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EVALUATION AND INTEGRAL TESTS OF FP NUCLEAR DATA FOR JENDL-3

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Abstract Neutron cross sections of 172 nuclides in fission product mass region from As to Tb in the energy range between 0.01 meV and 20 MeV were evaluated for JENDL-3. Compared to JENDL-2 which contains 100 nuclides, the isotopes of As, Se, Br, Sn and Te and several short lived nuclides were added. Threshold reaction cross sections were newly entried. Recent experimental data of resonance parameters and cross sections up to 1987 were utilized. Above unresolved resonance region, cross sections were calculated with spherical optical model, the preequilibrium and statistical theory. The systematics of nuclear model parameters was investigated. Integral test of JENDL-2 FP data was performed using the integral data measured at EBR-II, CFRMF and STEK. For nuclides such as Xe-132,- 134, Eu-152, and Eu-154 whose differential data are not available, the capture cross sections were adjusted with integral data.

(neutron cross sections, nuclear model parameter, fission product nuclides, evaluation, integral test, JENDL-3)

Introduction

JENDL-2 fission product cross section library/1/ released in 1984 contains the data for 100 nuclides in FP mass region. It covers 99.6% captures and 195% yields for FBR burnup calculations. In the present evaluation for JENDL-3, it was aimed to apply the data for more general purposes besides reactor burnup calculation, i.e., the applications to dosimetry, activation, radiation damage, nuclide transmutation and fuel failure detection. The number of nulides was extended to 172 nuclides ranging Z = 35 - 65, by adding As, Se, Br, Sn and Te isotopes, and some short lived nuclides. Threshold reaction cross sections were newly entried for most nuclides. Also, recent capture and resonance data up to 1987 were taken into account to update the JENDL-2 data. Integral test results on neutron capture were reflected on the cross section revision, particularly for nuclides whose differential data were not available.

Method of calculation and evaluation

The MLBW formula was used for resolved resonances. Unresolved resonance parameters were given for energy below 100 keV using ASREP code/2/. Above unresolved resonance region, CASTHY /3/ , a spherical optical model and the statistical theory code, was used to calculate the total, capture, elastic and inelastic scattering cross sections.

Threshold reaction cross sections of (n,2n), (n,p), (n,a), (n,n'p), (n,n'a), (n,d) and (n,t) reactions and the competing cross sections for CASTHY were calculated with PEGASUS/4/, a preequilibrium and multi-step evaporation code. An extensive data file containing level density parameters and inverse cross sections for neutrons and charged particles was prepared for massive computation. The code is particulary suited to the scoping calculations.

Integral test of JENDL-2 was performed by using the CFRMF and the EBR-II irradiation data/5,6/ and the STEK sample worth data/7/. The cross sections were adjusted for Xe-132. Xe-134, Eu-152 and Eu-154 for which the differential capture data are not reported.

Calculational parameters

Resonance parameters

Resolved resonance parameters were adopted mostly from JENDL-2 and Mughabghab et al./8,9/. New evaluation was made for Kr-86, Zr-93, Ag-110m, Sn-122, Sb-121, Sb-123, Xe-136, Ba-135, Ba-137, Ba-138, Ce-140, Ce-141, Ce-142, Sm-147, Sm-148, Gd-152, Gd-154 by using recent resonance data measured at JAERI, ORNL and NIR. The consistency between partial and total widths and the conservation of the capture area have been checked. The unassigned value of the neutron angular momentum of resonance level was determined based on Bayesian theorem. The unassigned resonance level spin 'J' was determined statistically.

Theoretical model parameters

For most nuclides, the spherical optical potentials used in JENDL-2/10/ were adopted which were determined to fit the total cross section data taking acount of the semi-local systematics of total cross sections as shown in Fig. 1. Optical potential parameters were revised for the elememts Pr, Pm and Eu to improve the fit with total and nonelastic cross sections. To calculate the inverse-reaction cross sections due to charged particles for PEGASUS calculations, grobal fit optical model parameters were adopted.

