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Evaluation of Neutron Cross Sections for Nd-143, Nd-145, Sm-147 and Sm-149 from 1 keV to 20 MeV

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Abstract

The neutron induced nuclear data for Nd-143, Nd-145, Sm-147 and Sm-149 were calculated and evaluated from 1 keV to 20 MeV. The energy dependent optical model potential parameters were extracted based on the recent experimental data and the s-wave strength function was calculated. Spherical optical model and statistical model in equilibrium energy and multistep direct and multistep compound model in preequilibrium energy were introduced in EMPIRE. The theoretically calculated cross sections were compared with the experimental data and the evaluated files on (n, tot), (n, n), (n, n'), (n, g), (n, p), (n, a), (n, 2n), (n, 3n), (n, np), (n, n) reactions. The model calculated cross sections gave quite well agreement with the reference experimental data. The evaluated cross sections were compiled to ENDF-6 format.

1. Introduction

The 19 priority fission products were decided in the neutron cross section evaluation, which mainly influenced on reactivity in a fission reactor. In this paper, the neutron cross sections on Nd-143, Nd-145, Sm-147 and Sm-149 among them were evaluated, using EMPIRE-II code package from 1 keV to 20 MeV. In ENDF/B-VI, Nd-143 and Nd-145 were evaluated in 1992. Sm-147 was evaluated in 1989 and Sm-149 in 1978. Table I shows the property of each nuclide.

Neutron induced nuclear reaction data for fission products are important to predict burnup performance in a fission reactor, to calculate criticality for spent fuel storage design and to study radiation damage estimation of structural material. The absorbed neutrons by fission products have a large portion in the total loss of neutrons. Neutron

Table I : Property of each fission product

Fission product	Mass	Half-life	Binding energy (MeV)	1st excited level (MeV)
Nd-143	142.9098	stable	8.330	0.7421
Nd-145	144.9125	stable	8.309	0.0671
Sm-147	146.9148	1.06E+11 yrs	8.280	0.1213
Sm-149	148.9171	2.00E+15 yrs	8.263	0.0225

capture cross sections of neodymium isotopes in several keV region are important because these isotopes are significant fission products in a fission reactor concerning neutron absorption loss and decay heat. The selected samarium has high yield, long lifetime and high capture rate in a reactor.

The optical model potential depending on the incident neutron energy was searched using a graphical interface[1] to the ABAREX[2]. Parameters were selected by comparing the model calculated total and elastic scattering cross sections with the reference experimental data. The calculated s-wave strength function by the parameters was compared with that of the evaluated in the resonance region.

Nuclear reaction cross sections were calculated by using recently released EMPIRE-II code[3]. This code consists of several modules for the spherical optical model calculation, equilibrium calculation and quantumn mechanical preequilibrium calculation. The width fluctuation correction influenced on the capture and inelastic scattering cross sections. The code offers several built-in libraries including the ENSDF nuclear level and decay information. The cross sections are evaluated on (n, tot), (n, n), (n, n'), (n, 2n), (n, 3n), (n, na), (n, np), (n, g), (n, p) and (n, a). The calculated cross sections are graphically compared with the experimental data and the evaluated files (ENDF/B-VI, JENDL-3.2, JEF-2.2, BROND-2 and CENDL-2).

2. Optical Model Potential Parameters

The incident neutron energy dependent potential was searched in spherical optical model based on the reference experimental data and the produced s-wave strength function compared with that of compiled for resonance region. To obtain proper potential parameters, the Woods-Saxon well is used for the real optical model potential

$$V(r) = -V/(1+\exp((r-R_v)/a_v)) \tag{1}$$

where V, a_v are the strength and diffuseness of the potential and the nuclear radius R_v,

