITH PEREY AND BUCK PARAMETERS (CURVE A), (ii) COMPOUND ELASTIC SCATTERING CONTRIBUTIONS FROM THE HAUSER-FESHBACH THEORY WITHOUT FLUCTUATIONS (CURVE B), AND (iii) COMPOUND ELASTIC SCATTERING CONTRIBUTIONS FROM THE HAUSER FESHBACH THEORY WITH FLUCTUATION CORRECTIONS (CURVE C)

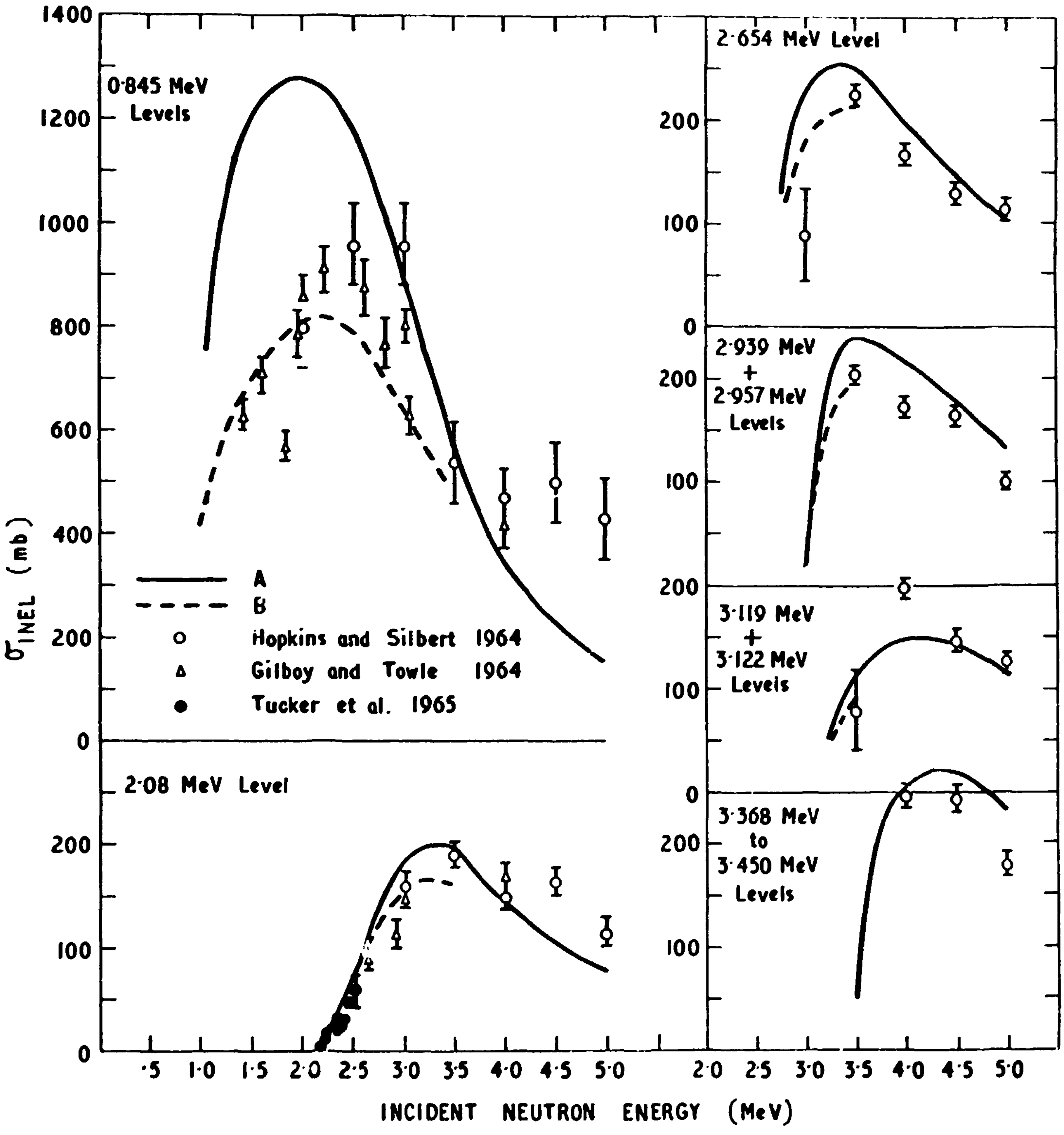