Level density parameters of the Gilbert-Cameron type were newly determined from the low-lying level scheme and the observed resonance level spacings. When these data are not available, the systematics /11/ was used to estimate 'a' parameter and the constant nuclear temperature parameter, T. The latter systematics is depicted in Fig. 2.

The gamma-ray strenth function was adjusted

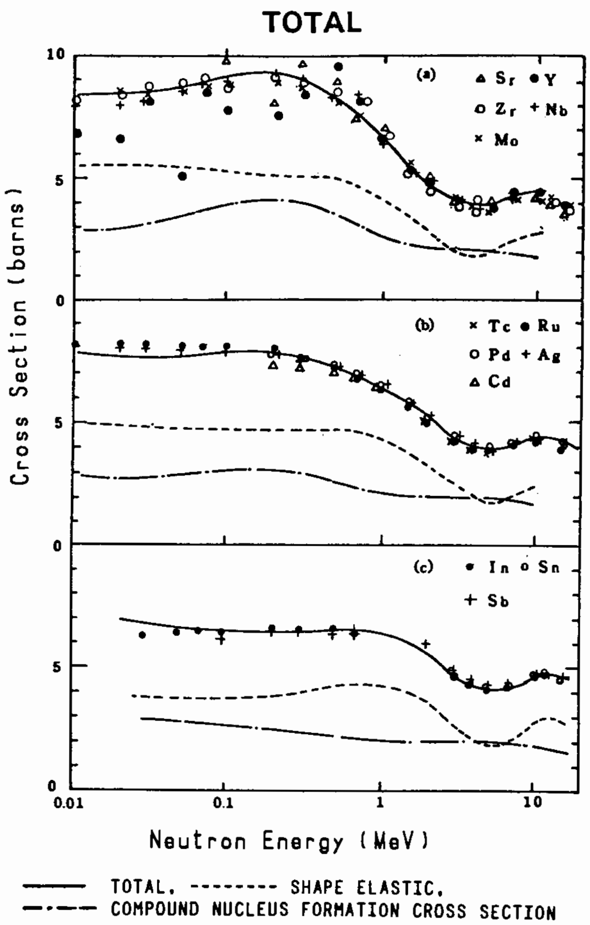

Fig. 1 Neutron total cross sections and the optical model fit.