Table II : Parameters of energy dependent spherical optical model potential

Parameter (unit)	Nd-143	Nd-145	Sm-147	Sm-149
V_o(MeV)	46.6600	48.7900	52.1870	52.6878
V_1(MeV)	-0.2000	-0.2000	-0.0330	-0.0330
r_o(fm)	1.2639	1.2526	1.2450	1.2220
a_v(fm)	0.638	0.580	0.739	0.635
W_o(MeV)	7.490	6.330	7.670	9.130
r_{wo}(fm)	1.1852	1.2500	1.2420	1.2200
a_w(fm)	0.614	0.536	0.568	0.590
V_{so}(MeV)	7.000	7.000	9.600	8.200
r_{so}(fm)	1.280	1.280	1.231	1.231
a_{so}(fm)	0.600	0.600	0.683	0.683
W_1(MeV)	0.0000	0.0000	-0.1020	-0.1020
r_{w1}(fm)	0.000	0.000	0.000	0.000
r_1(fm)	0.000	0.000	-0.010	-0.010

related to mass number A, is given by

$$R_v = r_v A^{1/3}. \qquad (2)$$

The derivative Woods-Saxon shape is used for the imaginary potential,

$$W(r) = -4W\exp((r-R_w)/a_w) / 1+ \exp((r-R_w)/a_w)^2 \qquad (3)$$

where W, R_w, a_w are potential strength, radius and diffuseness, respectively. Generally, Thomas form is taken in the optical model potential for spin-orbit coupling

$$V_{s\text{-}o}(r) = (2L*S)V_{so}(2/r)d/dr(1/[1+\exp((r-R_{so})/a_{so})]) \qquad (4)$$

where $L*S$ is the dot product of the orbital and spin angular momentum operator.

The real and imaginary potential depth and radius are expanded as a function of incident neutron energy

$$V = V_o + V_1 \times E_n , \quad r_v = r_o + r_1 \times E_n \qquad (5a)$$

$$W = W_o + W_1 \times E_n , \quad r_w = r_{wo} + r_{w1} \times E_n . \qquad (5b)$$

E_n is an incident neutron energy. The 13 potential parameters were searched simultaneously and the result was summarized in Table II. Table III shows s-wave strength function (So) calculated from the selected potential parameters at 1 keV. From the table, the calculated values are close to the recent evaluation at resonance energy region.

3. Calculation

EMPIRE-II code was used in calculation of total, elastic and threshold reaction cross sections. EMPIRE-II is a nuclear reaction code, comprising various nuclear models, and designed for calculations in the broad range of energies and incident particles. The code accounts for the major nuclear reaction mechanisms, such as optical model, Multistep Direct (MSD), Multistep Compound (MSC) and the full featured Hauser-Feshbach model. The Hauser-Feshbach decay for particles and gamma rays with the width fluctuation corrections was introduced in the calculation of cross sections. The multi-step direct model takes care of the inelastic scattering to vibrational collective levels and decay information.

Calculations were performed as follows. The selected energy dependent potential was expanded in the whole evaluation energy range. Spherical OM SCAT2 in EMPIRE was used with the neutron parameters. Then, discrete levels to be used were selected by EMPIRE. Afterwards, all other input parameters for EMPIRE were prepared and tuning of parameters was necessary. The calculated cross sections are graphically compared with the experimental data and evaluated files for all reaction channels.

Nd-143

Fig. 1 shows the calculated total cross section with the experimental data[4,5] and the evaluated files[]. The model calculation follows the reference total experimental data very well. Fig. 2 shows the capture cross section. Above 100 keV, the difference between the calculation and ENDF/B-VI is started.

Nd-145

The calculated total cross section follows the experimental data well in Fig. 3. Fig. 4 shows the calculated and measured capture cross section. The calculated capture cross section is in good agreement with the reference experimental data[4] above 20 keV. The capture cross section at low energy region might be substituted by resonance parameters.

Sm-147

Fig. 5 shows the calculated total cross section with the reference experimental data[6]. The calculated total cross section is lower than the experimental data. The s-wave strength function value evaluated from the resonance region was crucial in the total cross section generation. Model calculation shows the poor capture cross section below 20 keV as shown in Fig. 6. The capture cross section calculated by the resonance parameters will replace the model calculation at this energy region.

Sm-149

The model calculated total cross section follows the experimental data[5,6] well in Fig. 7. There is no much difference between the current evaluation and the ENDF/B-VI

Table III : Comparison of s-wave strength function

Fission product	s-wave strength function	
	by OM*	by evaluation**
Nd-143	3.303E-4	3.620E-4
Nd-145	4.000E-4	4.750E-4
Sm-147	5.020E-4	4.860E-4
Sm-149	4.689E-4	4.530E-4

*By ABAREX at 1keV

**from resonance parameters[11]

in the measured energy range. However, in capture cross section, the calculation has the lower value than the experimental data[7,8,9,10] and ENDF/B-BI in Fig. 8, around 20 keV.

