EVALUATION OF NEUTRON CROSS SECTIONS: CALCULATIONAL METHODS AND EVALUATED LIBRARIES

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A Paper to be Presented at the Conference on Nuclear Data - Microscopic Cross Sections and Other Data Basic for Reactors, in Paris, France, October 17-21, 1966.

*Operated for the United States Atomic Energy Commission by the General Electric Company, Contract No. W-31-109-Eng.-52

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In this paper we will outline two theoretical models which are useful, in conjunction with experimental data, in providing neutron cross sections for reactor and shielding calculations. We will also describe several derived data sets which we currently recommend.

1. OPTIC - A program for the calculation of nuclear cross sections using the optical model plus resonant phase shifts

OPTIC [1] calculates total, shape-elastic, and reaction cross sections, using an optical model plus resonant contributions described by R-matrix theory. By including the resonance contributions, OPTIC is able to describe fluctuations in the scattering (total) cross section which cannot be accounted for with a simple optical model.

For light nuclei like carbon and oxygen, resonance structure is clearly resolved below 10 Mev. Optical-model fits tend to become unsatisfactory below this energy. On the other hand, R-matrix theory has difficulties, stemming from the assumption that the nucleus scatters like a hard sphere. OPTIC therefore calculates the scattering from an optical potential instead of a hard-sphere model. This particular combination of optical and resonant phase shifts has no rigorous justification, but it is clear that a relationship exists between the optical model and the infinity of levels in R-matrix theory. Replacing the hard-sphere phase shift by an optical one is a reasonable way of accounting for these distant levels.

At energies sufficiently low so that only elastic scattering can occur, the quantum numbers j and ℓ (total and orbital angular momentum) characterize the phase shift, which for chargeless particles is given by

$$\tan^{-1}\left[R_{j\ell}(E)P_\ell(kR)/(1 - R_{j\ell}(E)\tilde{S}_\ell(kR))\right] + \phi_{j\ell}(kR)$$

with the following notation:

$R_{j\ell}(E)$ is the single-channel R-function: $\sum_\lambda \gamma_\lambda^2/(E_\lambda - E) + R_{j\ell o}$ ($R_{j\ell o}$ reflects the effect of distant levels);

R is the nuclear radius;

$P_\ell(kR)$ is the penetration factor, $P_\ell(kR) = kR\left[F_\ell(kR)^2 + G_\ell(kR)^2\right]^{-1}$ (F_ℓ and G_ℓ are spherical Bessel functions);

$\tilde{S}_\ell(kR)$ is the shift factor, $-b_\ell + kR(F_\ell F_\ell' + G_\ell G_\ell')(F_\ell^2 + G_\ell^2)^{-1}$

and $\phi_{j\ell}(kR)$ is either an optical model or a hard-sphere phase shift.

2. Oxygen 16 cross sections based on an optical model plus resonant phase shifts

A. Summary of data sources and fitting procedures.

I. Total Cross Section

Energy (Mev)	Experimental Data Source	Fitting Procedure
0 - 2.6	BNL 325, KFK 120	OPTIC
2.6 - 15.0	Bockelman, Fossan	EXPERIMENT

II. Elastic Cross Section

0 - 15	Total minus non-elastic (Summed over reactions)	EXPERIMENT

III. Inelastic Cross Section

0 - 10	KFK 120, Hall and Bonner	EXPERIMENT
14	Conner	
10 - 15		INTERPOLATION

IV. (n,α) Cross Section

0 - 5	BNL 325	EXPERIMENT
5 - 8.8	Davis, Bonner, et al.	EXPERIMENT
8.8 - 12	- - -	INTERPOLATION
12 - 15	Bormann, Cierjacks, et al.	EXPERIMENT

V. (n,p) Cross Section

10.2 - 15	BNL 325	Hauser-Feshbach plus experiment

VI. Legendre Moments

0 - 2.6	Lane, Langsdorf et al. Fowler and Cohn BNL 325, BNL 400	OPTIC
2.6 - 3.1	- - -	INTERPOLATION
3.1 - 4.7	Lister and Sayres	EXPERIMENT
4.7 - 5.0	- - -	INTERPOLATION
5.0 - 15.0	Chase, et al. Bauer, et al.	OPTICAL MODEL

B. Parameters used for the resonances

E (lab, Mev)	E (CM, Mev)	ℓ	J	γ^2 (Mev)
0.4444	0.4180	1	3/2	0.3340
1.000	0.94068 a	2	3/2	a
1.3161	1.2380	1	3/2	0.0756
1.6594	1.5610	3	7/2	0.8100
1.8295	1.7210	2	5/2	0.0676
1.9029	1.7900	1	1/2	0.0350
2.3700	2.2294	0	1/2	0.0484
3.2423	3.0500	2	3/2	1.4400
3.8270	3.6000	1	3/2	0.3600

$R^{3/2}_{0\,1}$ = -0.54 (distant level contribution)

a This is a single-particle resonance and is obtained from a potential well instead of from the R function.

