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Evaluation of Neutron Cross Sections for Eu-153, Gd-155 and Gd-157

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Abstract

The neutron induced nuclear data for Eu-153, Gd-155 and Gd-157 are calculated and evaluated in the high energy region. The evaluation procedure for deformed nuclei is setup by using Ecis-Empire codes. The energy dependent optical model potential parameters are searched based on the recent experimental data and applied up to 20 MeV. Optical model, full featured Hauser-Feshbach model and multistep direct and multistep compound model are used in the calculation. The direct-semidirect capture model and the direct coupled-channels contribution to discrete levels are introduced to improve the capture and inelastic scattering cross sections. The theoretically calculated cross sections are compared with the experimental data and the evaluated files. The model-calculated total and capture cross sections are in good agreement with the reference experimental data. The evaluated cross section results are compiled to ENDF-6 format and are expected to improve the ENDF/B-VI.

Key Words : neutron, cross section, evaluation, deformed nuclei

1. Introduction

Neutron induced nuclear reaction data for fission products are important for predicting burnup performance in a fission reactor, criticality for spent fuel storage design, advanced fuel performance and radiation damage estimation of structural material. The neutron capture cross section of Eu and Gd is important in their applications concerning neutron absorption.

The priori fission products[1] were selected in the current neutron cross section evaluation. The evaluation for the selected fission products has been jointly performed with National Nuclear Data Center (NNDC) of Brookhaven National Laboratory (BNL). The joint work is divided into two regions: resonance region including thermal region and upper resonance region up to 20 MeV. For resonance energy region, the evaluation was done[1] for all the selected fission products and the results were adopted in the release 8 of ENDF/B-VI last year up to 1st excited energy. In the region above the resonance, a series of the evaluation works was performed on the spherical nuclei[2,3,4] and the results were compiled to ENDF-6 format. Unresolved resonance region is extended up to several keV or hundreds of keV for the fission products. Therefore, the current evaluation results will complement the evaluation of the resonance region from the 1^{st} excited energy level, where the inelastic scattering reaction channel opens, which corresponds to 83 keV, 60 keV and 55 keV for Eu-153, Gd-155 and Gd-157, respectively.

Eu and Gd have a strong neutron absorption property. Especially, Gd has a very strong neutron capture property. Therefore, these materials are considered as burnable poison. On Eu-153, the evaluation above the resonance was carried out in 1986 for ENDF/B-VI. Ecis code was used to calculate neutron transmission coefficients. Hauser-Feshbach statistical theory calculations were carried out with the GNASH[5] and COMNUC[6] code systems. Systematics were used to obtain parameters for the exciton preequilibrium model with small adjustments. The evaluation on Gd-155 and Gd-157 was done in 1977 for ENDF/B-VI. The natural Gd experimental data was used instead for total cross section. Inelastic and capture cross sections were calculated with COMNUC. Therefore, a new evaluation without systematic approach or simplified theory is necessary for accurate cross section data.

Ecis-Empire[7,8] code combination was used in cross section calculation of the deformed nuclei for total, elastic scattering and reaction cross sections. The optical model potential parameters depending on the incident neutron energy were searched and applied in the whole evaluation energy range. Ecis is well known and highly respected code based on generalized optical model and coupled-channels model (CCM) by J. Raynal (CEA Saclay, France). Ecis is useful for reactions on deformed nuclei, in particular, for description of strong population of collective discrete levels in the (n, n') channel, taking into account symmetric rotational, vibrational-rotational and harmonic vibrational CCM modes.