The elastic and other threshold reaction cross sections are not shown here, but the results are summarized in ENDF-6 formatted files. New evaluated total cross section improves ENDF/B-VI substantially.

4. Discussion

The selected energy dependent optical model potential was proper to produce the model calculated cross sections in the evaluation energy range. s-wave strength function was helpful to get the total cross section closer to the experimental data. EMPIRE was successful to produce the reaction cross sections. Evaluated cross sections are in good agreement with the experimental data. They represented improvement over current ENDF/B-VI and the results were converted into the ENDF-6 format. The results should be considered in a new release of the ENDF/B-VI libraries.

Acknowledgements

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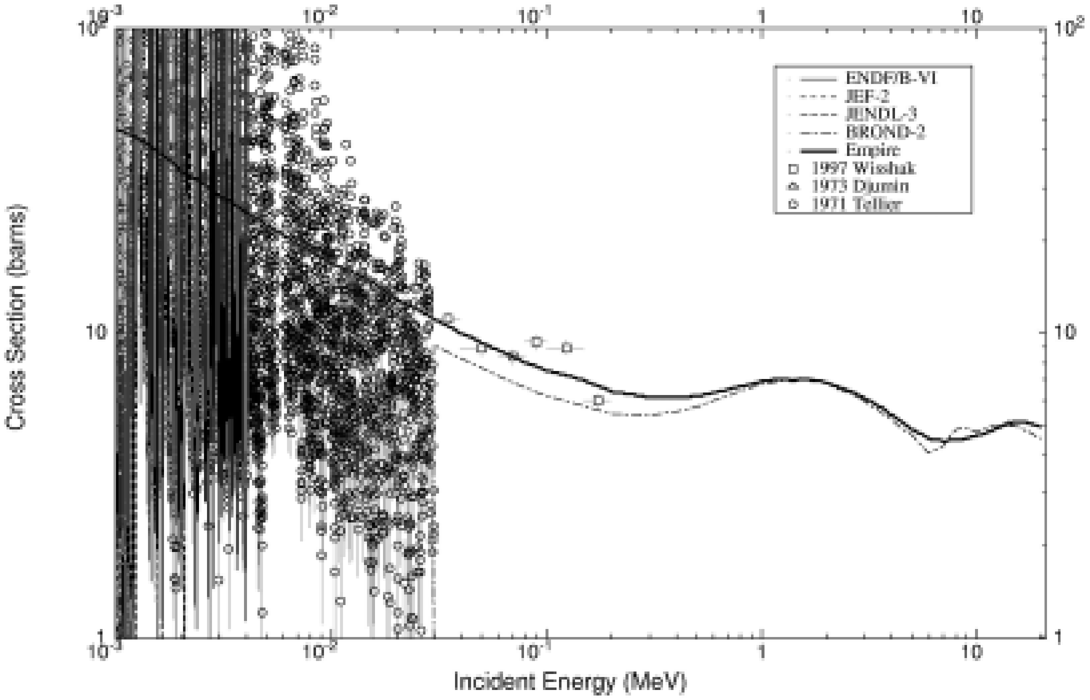

Fig. 1. Total cross section for Nd-143.