In conjunction with our currently recommended hydrogen library, this set of oxygen cross sections gives a water age of 26.5 cm^2 to indium, in good agreement with experiment. The fit to the total cross section below 3 Mev is shown in Fig. 1.

Complete references are available in Reference [2] which also gives the optical model parameters used in the calculation.

3. Carbon 12 cross sections based on an optical model plus resonant phase shifts

A. Summary of data sources and fitting procedures

I. Total Cross Section

Energy (Mev)	Experimental Data Source	Fitting Procedure
0 - 4	BNL 325, Bockelman, Wills KFK 120	OPTIC
4 - 15	BNL 325, Fossan	EXPERIMENT

II. Elastic Cross Section

0 - 9.2	Total - NE (Summed over reactions)	OPTIC
9.2 - 15	Total - NE (MacGregor and Booth)	INTERPOLATION, 2 PLUS

III. Legendre Moments

0 - 7 Mev	OPTIC
7. - 8.4	INTERPOLATION
8.4 - 15	2 PLUS

IV. Inelastic Cross Section

0 - 9.2	Hall and Bonner	EXPERIMENT
9.2 - 15	NE - other processes	

V. (n,α) Cross Section

6.18 - 7.9	Coulomb penetrability	
7.9 - 8.65	Davis, Bonner et al.	EXPERIMENT
7.7 - 9.9	Risser, Price, et al. (inverse)	
9.9 - 15		INTERPOLATION
14.0	Al-Kital and Peck	

VI. $(n,n',3\alpha)$ Cross Section

Threshold -15 Mev	Vasilev et al. Frye, Rosen, et al.	EXPERIMENT

B. Summary of fitting parameters

I. $E < 3.4$ Mev

E(CM)	ℓ	j	γ^2
-6.0	0	1/2	4.C
1.915	2	5/2	.025
2.733	2	3/2	.175
3.383	2	3/2	1.638
3.55	2	3/2	optical
3.967	1	1/2	.087

+ Hard-sphere phase Shift: R = 3.719 ,

$R_{1\frac{1}{2}0} = .05$, $R_{1\frac{3}{2}0} = .15$

II. $2.9 < E < 7.0$ Mev

E(CM)	ℓ	j	γ^2
2.733	2	3/2	.3925
3.940	1	1/2	.1415
4.548	1	1/2	.00622
4.944	1	3/2	.01736
5.800	3	7/2	.9058

+ optical phase shift with energy dependent parameters
(D 3/2 resonance at 3.55 Mev due to potential well)

III. $8.4 < E < 15$ Mev (2 PLUS parameters)

$V_R = 50.36$ $V_I = 0$ $V_{GAUS} = 6.76$ $V_S = 5.0$ $R = 2.7$
$a = .51$ $b = .81$ $\beta = .57$ (coulomb excitation)

A segment of the fit to the total cross section is shown in Fig. 2. Complete references are available in Reference 3. The program 2 PLUS performs the coupled channel calculation described in the following section.

4. Coupled-channel calculation of neutron cross sections

For nuclei with low-lying collective states, the latter's coupling to the ground state is not negligible and the single-channel optical model requires generalization to a coupled-channel theory. We have made coupled-channel calculations for even-even nuclei with first excited 2 + states using the vibrational nuclear model to obtain the coupling between the two channels. In the vibrational model of Bohr and Mottelson the nuclear surface is assumed to be deformed dynamically and the radial coordinate of the surface may be defined by

$$R(\hat{r}) = R\left[1 - \sum_M \alpha_{2M} Y_2^M(\hat{r})\right].$$

The optical potential experienced by a neutron at $\vec{r}_o$ is assumed to depend only on the distance from the neutron to the nuclear surface and may be expanded to first order in the α_{2M}'s to yield

$$V(r_o - R(\hat{r}_o)) \cong V_o(r_o) + R\frac{dV_o}{dr_o}\sum_M \alpha_{2M} Y_2^M(\hat{r}_o)$$

$$\langle\Psi_{oo}|\alpha_{2M}|\Psi_{2\mu}\rangle = (-1)^M\langle\Psi_{2-\mu}|\alpha_{2M}|\Psi_{oo}\rangle = -\frac{\beta}{\sqrt{5}}\delta_{M\mu}$$

$$\langle\Psi_{2\mu}|\alpha_{2M}|\Psi_{2\mu'}\rangle = \langle\Psi_{oo}|\alpha_{2M}|\Psi_{oo}\rangle = 0$$

The central potential $V_o(r_o)$ is a Saxon-Woods well plus an imaginary Gaussian well and spin-orbit coupling. Also shown are the nuclear matrix elements which define the operators α_{2M} where ψ_{oo} and the $\psi_{2\mu}$'s are the nuclear ground and first excited states. The parameter β is a measure of the distortion of the nuclear surface. The coupling potential can then be written

$$\left\langle \psi_{2M} \middle| V(r_o - R(\hat{r}_o)) \middle| \psi_{oo} \right\rangle = - \frac{\beta}{\sqrt{5}} R \frac{dV_o}{dr_o} Y_2^M(\hat{r}_o)$$

The compound elastic and inelastic scattering are calculated using Hauser-Feshbach theory and the coupled equations are solved using the program 2 PLUS[4].