FIGURE 3. INELASTIC SCATTERING CROSS SECTIONS FOR ^{56}Fe

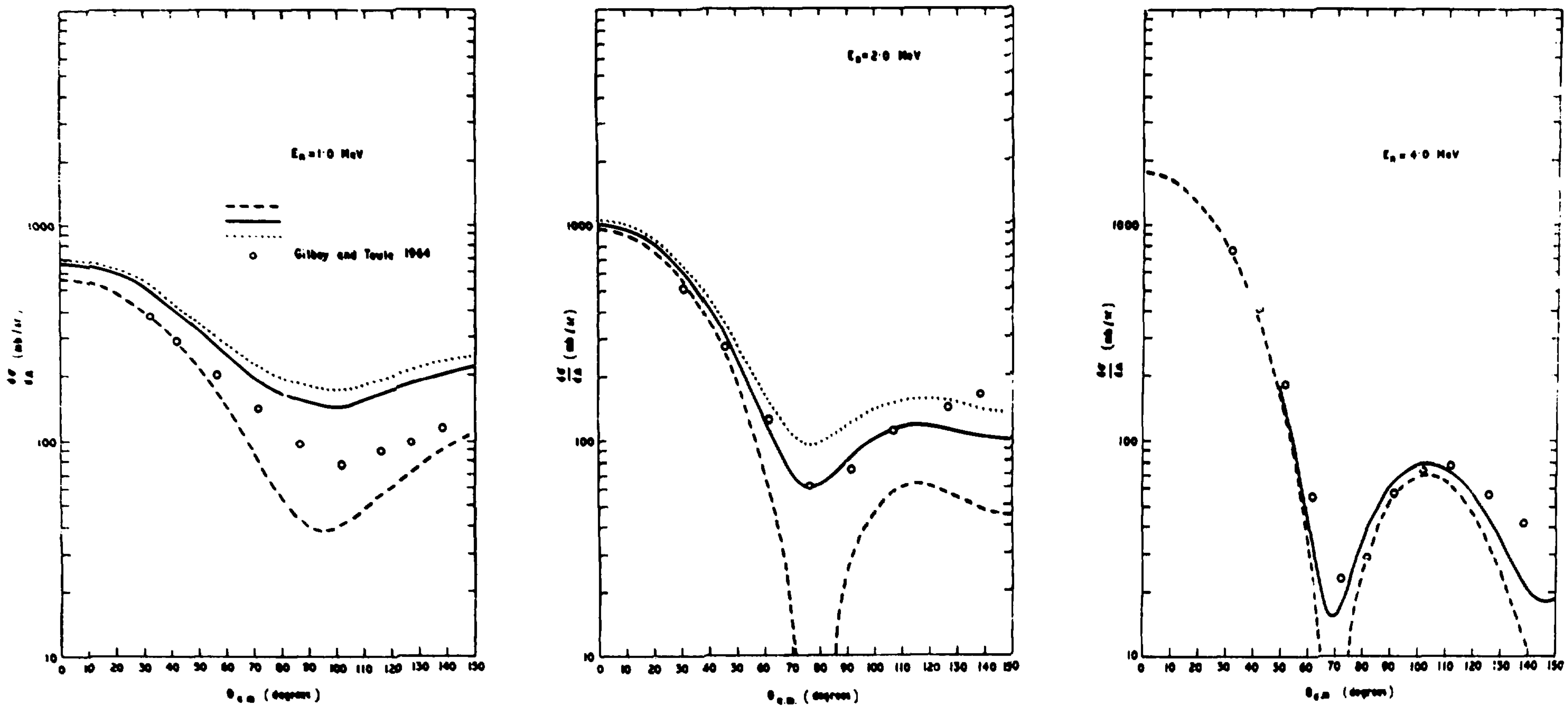

FIGURE 4. DIFFERENTIAL ELASTIC SCATTERING