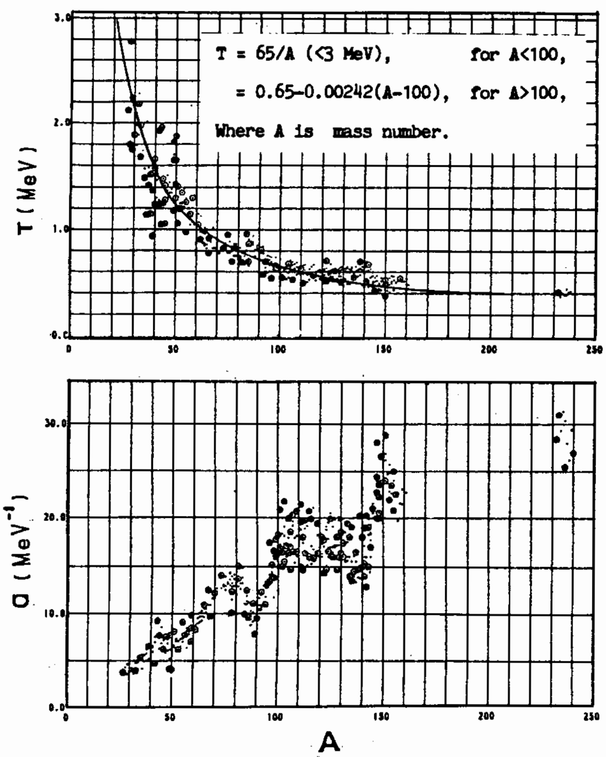

Fig. 2 Mass number dependence of level density parameters

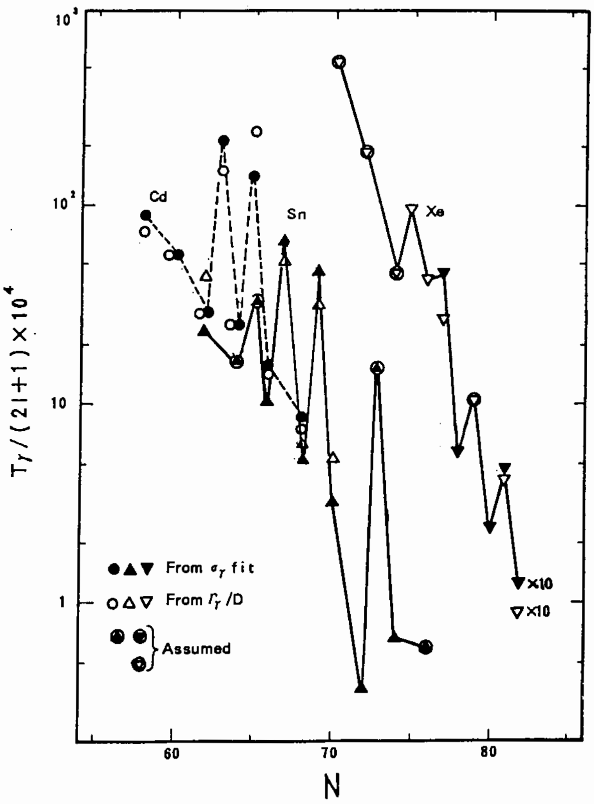

Fig. 3 Systematics of gamma-ray transmission coefficients for Cd, Sn and Xe isotopes.

to fit the capture data. Its systematics was investigated by using the values determined from capture fit and the ones from the average resonance parameters either measured or estimated based on the above-mentioned systematics of the level density. The trends are shown in Fig. 3 for Cd, Sn and Xe isotopes. The values obtained by different methods are generally consistent with each other. The systematics of the gamma-ray strength functions was used for the nuclides whose capture data are not reported.

The Kalbach's constant K, which represents the strength of the pre-equilibrium transition rate, was estimated as $K = 0.1/(g/A)^3$ (±50%), where g is the single particle level density of the composite nucleus. The estimation is based on the expression of two-body interacion in nuclear matter by Kikuchi and Kawai. The value of K and level density parameters were adjusted to fit the measured (n,2n) cross sections.

Integral test and cross section adjustment

The JENDL-2 FP data were tested with STEK, CFRMF and EBR-II integral data. In case of STEK data analysis, the correction to flux depression for strong low energy resonances was made using the neutron escape probability. The correction was effective for a consistent comparison of the calculated and measured reactivities of strong absorber samples. Table 1 shows the calculation-to-experiment ratios for STEK sample worth and reaction rates measured in CFRMF and EBR-II. Agreement between calculation and experiment is generally good, except for Pd-104, Ag-109, Xe-132, Xe-134, Eu-151,Eu-152, and Eu-154. For Tc-99 and Pm-147

Table 1 JENDL-2 integral test result (C/E Values)

Nuclide	STEK	CFRMF	EBR-II Core	EBR-II Reflector
Nb-93	1.03 - 1.20	-	-	-
Mo-95	0.97 - 1.11	-	-	-
Tc-99	0.88 - 0.91	1.23(15%)	-	-
Ru-101	0.98 - 1.06	-	-	-
Rh-103	1.01 - 1.14	-	-	-
Pd-104	1.07 - 2.09	-	-	-
Pd-107	0.94 - 1.04	-	-	-
Ag-109	0.76 - 0.96	0.67(10%)	-	-
Xe-131	0.93 - 1.18	-	-	-
Xe-132	-	1.29(8%)	-	-
Xe-134	-	1.38(7%)	-	-
Cs-133	0.76 - 0.85	0.91(7%)	-	-
Nd-143	0.89 - 0.93	-	0.85(6%)	0.86(14%)
Pm-147	0.88 - 0.93	1.10(13%)	-	-
Sm-149	0.92 - 1.05	-	0.88(6%)	1.01(14%)
Sm-152	0.81 - 1.09	1.00(6%)	-	-
Eu-151	-	0.83(6%)	0.68(8%)	0.70(15%)
Eu-152	-	-	0.64(11%)	0.90(16%)
Eu-153	0.89 - 0.96	0.91(7%)	0.83(7%)	0.87(14%)
Eu-154	-	-	0.70(10%)	0.84(15%)
Gd-157	0.82 - 1.01	-	-	-