Figure 3 shows fits obtained with this model for titanium and iron at 2.45 Mev. On the top is the fit to elastic differential cross section data for natural Ti and inelastic cross section data for exciting the .99 Mev 2 + level in Ti^{48}. The difference in the elastic cross section for natural Ti and Ti^{48} is expected to be small. In the bottom curve the elastic data are for natural Fe and the inelastic data are for exciting the .845 Mev level in Fe^{56}. The values for the distortion parameter required for the Ti and Fe fits were .21 and .28 respectively. The direct inelastic scattering cross section calculated was significant, being about 20% of the total inelastic cross section for both nuclei. The non-spherical part of the optical potential also had an appreciable effect on the shape of the differential elastic cross section, decreasing it at the very forward and backward angles and at the diffraction minimum. The resulting shape is not easily fit with a spherical optical potential. Fits were also obtained for these nuclei at different energies and for Cr, Zr, and C. In all cases the calculated direct inelastic scattering was significant.

We have also calculated cross sections for Ti and Fe using the shell model with residual pairing and quadrupole forces to describe these nuclei. The single-particle wave functions used in the nuclear wave function were calculated from a Saxon-Woods well with coulomb and spin-orbit forces. The single-particle energies used were those measured in deuteron stripping experiments and the pairing force coupling constant was taken to be 23/A Mev where A is the atomic number. The nuclear wave functions were then calculated in the Boson approximation with the strength of the quadrupole force determined by matching the energy of the first excited 2 + state.

The interaction between the scattered neutron and the target nucleons is represented by a two-body, central, non-exchange potential with a Yukawa shape given by

$$V_I = \frac{C}{4\pi} \sum_i \frac{e^{-|\vec{r}_o - \vec{r}_i|/\mu}}{|\vec{r}_o - \vec{r}_i|/\mu}$$

The sum is over all nucleons in the nucleus and the range μ is taken to be

1 fm. The coupled-channel equations arising in these calculations have exactly the same form as those based on the vibrational model just discussed. The spherical and non-spherical parts of the optical potential in this case are matrix elements of V_I and the potentials shown above become

$$V_o(r_o) = \langle \psi_{oo} | V_I | \psi_{oo} \rangle$$

$$-\frac{\beta}{\sqrt{5}} R \frac{dV_o}{dr_o} Y_2^M(\hat{r}_o) \rightarrow \langle \psi_{oo} | V_I | \psi_{2M} \rangle$$

The main difficulty with the formulation of the scattering problem at this point is that the spherical part of the optical potential is real and there is thus no compound nuclear reaction. We therefore assume that the imaginary potential arises from interactions with nucleons outside the closed shells, and consider it to arise from a two-body interaction with the same Yukawa shape between the neutron and extra-core nucleons (nucleons in the $f_{7/2}$ and higher shells). It thus has the form $iN\langle \psi'_{oo} | V_I | \psi'_{oo} \rangle$. Here ψ_{oo}' is the ground state wave function with the core nucleons removed and N is a normalization constant.

We therefore have two adjustable parameters, C and N, to fit both the elastic and inelastic cross sections. A value of 400 Mev was used for C and the strength of the imaginary potential was determined by fitting the total inelastic cross section.

Figure 4 shows fits obtained in this way to the Ti and Fe data just shown. Here the calculated direct inelastic scattering was again about 20% of the total inelastic.

Therefore the calculations with both nuclear models used here indicate that the direct inelastic scattering is important for these nuclei even at 2.45 Mev and should be taken into account in order to make accurate calculations. Also, care should be used when calculating the elastic cross sections of nuclei with low-lying collective states since removal of the non-spherical potential destroys the fits presented here.

5. Uranium 235 cross sections

No existing set of pointwise evaluated U235 cross sections that we are aware of has an epithermal alpha (= capture/fission ratio) as low as .50, the latest recommendation based on integral measurements [5]. (Typical values run from around .6 to around .7.)