CROSS SECTIONS FOR ^{56}Fe

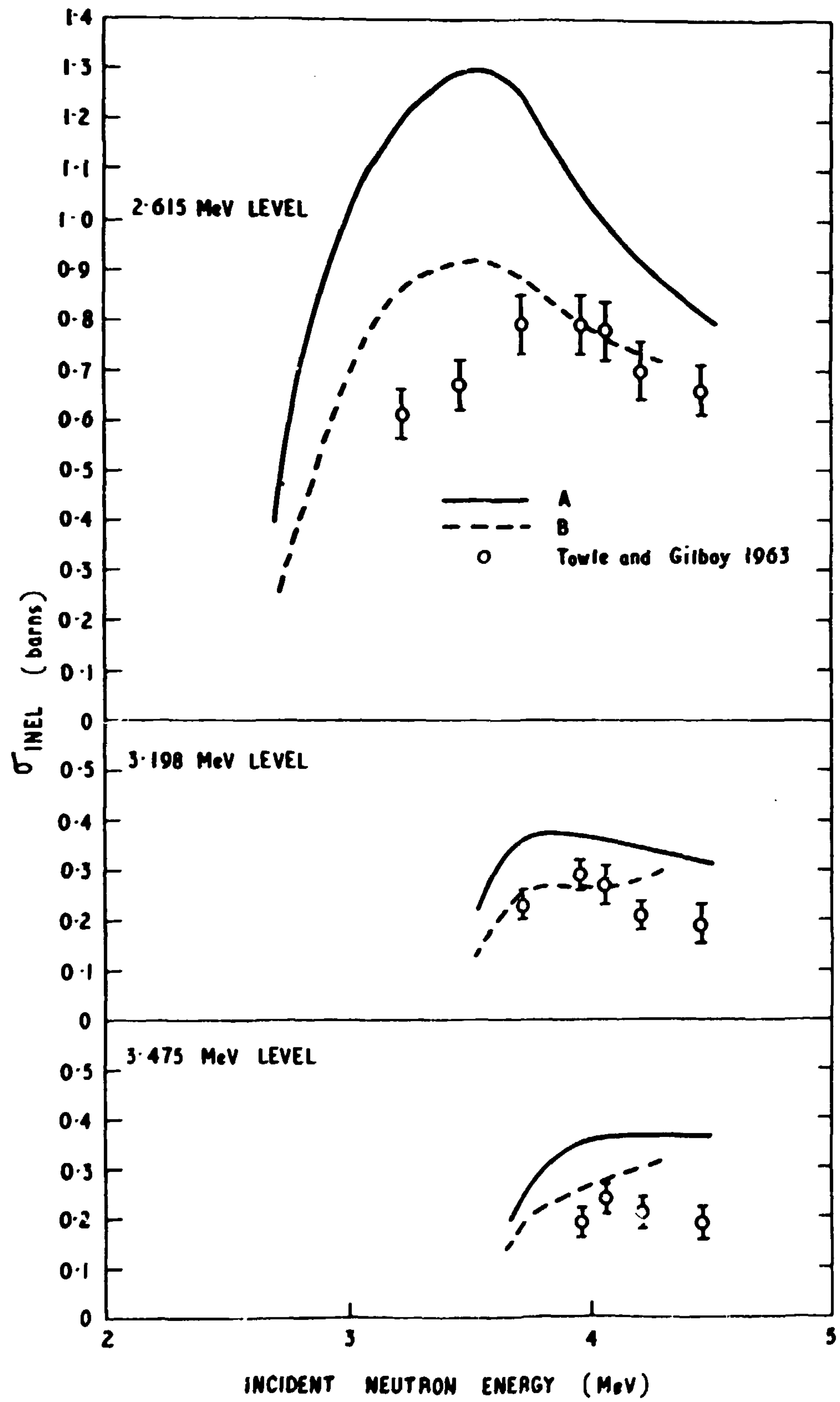

FIGURE 5. INELASTIC SCATTERING CROSS SECTIONS FOR ^{208}Pb