Nuclear reaction cross sections were calculated using the Hauser-Feshbach model for equilibrium energy region and the quantumn mechanical approach in pre-equilibrium energy region. The width fluctuation correction was considered in Hauser-Feshbach particle decay. The direct and semi-direct capture model was introduced to increase the accuracy of the pre-equilibrium capture cross section. The Empire offers several built-in libraries including the ENSDF nuclear level, deformation parameters and decay information. Empire becomes a highly competitive tool for the evaluation of nuclear reaction data with fully inserted nuclear models. The cross sections are evaluated on (n, tot), (n, n), (n, n'), (n, 2n), (n, 3n), (n, nα), (n, np), (n, γ), (n, p) and (n, α). 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. Model Theory

2.1. Empire

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 Multistep direct model takes care of the inelastic scattering to vibrational collective levels and decay information. In Multistep Direct approach, continuum scattering is considered as a sequence of 1p-1h transitions and the transition strength functions correspond to response functions of an external one-body operator acting repeatedly on a nucleus. The modeling of Multistep Compound processes follows the approach of Nishioka et at. (NVWY)[8]. Like most of the pre-compound models, the NVWY theory describes the equilibration of the composite nucleus as a series of transitions along the chain of classes of closed channels of increasing complexity. The direct-semidirect (DSD) capture model was recently incorporated in Empire. The primary motivation was to improve the capture reactions for fast neutrons.

In the statistical model of nuclear reactions, the Compound Nucleus (CN) state a with spin J, parity Π and excitation energy E to a channel b is given by the ratio of the channel width Γ_b to the total width $\Gamma_{tot} = \Sigma_c \Gamma_c$ multiplied by the population of this state $\sigma_a(E,J,\Pi)$. This also holds for secondary Compound Nuclei which are formed due to subsequent emissions of particles. Each of such states contributes to the cross section.

$$\sigma_b(E,J,\Pi) = \sigma_a(E,J,\Pi)\frac{\Gamma_b(E,J,\Pi)}{\sum_c \Gamma_c(E,J,\Pi)} \tag{1}$$

These have to be summed over spin J and parity Π and integrated over excitation energy E (in case of daughter CN) to obtain observable cross sections.

The particle decay width[8] is given by

$$\Gamma_c(E,J,\Pi) = \frac{1}{2\pi\rho_{CN}(E,J,\Pi)}\sum_{J'=0}^{\infty}\sum_{\Pi'}\sum_{j=J'-J}^{J+J'}\int^{E-B_c} \rho_c(E',J',\Pi')T_c^{l,j}(E-B_c-E')dE' \tag{2}$$

where B_c is the binding energy of particle c in the compound nucleus, ρ_c is the level density, and $T_c^{l,j}(\varepsilon)$ stands for the transmission coefficient for particle c having channel energy $\varepsilon = E - B_c - E'$ and orbital angular momentum l, which together with the particle spin s couples to the channel angular momentum j. For the discrete levels, characterized by the energy E_i, spin J_i and parity Π_i, the level density $\rho_c(E, J', \Pi')$ reduces to $\delta(E - E_i)\delta_{J', J_i}\delta_{\Pi', \Pi_i}$.

The shape of each nucleus affects the parameters of the Giant Dipole Resonance, level density parameter (a) and rotational enhancement of the level densities. The deformation in Empire enters level densities formulae through moments of inertia and through the level density parameter that increases with the increasing nucleus surface. The code estimates this shape by summing up ground state deformation and dynamical deformation induced by the rotation of the nucleus. The Gilbert-Cameron[9] level density formula was used for the current evaluation. The a in Empire is assumed to be energy dependent and calculated following Ignatyuk *et al*[10] as

$$a(U) = \tilde{a}[1 + f(U)\frac{\delta_W}{U}] \tag{3}$$

δ_W is the shell correction which fades out with increasing energy and $\tilde{a}$ is the asymptotic value of the a parameter. $\tilde{a}$ has surface factor, which is the ratio of nuclear radius in R_{max} and R_{min}, to account for the dependence of the level density parameter on nuclear deformation. U is the excitation energy less pairing energy. In Empire, $f(U)$ is used as a function of U,

$$f(U) = 1 - \exp(-\gamma U) \tag{4}$$

where $\gamma = 0.054$ from Ignatyuk.