It appears that the usual procedure of subtracting fission and scattering from the total cross section to get capture values systematically overestimates the latter. This procedure also tends to obscure the characteristic differences in shape between capture and fission resonances which are ascribable to multilevel effects in the fission channels. Both of these difficulties are avoided in the present work, by relying where possible on the direct capture measurements made earlier this year by the Oak Ridge/Rensselaer Polytechnic Institute group. [13]

Starting with Wescott's recent recommended set of 2200 m/s cross sections [6], we used the fission measurements of Leonard [7] and the Livermore group's [8] 1966 data in the region up to .4 eV, fitting these, as needed, by least squares polynomial fits. From .4 eV to 62 eV, we used the Oak Ridge-RPI fission data, normalizing it so that its integrated value from .4 - 62 eV matched the Livermore value. The latter has the advantage of being directly normalized to the 2200 m/s value. From 62 - 10,000 eV we used Saclay data [9], and from 10,000 - 2 x 10^7 eV a curve similar to the BNL 325 eyeguide, but adjusted to pass through the 24 keV value of Perkin, et al. [10] This composite curve gave a resonance integral of 281 barns from .5 to 10^7 eV, compared to the Feiner and Esch value of 280 ± 11.

For capture, we again used the ORNL-RPI data from .4 - 62 eV, but above and below that region used capture/fission ratios times the previous fission curve. Below .4 eV the alpha values came from BNL 325 and Wescott [6]. From 62 - 10,000 eV we used the values in KFK 120 [11]. From 10,000 - 2 x 10^7 eV we used BNL 325 plus a smooth extrapolation.

This composite cross section has a resonance integral of 139.8 barns from .5 to 10^7 eV, compared to the Feiner-Esch value of 140 ± 8. The alpha value of these two sets is .497, in good agreement with the Feiner-Esch value of .50 ± .02. If the ORNL-RPI capture measurements can be independently verified, this will resolve the long-standing discrepancy between the differential and integral alpha values.

We are carrying out both Breit-Wigner single-level and Reich and Moore multilevel fitting to this set of cross sections. The single-level procedure is relatively simple, but does not give a very good fit to the fission data. For example, the total widths of some resonances are 15% larger when seen in fission than when seen in capture. The two-channel Reich and Moore procedure can reproduce this type of behavior but is difficult to parameterize. We are programming a version of the Reich and Moore procedure which will utilize an automatic parameter search but this program is not yet operating. An interesting fact which emerges from even the preliminary analysis is that there is considerable fluctuation in the capture width distribution, suggesting collective effects in the gamma transitions.

6. Activation cross sections

The procedure of using Hauser-Feshbach theory to generate the threshold dependence of (n,p) cross sections has been described previously [12]. In Figure 5 we show the results of combining this procedure with experimental data at higher energy, and then adjusting each curve to yield a recommended average value in a fission spectrum. The square bracket following the isotope designation on each curve gives the fission spectrum average. We show two curves for Ti 46 since the literature is evenly split on whether the fission average is about 8 mb or about 13 mb.

Evaluated cross sections have also been adopted for Al27(n,α), S32(n,p), Np237(n,f) and U238(n,f), but these were based entirely on experimental data.

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Figure Captions

1. Resonance-plus-potential well fit to O^{16} total neutron cross section below 3.0 Mev.

2. Resonance-plus-potential well fit to C^{12} total neutron cross section from 2.8 to 5.0 Mev.

3. Coupled-channel fit to Ti^{48} and Fe^{56} elastic and inelastic cross sections at 2.45 Mev (Conventional potential wells plus deformation).

4. Coupled-channel fit to Ti^{48} and Fe^{56} elastic and inelastic cross sections at 2.45 Mev (Potential wells derived from a Yukawa two-body interaction).