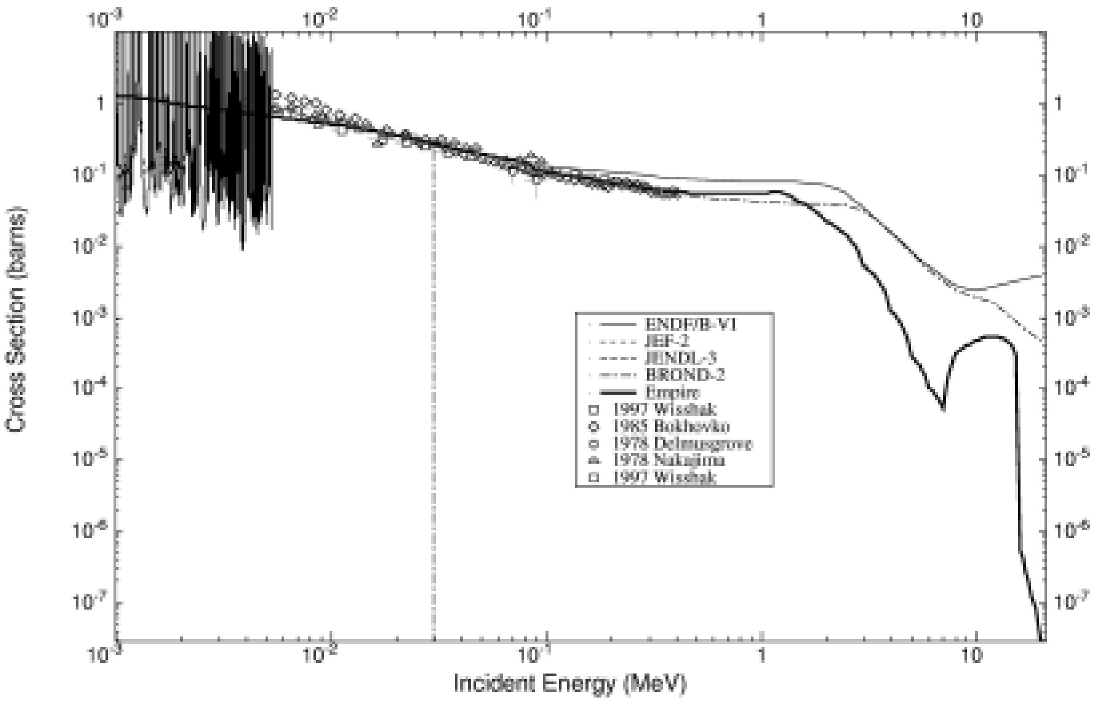

Fig. 2. Capture cross section for Nd-143.

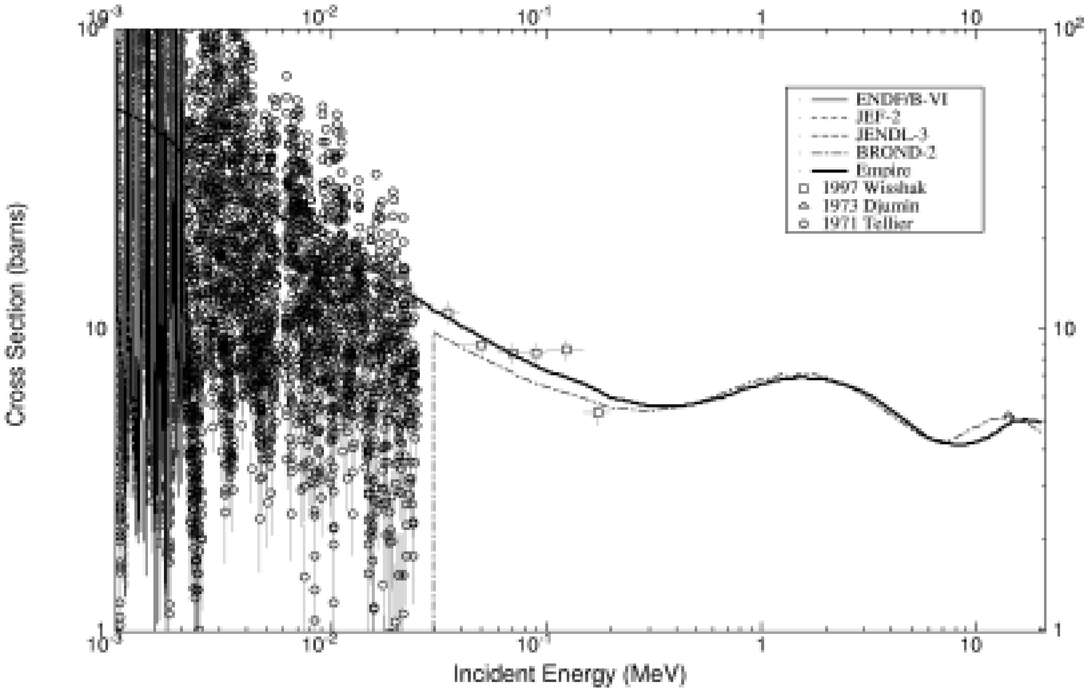

Fig. 3. Total cross section for Nd-145.