2.2. Ecis

Ecis was added to Empire as its new extensive module by R. Capote (CEADEN, Habana, Cuba and University of Seville, Spain) in February 2001[8]. Ecis can handle deformed nuclei as well as spherical ones. Majority of deformed nuclei is covered, such as rotational and vibrational, even-even and even-A with integer spins, as well as odd-A with half-integer spins. Vibrational even-even nuclei are also covered. An important feature is an automatized preparation of detailed input for Ecis. This is carried out by Empire: A comprehensive library of input parameters including nuclear masses, optical model parameters, ground state deformations, discrete levels and decay schemes, level densities and γ-ray strength functions. Effects of the dynamic deformation of a fast rotating nucleus can be taken into account in the calculations.

Ecis can be invoked by Empire for deformed nuclei in different ways: One option is that population of (n, n′) discrete collective levels are calculated by CCM. This gives exact direct cross section. However, spherical transmission coefficients provided by SCAT2 are used for whole energy grid, that is, for subsequent pre-equilibrium and HF calculations. These results are renormalized at the transmission level by taking into account direct component. Elastic, absorption and inelastic total cross sections are taken from the CCM calculations. It should perform well for weakly coupled levels. For strong coupling, such as highly deformed rotational bands in heavy nuclei, it should be used with caution. Another option is that population of (n, n′) collective levels is calculated by CCM as above. Importantly, CCM is used consistently, considering ground state and coupled levels, to calculate all necessary transmission coefficients for subsequent pre-equilibrium and HF calculations. These CCM transmission coefficients sum to an absorption cross section which is available for pre-equilibrium + HF decay. This absorption cross section and coupled-channels excitation of collective levels give together reaction cross section. It is the recommended option for very accurate calculation.

3. Procedure

Fig. 1 shows the procedure of neutron cross

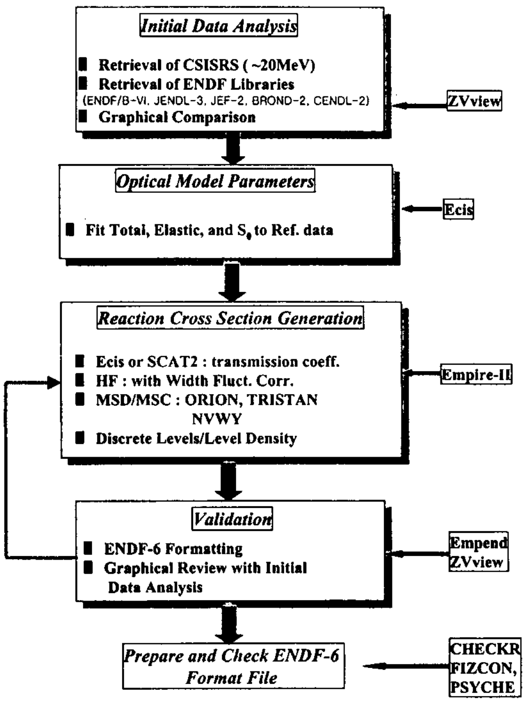

Fig. 1. Schematic Diagram for Evaluation Procedure

section evaluation for deformed nuclei. As a preliminary step, we retrieve and analyze the available experimental data and the evaluated files (ENDF/B-VI, JENDL-3, JEF-2, BROND-2 and CENDL-2) in the evaluation energy range. The analysis of experimental data is very important in the evaluation as a first step. Next step is to look into the proper optical model potential, for example, from Reference Input Parameter Library (RIPL). Empire can import the potential directly from RIPL[11] for spherical and deformed nuclei. However, the total and elastic scattering cross section value produced by the default must be checked with the reference experimental data. If the comparison is unsatisfied, the optical model potential based on the reference total and elastic scattering experimental data should be searched in the Ecis. In this case, the collective levels and deformation parameters are introduced.