5. Evaluated activation cross sections (Fission spectrum averages in mb given in square brackets).

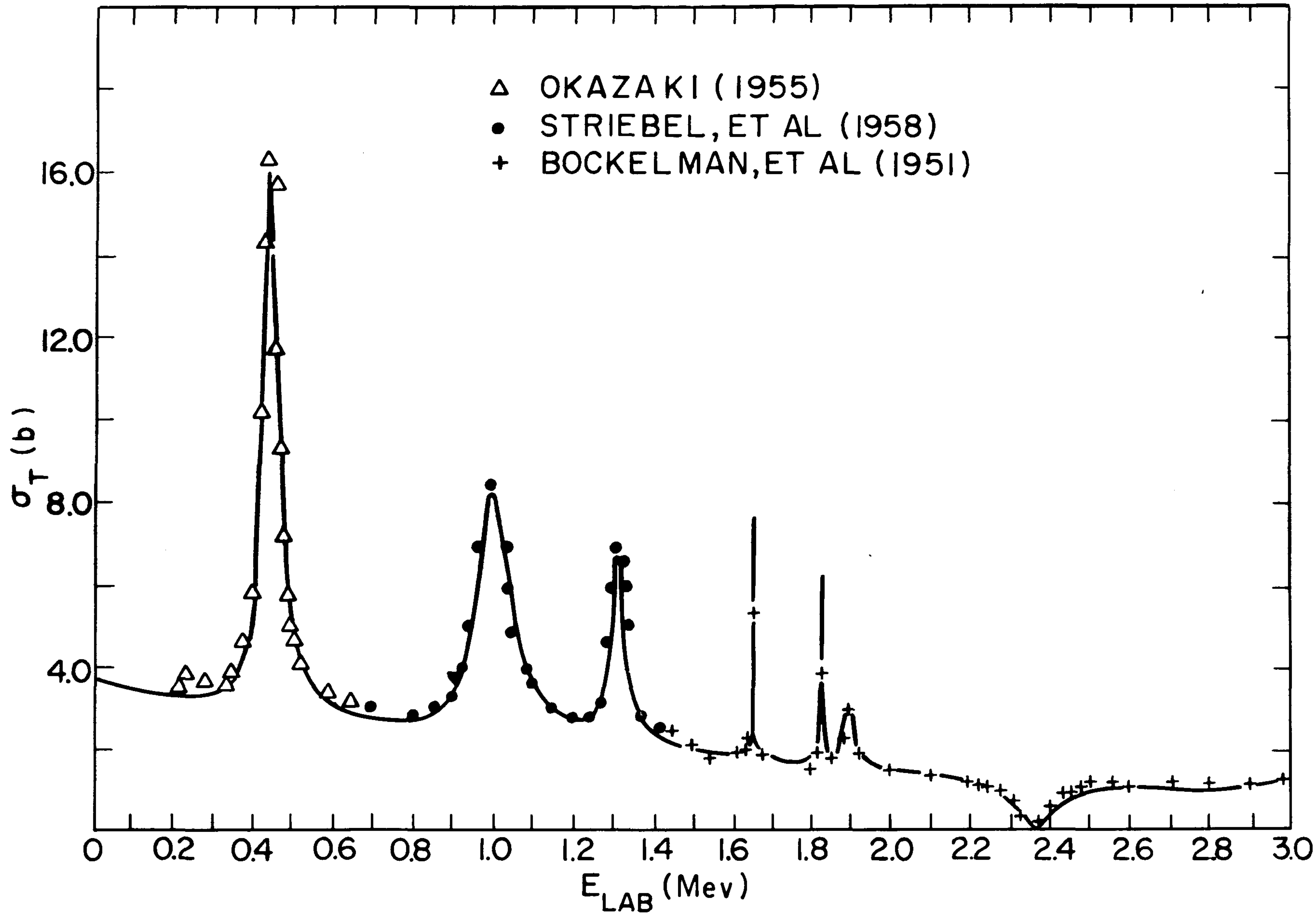

FIG. 1. RESONANCE-PLUS POTENTIAL WELL FIT TO O16 TOTAL NEUTRON CROSS SECTION BELOW 3.0 Mev

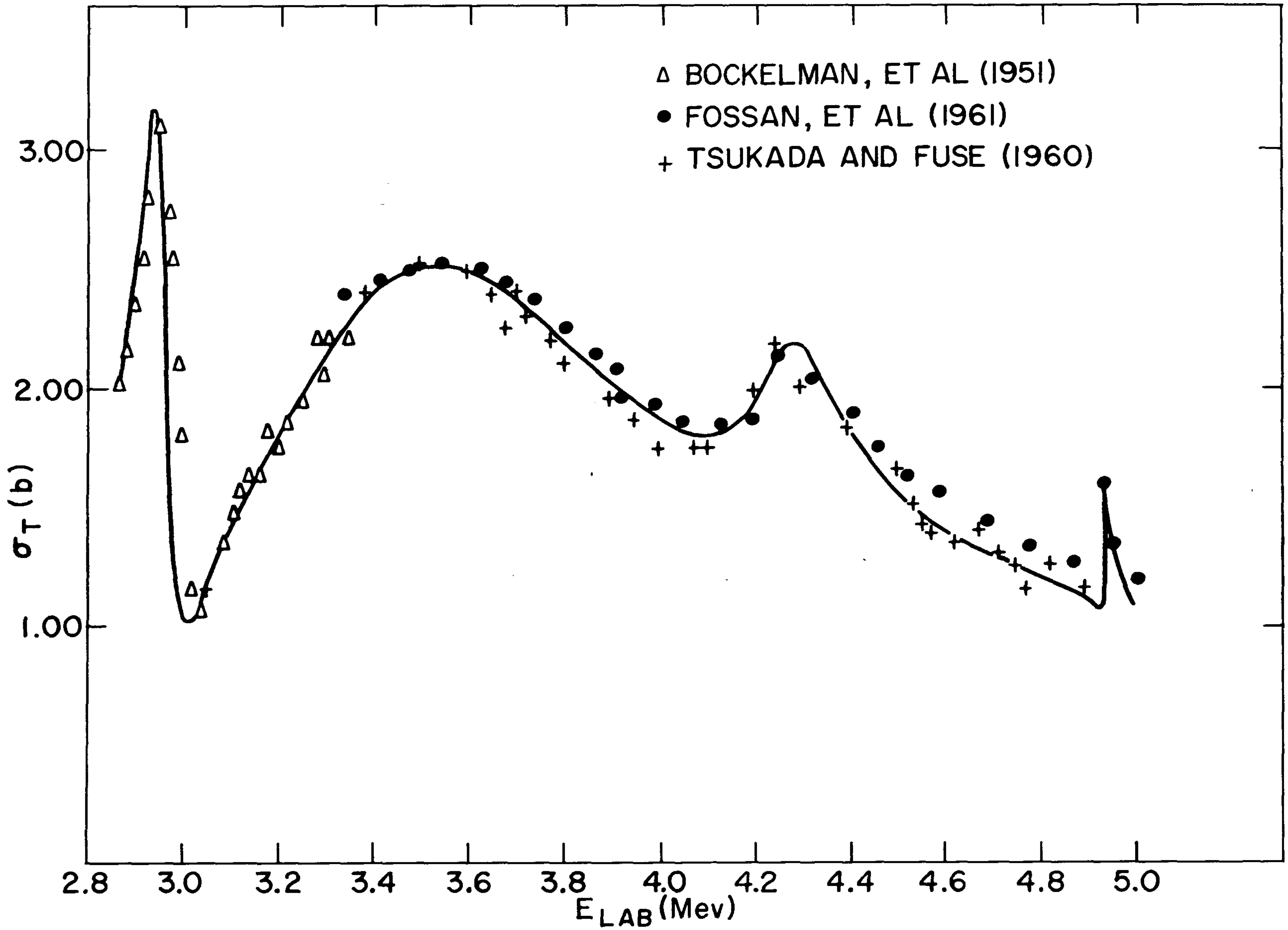