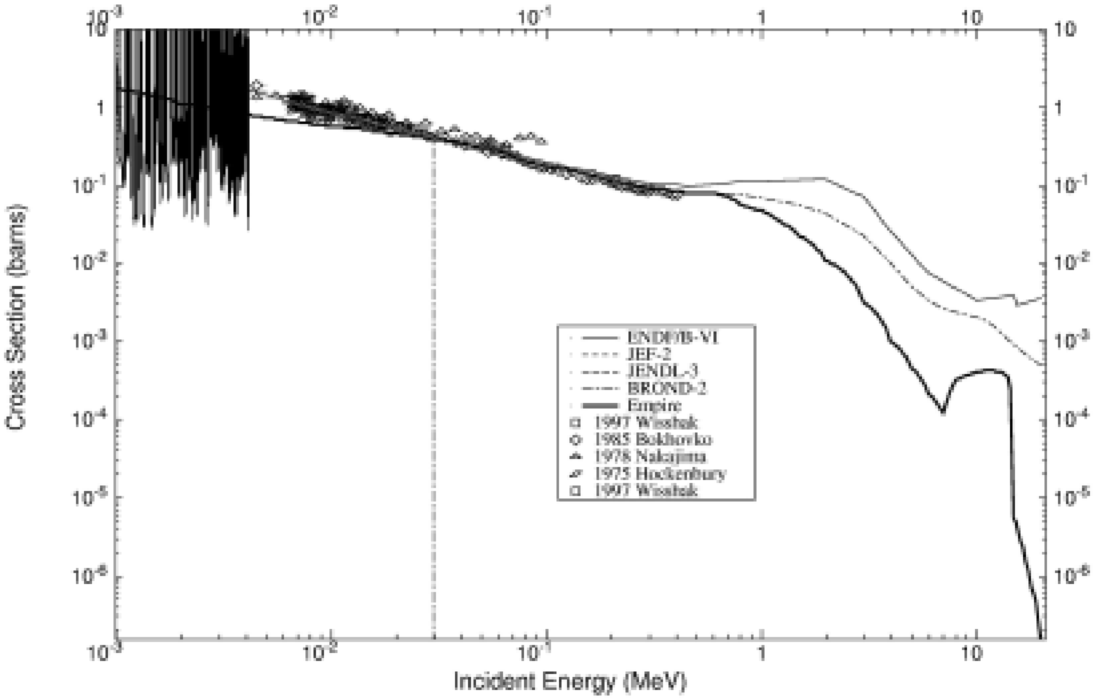

Fig. 4. Capture cross section for Nd-145

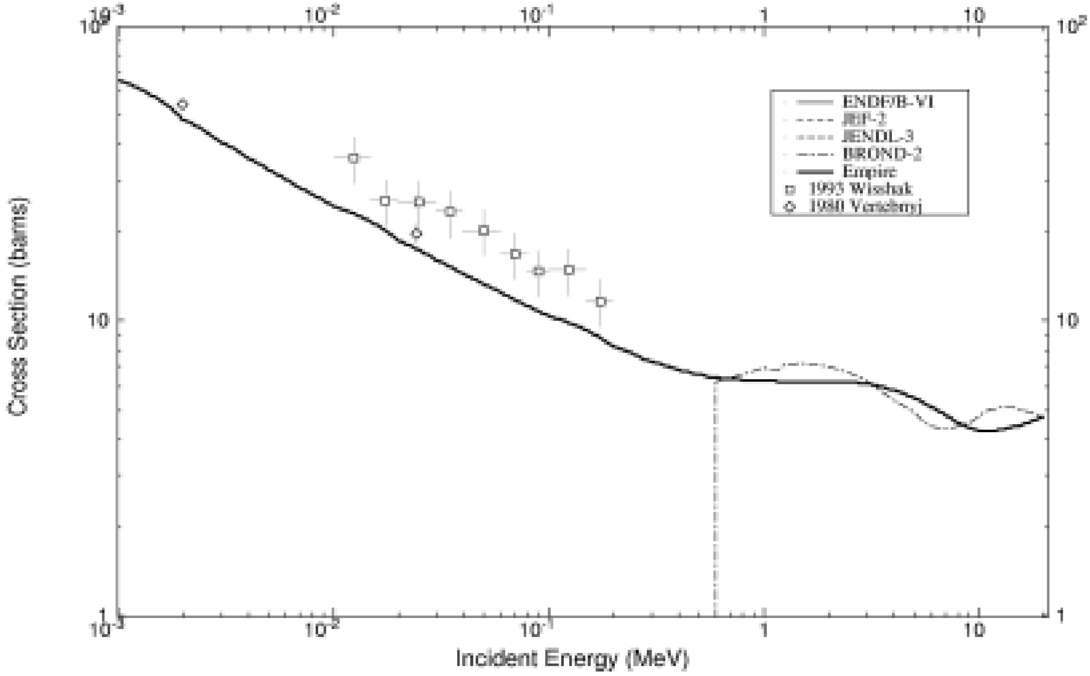

Fig. 5. Total cross section for Sm-147.