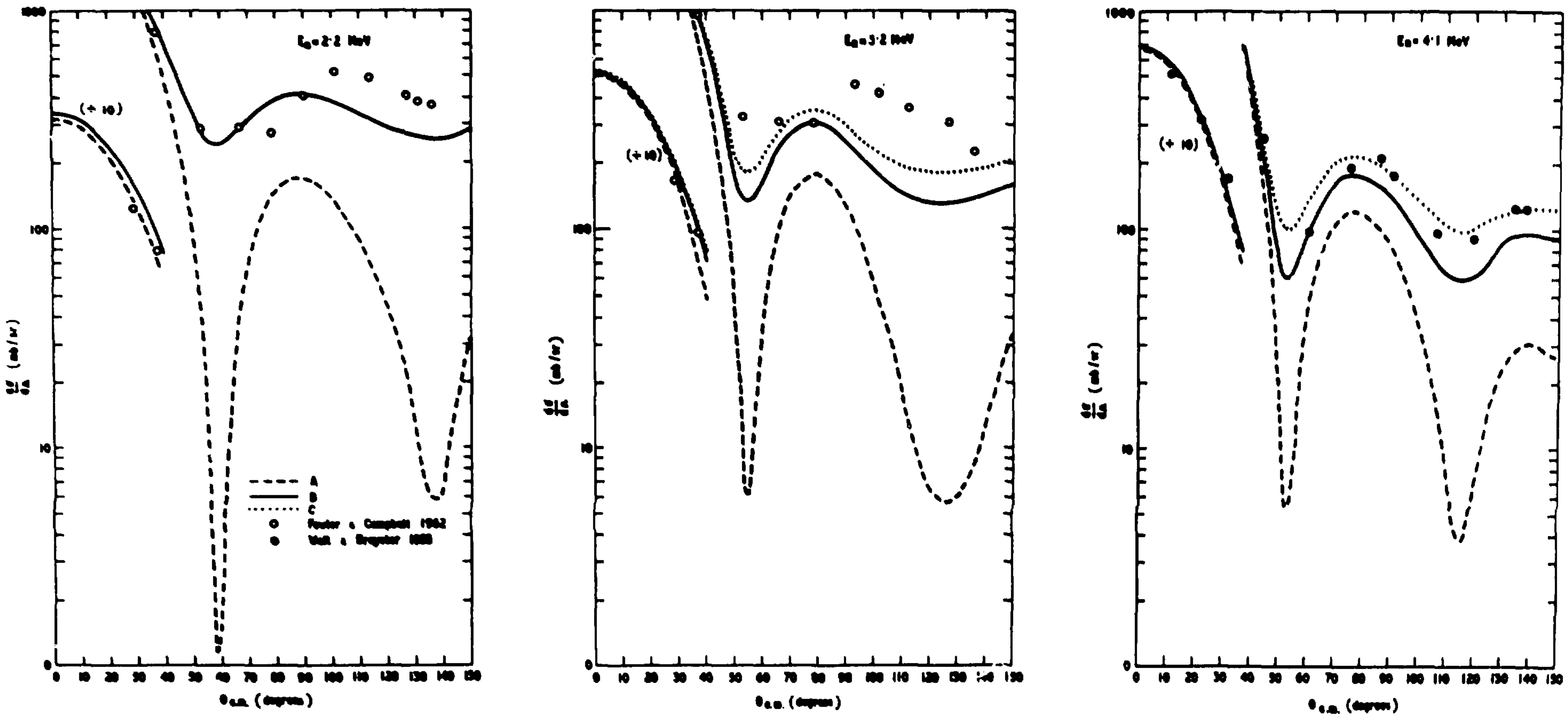

FIGURE 6. DIFFERENTIAL ELASTIC SCATTERING CROSS SECTIONS FOR ^{208}Pb

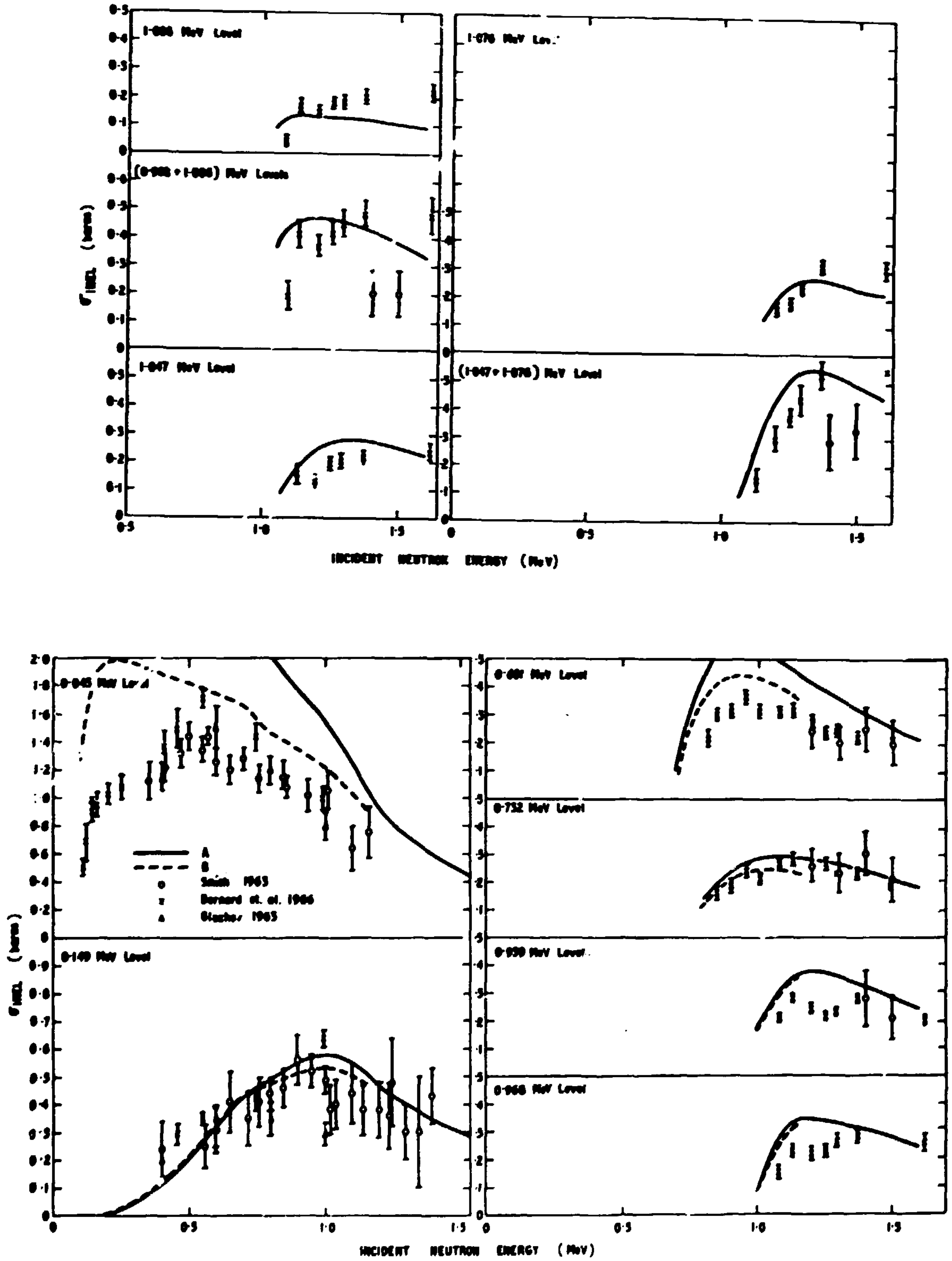