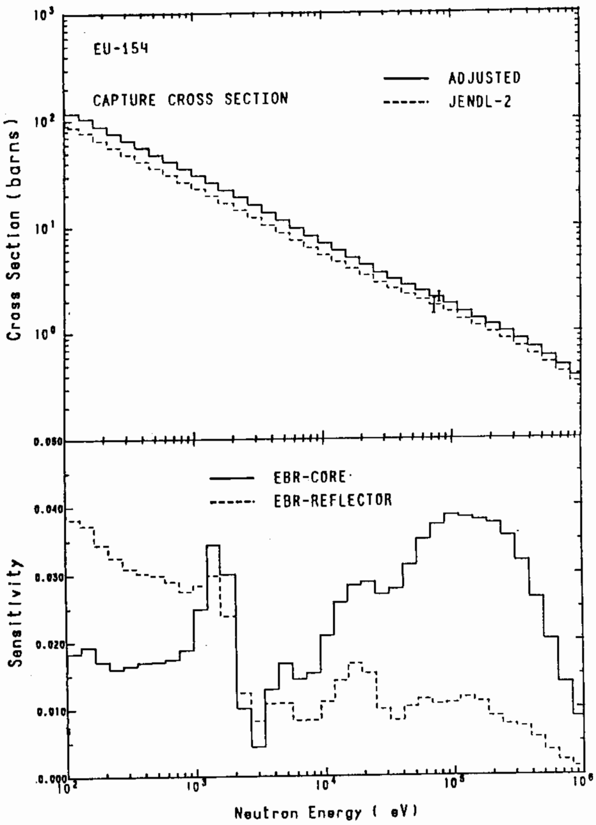

Fig. 4 A priori and adjusted capture cross section of Eu-154. Adjustment was made with EBR-II data.

Table 2 Results of cross section adjustment

Nuclide	Spectrum	C/E values before adjust	C/E values after adjust
Xe-131	STEK500	1.18 (14%)	0.96 (5%)
	STEK2000	1.18 (10%)	1.04 (2%)
Pm-147	STEK1000	0.94 (12%)	0.97 (4%)
	[CFRMF	1.10 (19%)	1.13 (7%)]
	CFRMF	1.10 (19%)	1.03 (10%)
Eu-151	EBR-II/C	0.67 (10%)	0.82 (5%)
	EBR-II/R	0.68 (12%)	0.81 (9%)
	CFRMF	0.84 (11%)	1.02 (5%)
Eu-153	EBR-II/C	0.91 (12%)	1.02 (6%)
	EBR-II/R	0.83 (11%)	0.92 (5%)
	CFRMF	0.87 (12%)	0.94 (9%)
Xe-132	CFRMF	1.29 (15%)	1.06 (5%)
Xe-134	CFRMF	1.37 (19%)	1.02 (5%)
Eu-152	EBR-II/C	0.64 (21%)	0.80 (11%)
	EBR-II/R	0.90 (28%)	1.12 (13%)
Eu-154	EBR-II/C	0.70 (18%)	0.87 (10%)
	EBR-II/R	0.84 (22%)	1.04 (12%)

N.B. 1) EBR-II/C: spectrum in EBR-II core.
2) EBR-II/R: spectrum in EBR-II reflector.
3) The value in parenthesis is a percent error.