FIG. 2 RESONANCE PLUS POTENTIAL WELL FIT TO C12 TOTAL NEUTRON CROSS SECTION FROM 2.8 TO 5.0 Mev

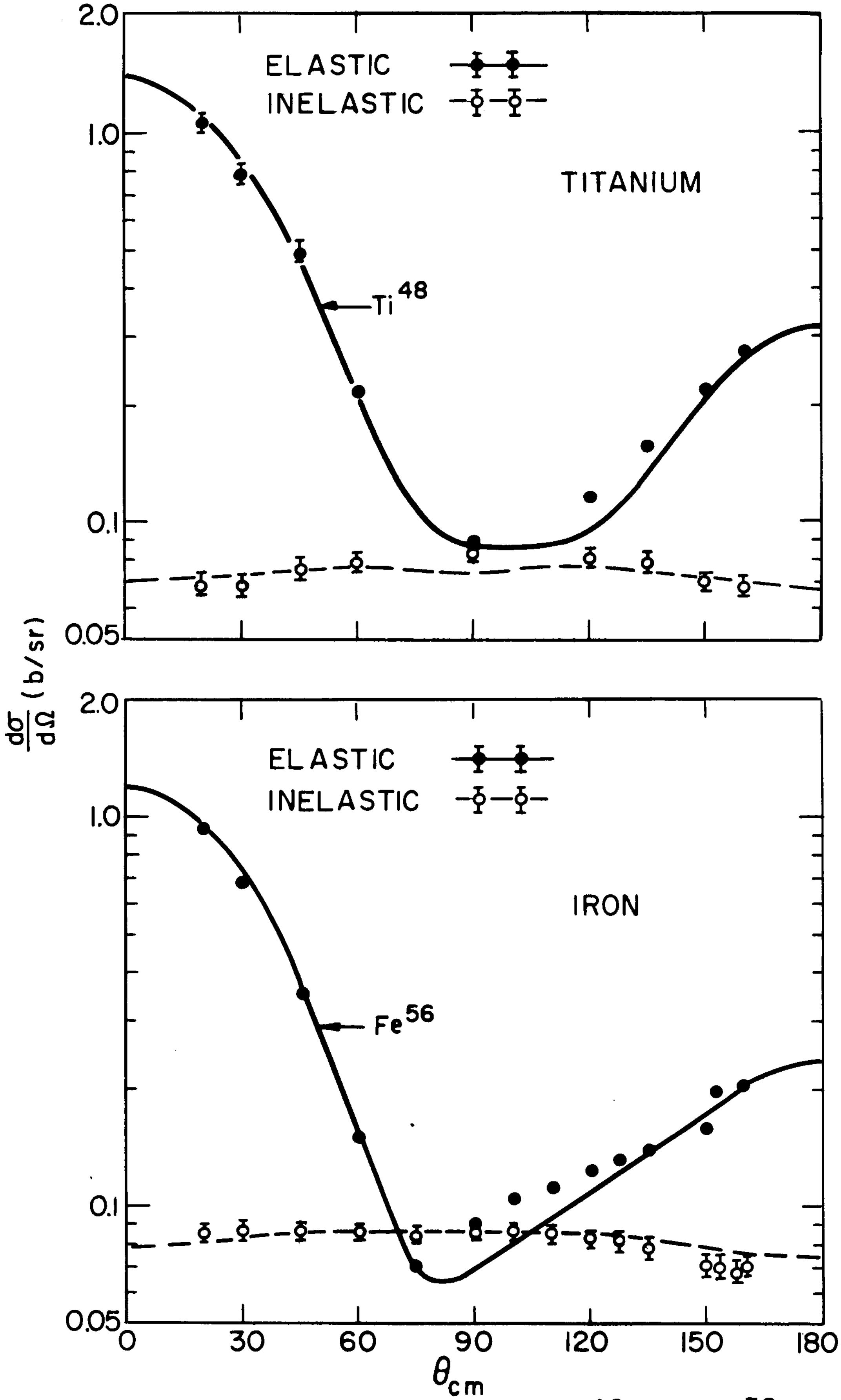

FIG. 3. COUPLED-CHANNEL FIT TO Ti^{48} AND Fe^{56} ELASTIC AND INELASTIC CROSS SECTIONS AT 2.45 Mev. (CONVENTIONAL POTENTIAL WELLS PLUS DEFORMATION)