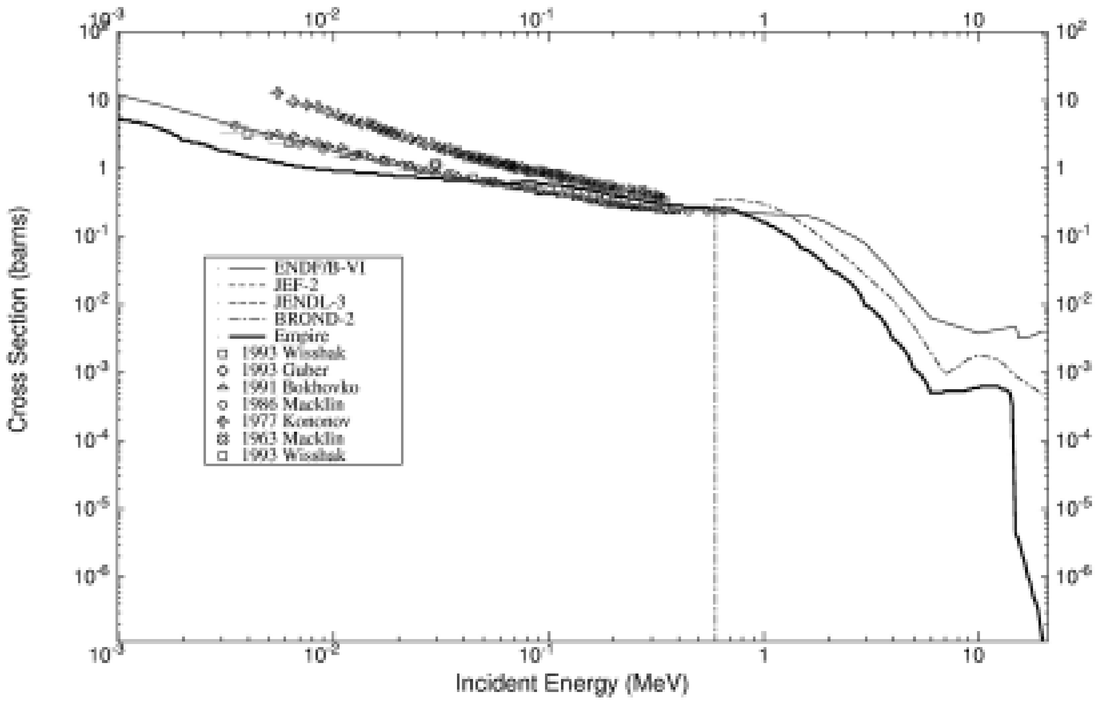

Fig. 6. Capture cross section for Sm-147.