Once Ecis is invoked to calculate cross sections for deformed nucleus, the searched potential form and parameters are applied and the code automatically prepares information for run. The potential is used for total, elastic scattering and reaction cross section data calculation as well as transmission coefficients for compound reaction calculation. Using these data, all initial input parameters for Empire are prepared and tuning of parameters is necessary to fit the calculation to the experimental data. Empire calculates the individual reaction cross sections with residual level density. The calculated cross sections are formatted in ENDF-6 format by Empend processing code. Zvview graphical interface helps to compare the results with experimental data and evaluated files in an evaluation energy region for all reaction channels. If the individual cross section results are satisfied with experimental data, the results are combined with the resonance parts. The created nuclear data full set experiences format and physics checking in the whole evaluation energy region using CHECKR, FIZCON and PSYCHE codes.

4. Calculation

The theoretically calculated cross sections are introduced and discussed on (n, tot), (n, n′), (n, γ, (n, p), (n, α), (n, 2n) cross sections in this paper. The major reference experimental data are summarized in Table 1. The present work will be merged at the 1st excited energy with the results of resonance region to make a nuclear data full set. Table 2 shows the summary of collective levels, spin, parity and deformation parameters for coupled channel calculation. Table 3 shows the energy dependent optical model potential parameters. The potential depth (V and W) and radius (r and r_w) for the real and imaginary part

Table 1. Reference Experimental Data

Isotope	Reference experimental data	
	Total cross section	(n, γ) cross section
Eu-153	-	Bokhovko[14]
Gd-155	Wisshak and Djumin[17,18]	Wisshak[17]
Gd-157	Wisshak and Djumin[17,18]	Wisshak[17]

Table 2. Levels for Coupled-channel Calculation

	Level (MeV)	Spin	Parity	Deformation Parameter (β)
Eu-153	0.0000 0.0834 0.1931	2.5 3.5 4.5	1 1 1	0.300
Gd-155	0.000 0.060 0.146 0.252	1.5 2.5 3.5 4.5	−1 −1 −1 −1	0.252
Gd-157	0.000 0.055 0.131 0.227	1.5 2.5 3.5 4.5	−1 −1 −1 −1	0.271

Table 3. Potential Parameters as a Function of Incident Neutron Energy

Parameter (unit)	Eu-153	Gd-155	Gd-157
V_0(MeV)	49.80	59.40	43.80
V_1(MeV)	-0.325	-0.250	-0.250
r_0(fm)	1.280	1.280	1.289
a_v(fm)	0.630	0.510	0.530
W_0(MeV)	4.020	5.020	8.820
r_{w0}(fm)	1.280	1.260	1.260
a_w(fm)	0.480	0.420	0.620
V_{so}(MeV)	6.000	6.000	7.000
r_{so}(fm)	1.280	1.260	1.260
a_{so}(fm)	0.630	0.630	0.630
W_1(MeV)	0.510	0.510	0.500
r_{w1}(fm)	0.000	0.000	0.000
r_1(fm)	0.000	0.010	0.00

were expanded as a function of incident neutron energy, E_n .

$$V = V_o + V_1 x E_n,\ r = r_o + r_1 x E_n \quad (5a)$$

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

The Table shows the much different potential depth of real and imaginary part for the nuclei. However, the radii were not changed much in real and imaginary part.

Fig. 2 shows the calculated total cross section with the evaluated files for Eu-153. There is only one experimental data in the evaluation energy range. The calculated total cross section agrees well with the ENDF/B-VI data. Fig. 3 shows the inelastic scattering cross section. ENDF/B-VI is higher than the calculation until 9 MeV. However, there is no experimental data. The calculated capture cross section is shown in Fig. 4. The calculation and ENDF/B-VI are in good agreement with the experimental data[12,13,14] until 2 MeV. However, above 2 MeV, there is the difference between the calculation and the ENDF/B-VI. Around 14 MeV, the calculation shows the improved capture shape following the giant dipole resonance. Fig. 5 is for the (n, p) cross section. The calculation and the ENDF/B-VI are in good agreement at 14.7 MeV with the measured data[15]. There is no (n, α) cross section data in ENDF/B-VI. The calculation follows the experimental data[15,16] in Fig. 6 for (n, α) cross section. Fig. 7 is the (n, 2n) cross section. The