FIGURE 7. INELASTIC SCATTERING CROSS SECTIONS FOR ^{238}U

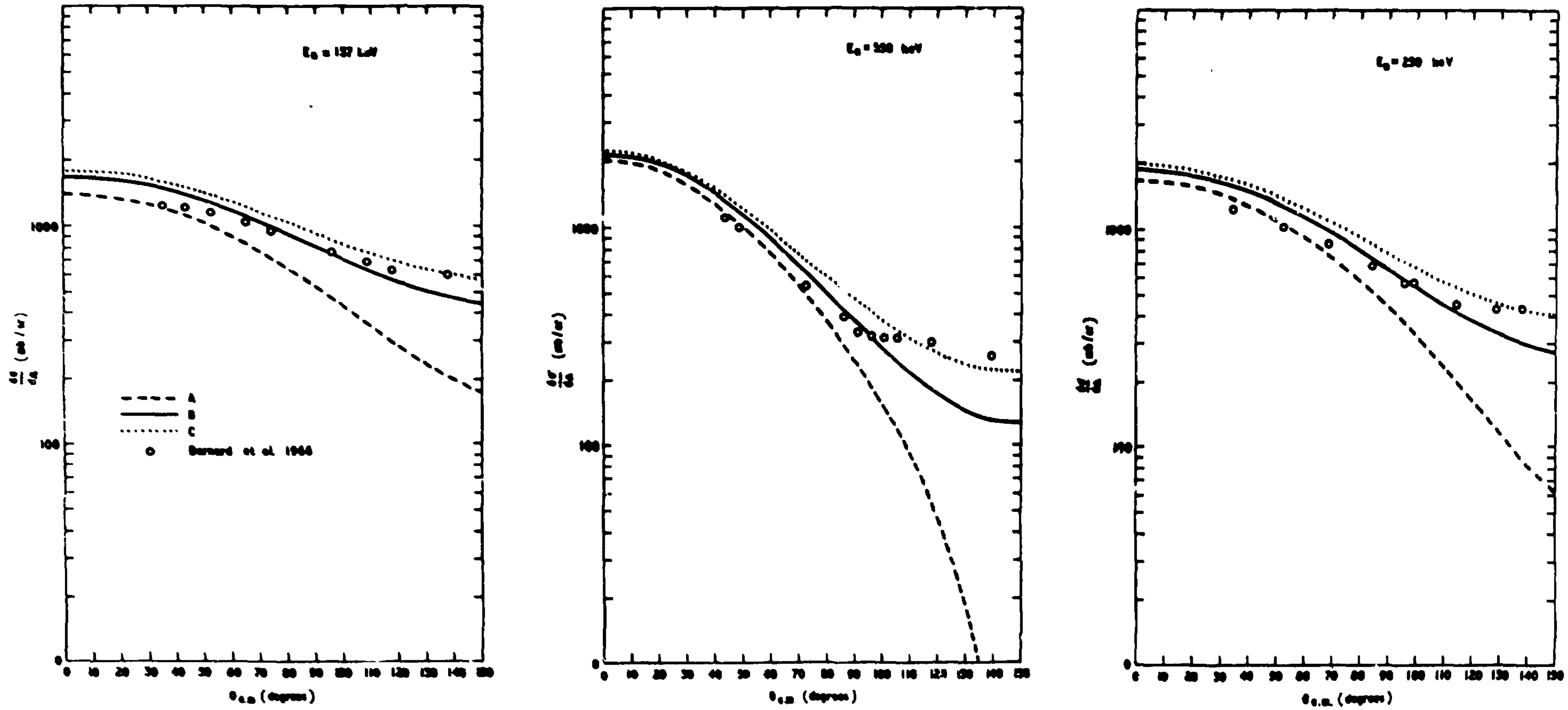

FIGURE 8. DIFFERENTIAL ELASTIC SCATTERING CROSS SECTIONS FOR ^{238}U