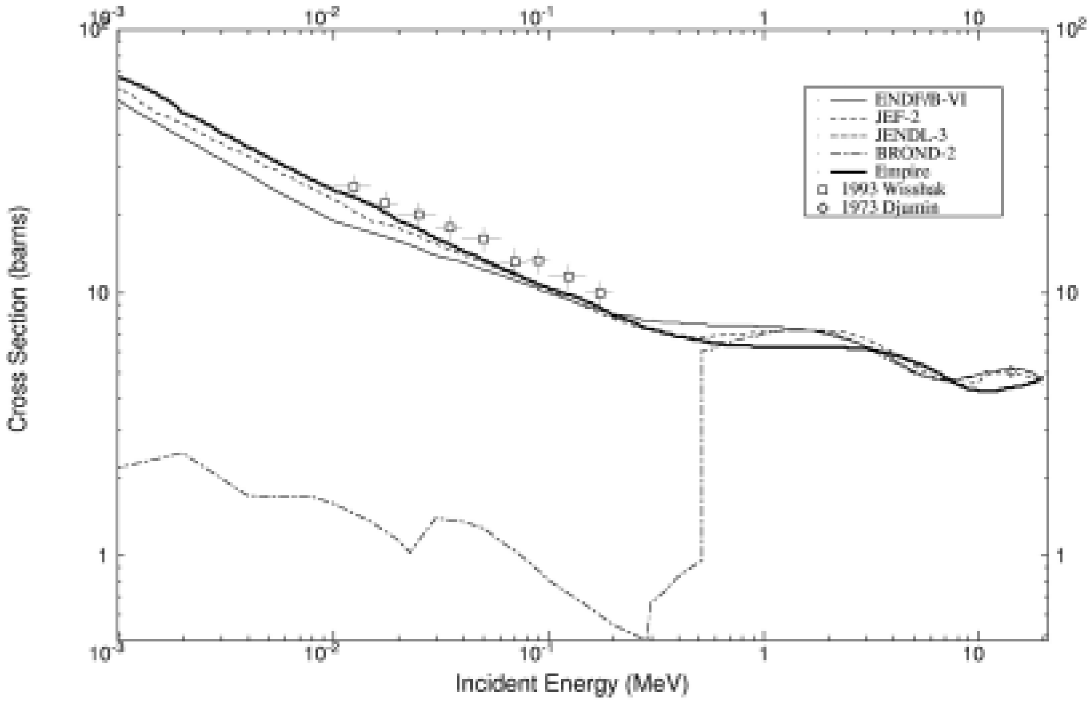

Fig. 7. Total cross section for Sm-149.

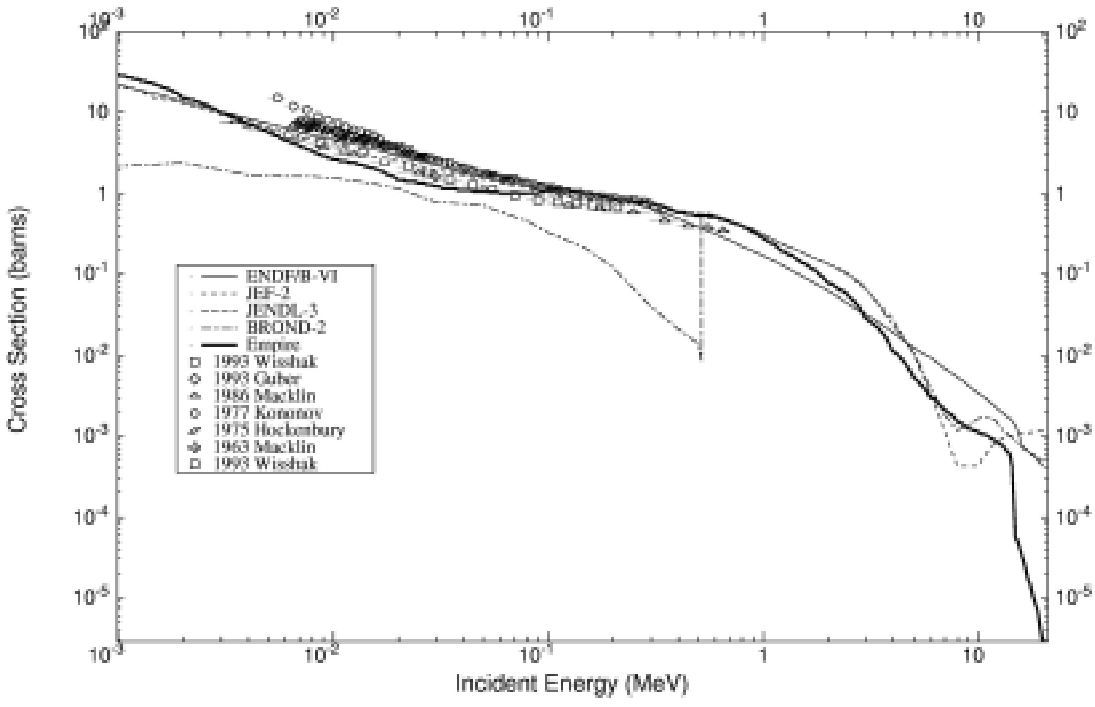

Fig. 8. Capture cross section for Sm-149.