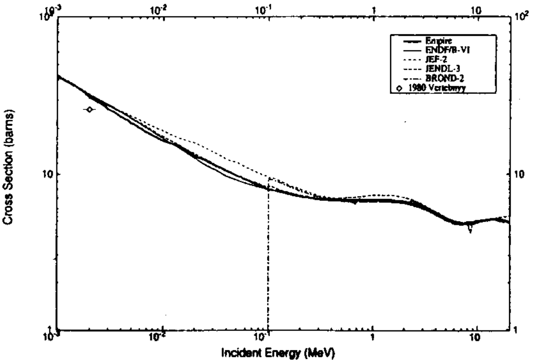

Fig. 2. Total Cross Section of Eu-153

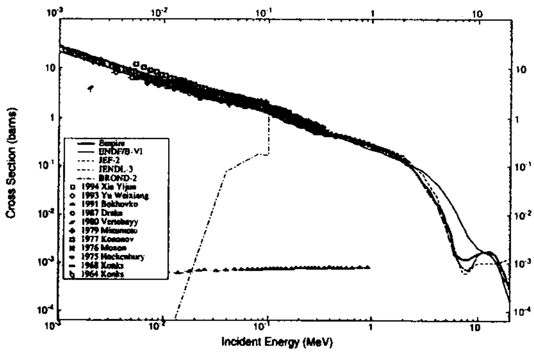

Fig. 4. (n, γ) Cross Section of Eu-153

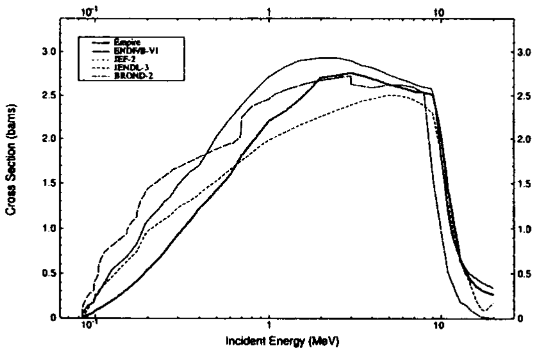

Fig. 3. (n, n′) Cross Section of Eu-153

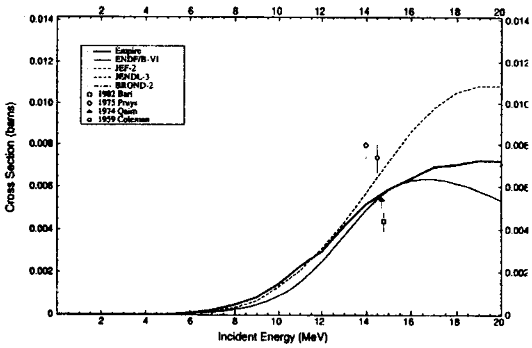

Fig. 5. (n, p) Cross Section of Eu-153

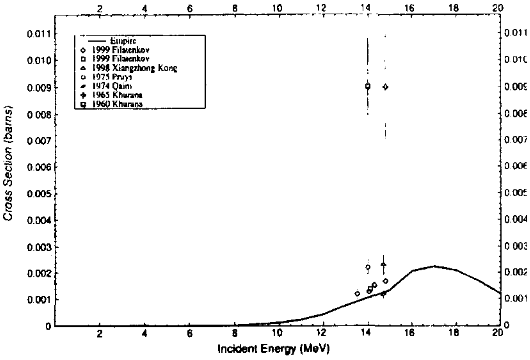

Fig. 6. (n, α) Cross Section of Eu-153

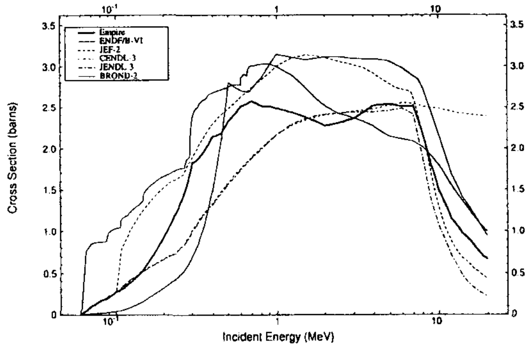