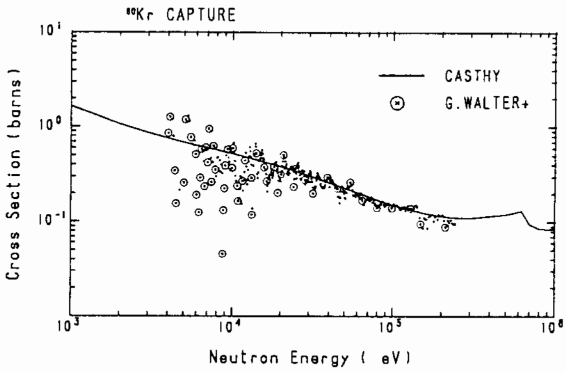

Fig. 5 Kr-80 capture cross section.

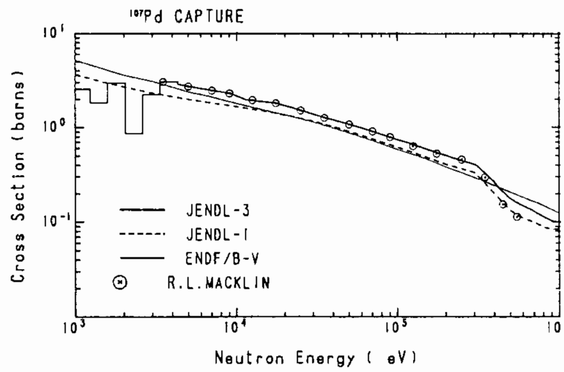

Fig. 6 Pd-107 capture cross section.

there seems to be inconsistency between the integral data of CFRMF and STEK. Capture cross sections of Xe-132, Xe- 134, Eu-152, and Eu-154 were adjusted based on integral data using Bayesian method. Only the integral data are available for these nuclides. The adjustment was also made for some other nuclides as the test of the method. Flux uncertainties are treated as "method uncertainty". Cross section covariance matrices were generated with the "strength function model".

Table 2 compares the C/E values before and after adjustment. The C/E values are mostly improved after adjustment as expected, although the solution which simultaneously satisfies the CFRMF and STEK data was not obtained in case of Pm-147. Figure 4 shows a priori and adjusted cross section of Eu-154 using EBR-II irradiation data.

<u>Evaluated cross sections</u>

Capture cross sections for Zr-93, Pd-107, Sm-149 and Kr isotopes were reevaluated based on recent capture data/12-15/. Figures 5 and 6 show the cross sections for Kr-80 and Pd-107.

Figure 7 gives the experiment-to- calculation ratios of (n,2n) and (n,p) cross sections at 14.5 MeV. The (n,2n) cross sections are predicted fairly well, while the prediction of (n,p) cross sections is rather diverging. In the final data file calculation was normalized to the experimental data or 14.5 MeV systematics. Figure 8 compares the evaluated and measured (n,2n) cross sections for Nd-144 and Nd-150.

Concluding remarks

Owing to the recent experimental data on capture cross sections, the discrepancies observed by the integral testing of JENDL-1 FP data have been largely removed. Conversely,for example, the adjusted capture cross section of Zr-93/1/ with STEK reactivity data was in good agreement with the later experimental data of Macklin/13/.

For resolved resonance parameters, many hitherto unknown new data were given by the ORELA measurements. Yet there exists often the energy gap between the minimum resonance energy of about 2.6 keV measured at ORELA and the maximum energy by other measurements. Since it is not allowed in ENDF/B format to give "resolved-unresolved-resolved" sequence of data, the ORELA resonance data above 2.6 keV were often not able to include in the evaluated data file. Some of recent experimental data at JAERI filled up this energy gap, hence making possible at the same time to include the ORELA data in the evaluated data file. Therefore, further measurements of resonance parameters filling this energy gap are requested. Evaluation is now at the final stage and will be completed by August 1988.