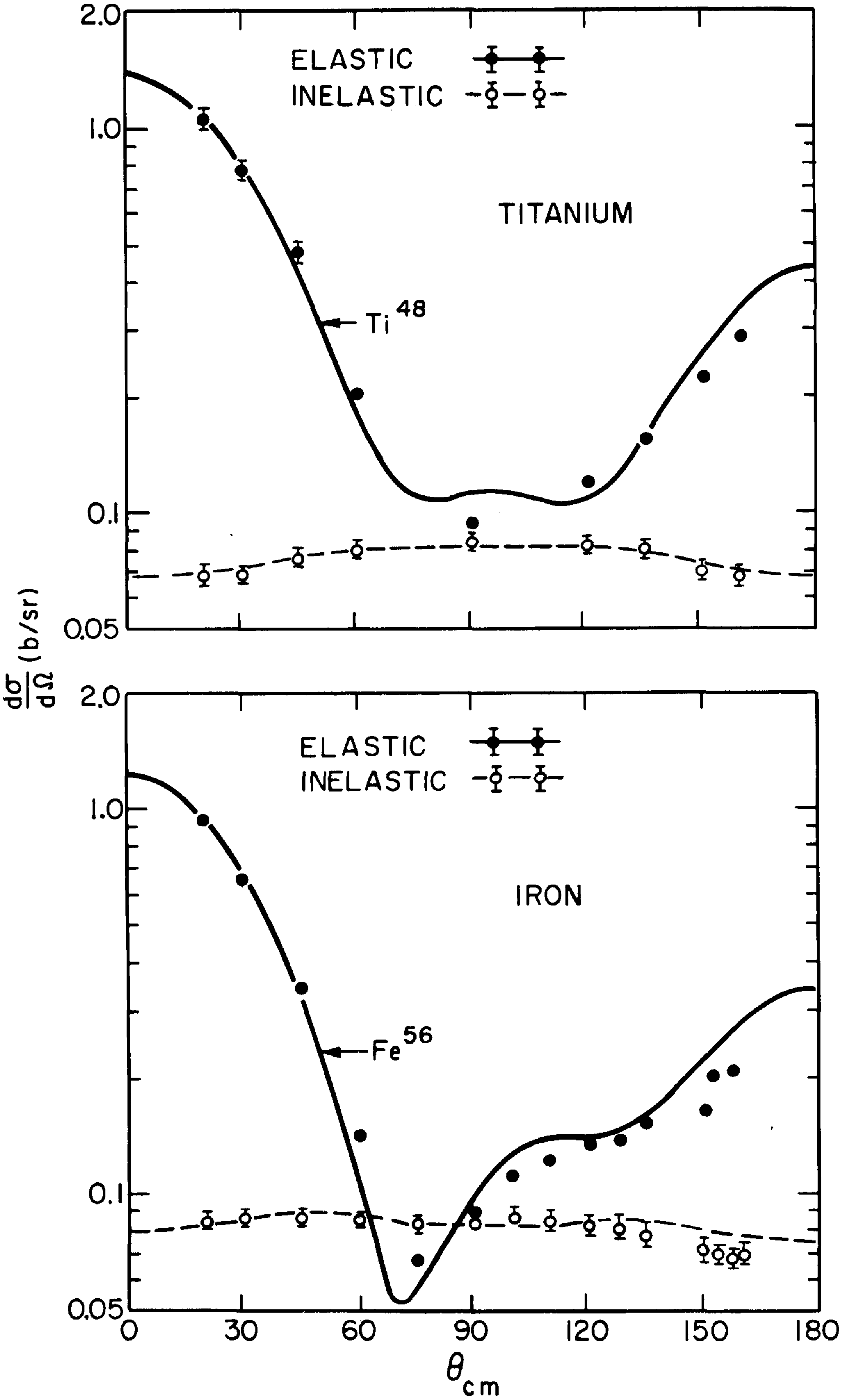

FIG. 4. COUPLED-CHANNEL FIT TO Ti^{48} AND Fe^{56} ELASTIC AND INELASTIC CROSS SECTIONS AT 2.45 Mev (POTENTIAL WELLS DERIVED FROM A