Fig. 9. (n, n′) Cross Section of Gd-155

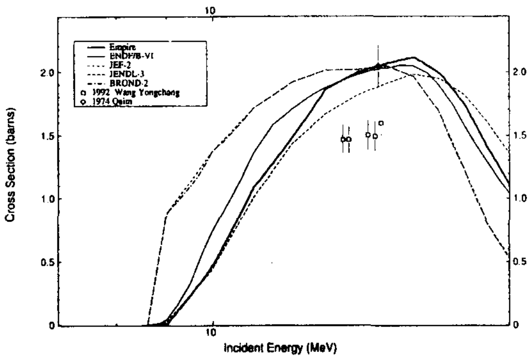

Fig. 7. (n, 2n) Cross Section of Eu-153

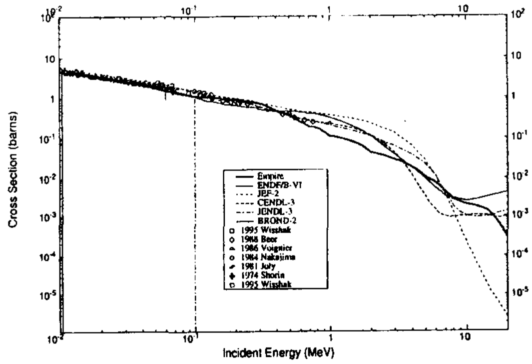

Fig. 10. (n, γ) Cross Section of Gd-155

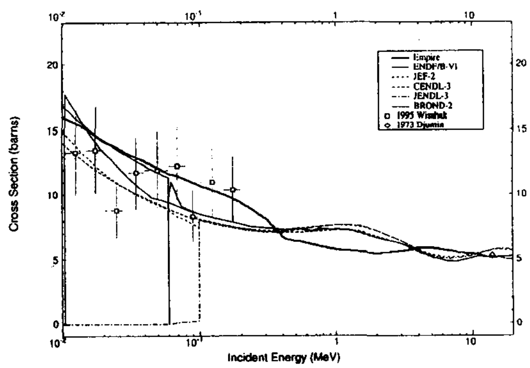

Fig. 8. Total Cross Section of Gd-155

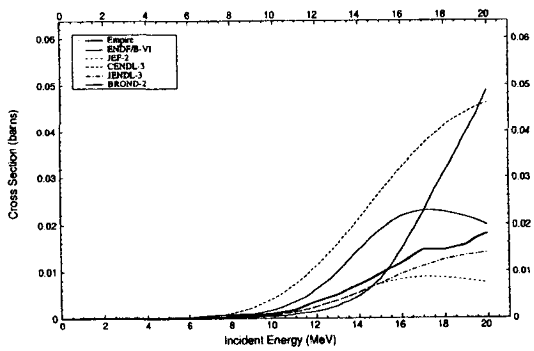

Fig. 11. (n, p) Cross Section of Gd-155

calculation is in good agreement with the measured data[15] at 14.7 MeV.