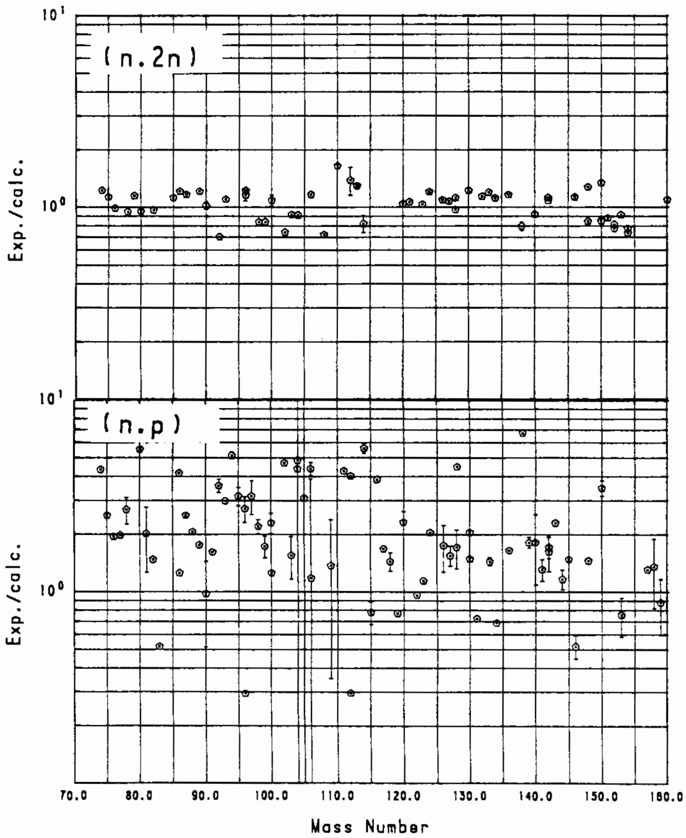

Fig. 7 Experiment-to-calculation ratios of 14.5 MeV (n,2n) and (n,p) cross sections

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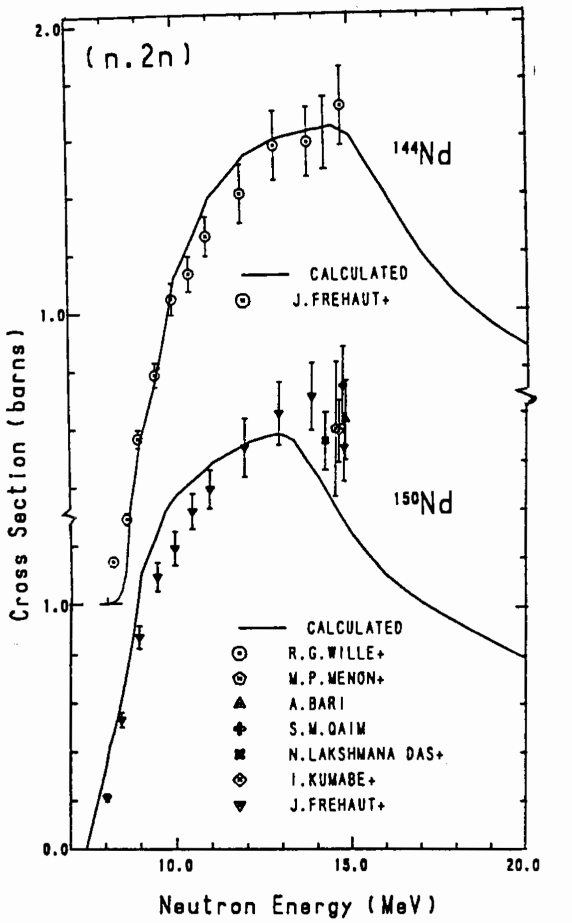

Fig. 8 Calculated (n,2n) cross sections for Nd-144 and Nd-150.