YUKAWA TWO-BODY INTERACTION)

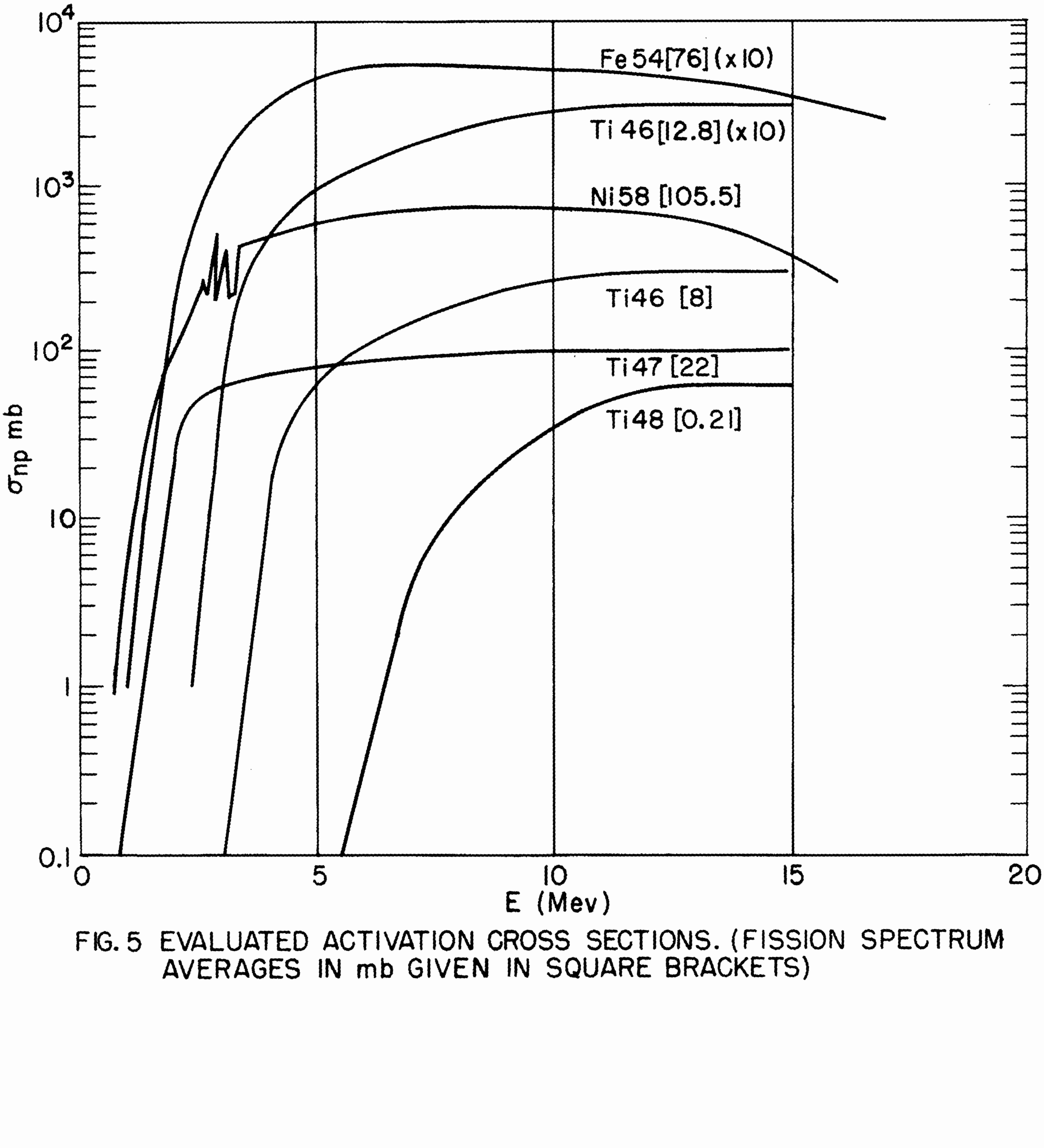

FIG. 5 EVALUATED ACTIVATION CROSS SECTIONS. (FISSION SPECTRUM AVERAGES IN mb GIVEN IN SQUARE BRACKETS)