Fig. 8 shows the total cross section on Gd-155. The calculation and the ENDF/B-VI are matched well with the experimental data[17,18] within the measurement error fluctuation. However, the

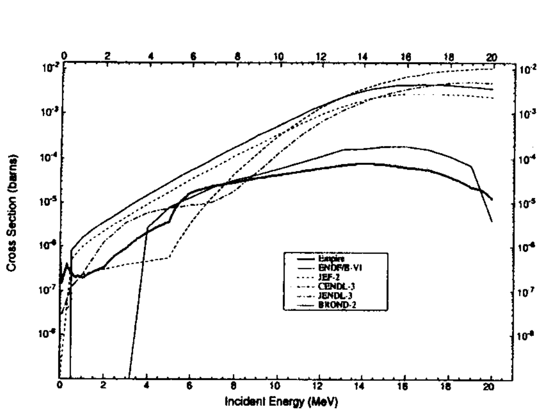

Fig. 12. (n, α) Cross Section of Gd-155

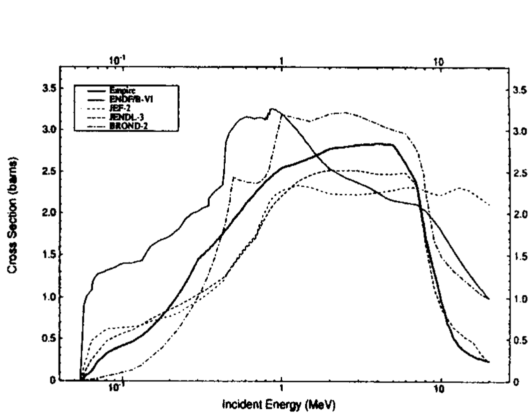

Fig. 15. (n, n′) Cross Section of Gd-157

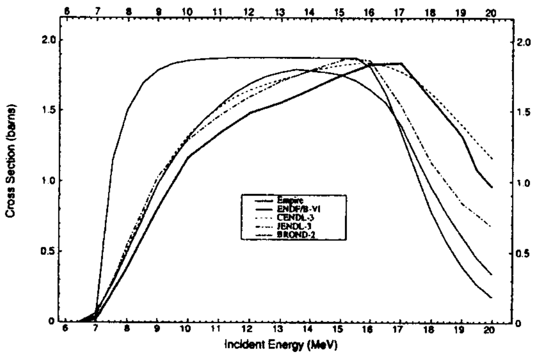

Fig. 13. (n, 2n) Cross Section of Gd-155

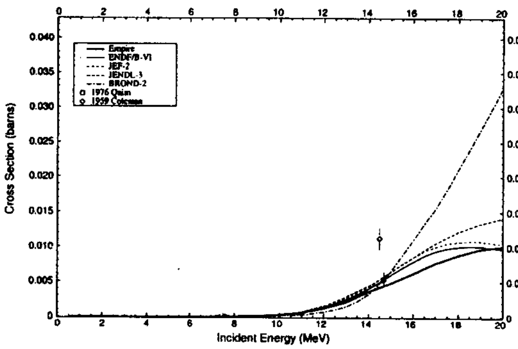

Fig. 16. (n, γ) Cross Section of Gd-157

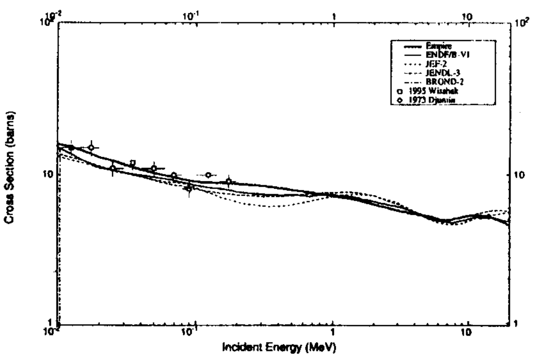

Fig. 14. Total Cross Section of Gd-157

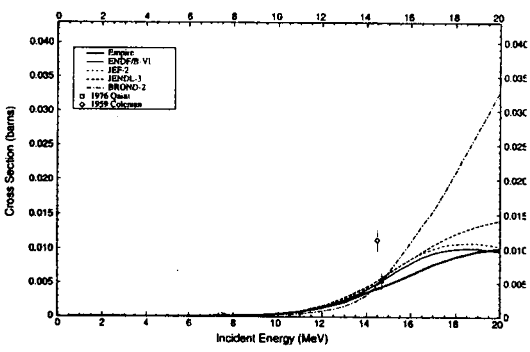

Fig. 17. (n, p) Cross Section of Gd-157

slope is totally different from the ENDF/B-VI in the whole evaluation range. Around 1 MeV, the current calculation is rather lower than the other evaluation files. Fig. 9 is the inelastic scattering cross section. There is no experimental data. Fig. 10 is the capture cross section. The calculation

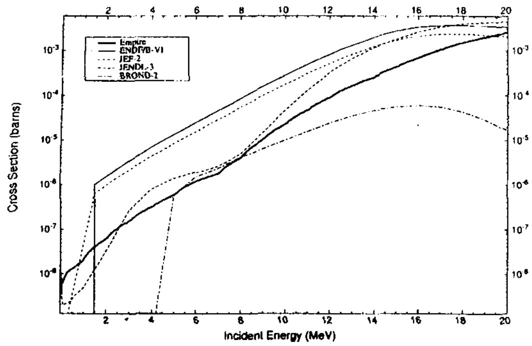

Fig. 18. (n, α) Cross Section of Gd-157

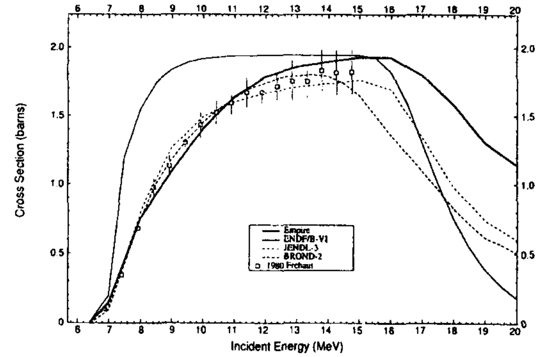

Fig. 19. (n, 2n) Cross Section of Gd-157

and ENDF/B-VI are in good agreement with the experimental data[17,19]. However, above 700 keV, there are different cross section between the calculation and the ENDF/B-VI. Figs. 11, 12 and 13 are for (n, p), (n, α) and (n, 2n) cross sections. There is no experimental data for those reactions.

Fig. 14 is the total cross section of Gd-157. In the measured region, the calculation has somewhat different cross section value from the ENDF/B-VI within the fluctuation,. However, the calculation and the ENDF/B-VI agree well with the experimental data[17,18]. Fig. 15 is for the inelastic scattering cross section. Fig. 16 shows the capture cross section. The calculation and the ENDF/B-VI are in good agreement with the measured data[17,19]. Around 14 MeV, the calculation shows the difference from the ENDF/B-VI. Fig. 17 is for (n, p) cross section. The calculation is in good agreement with the Qaim data[20]. Fig. 18 is (n, α) cross section. Fig. 19 is for (n, 2n) cross section. The calculation is in good agreement with the experimental data[21]. However, the ENDF/B-VI has totally different cross section values from the measured data.

5. Conclusions

The evaluation process for deformed nuclei was successfully setup and the most proper model theory was applied for the Eu-153, Gd-155 and Gd-157 evaluation. The calculation results were satisfactory in the coupled-channel calculation using Ecis. Further, fast neutron capture by direct and semi-direct capture model was substantially improved in the pre-equilibrium energy region. Therefore, the Empire package becomes a highly competitive tool for the evaluation of nuclear reaction data on spherical and deformed cases. The selected energy dependent optical model potential was proper to calculate the total and reaction cross sections in Ecis-Empire combination. Empire was successful in producing the threshold reaction cross sections. The evaluated cross sections are in good agreement with the experimental data. They will contribute to the improvement over ENDF/B-VI library.

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