TRANSMISSION FUNCTION MEASUREMENTS, EVALUATION OF MEAN RESONANCE PARAMETERS AND GROUP CONSTANTS FOR ^{235}U IN THE UNRESOLVED RESONANCE REGION

A.A. Van'kov, L.s. Gosteva, V.f. Ukraintsev, S. Toshkov, N. Yaneva

ABSTRACT

An analysis of experimental average transmission and cross-sections data for ^{235}U was carried out using the multilevel theory. A new evaluation for mean resonance parameters and group constants of ^{235}U was made in the energy region 0.1-21.5 keV.

Research is currently being done on analysing neutron cross-sections in the resonance energy region [1]. For fissile nuclides, the problem of the resonance region is complicated by the need to take account of the strong effects of inter-level interference. Uranium-235 is an example of one of these "difficult" nuclides. At the same time, the evaluation of its fission cross-section is taken as standard. The latest evaluation of the cross-sections for ^{235}U in the ENDF/B-V library [2] is connected with work [3] on the analysis of ^{235}U cross-sections for polarized neutrons. These results significantly affect the recommended values for mean resonance parameters: the mean distance between the levels D and the fission widths in the states J^{π}, equal to 3^-, 4^-.

The aim of the present work is to make a combined analysis of the data for ^{235}U using the mean cross-sections from Ref. [2] and of the results obtained by the authors of the present work for transmission function measurements of the type:

$$T(n) = 1/\Delta u \int exp\left[-\sigma_t(u)n\right]du\,; \qquad T_f(n) = 1/\langle\sigma_f\rangle \int \sigma_f(u) exp\left[\sigma_t(u)n\right]du\,,$$

and also to obtain an improved evaluation of the mean resonance parameters for ^{235}U. This will be used as the basis for calculating group constants (mean cross-sections and resonance self-shielding factors) for a system such as the BNAB-78 library [4].

Description of experimental data on transmission functions

The transmission T(n) and the self-indication functions of the fission reaction $T_f(n)$ were measured using the IBR-30 reactor neutron time-of-flight spectrometer. The neutron spectrum was close to the Fermi slowing-down spectrum. A description of the experimental conditions is given in Refs [5 and 6]. It should be noted that the sample filters, of metallic uranium, were 90% enriched and had high chemical purity.

We intend to analyse Garber's results [2] and the experimental data on the functions T(n) and $T_f(n)$ shown in Fig. 1, which also shows the data from Ref. [7]. Apart from ours, the latter is the only work in which the function $T_f(n)$ is measured for ^{235}U but it is measured only at neutron energies below 1 keV. There is good agreement between the results of Czirr's work [7] and our present data.

An evaluation of the errors in our results is given in Refs [5 and 6]. The main component of these errors is related to the background measurement. In analysing the experiment and in evaluating the mean resonance parameters, the errors for the experimental values T(n) and $T_f(n)$ emerged somewhat

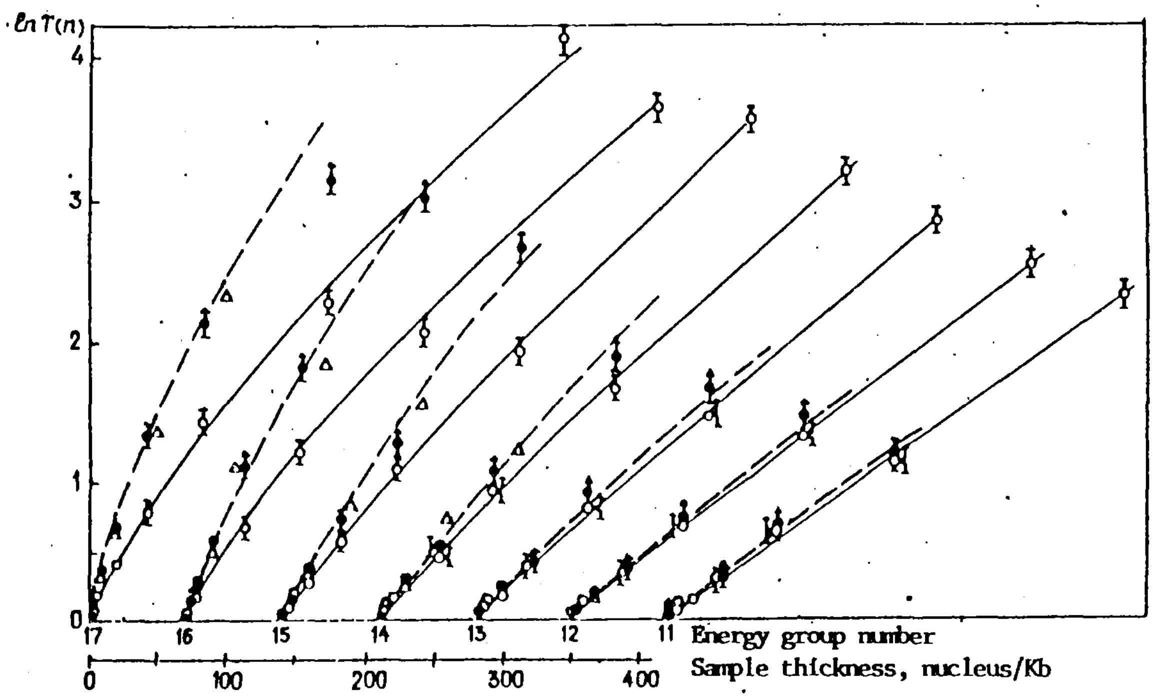

Fig. 1. Transmission functions (experimental points and optimized calculation) Data of the present work: ⧫ - $T(n)$; ◊ - $T_f(n)$. Data of Ref: [7]: Δ - $T_f(n)$

higher than those stated in Ref. [5]. These errors correspond to a confidence level of 95%.

Calculation-theoretical method. Calculation of the mean cross-sections based on the evaluated mean resonance parameters is usually performed using the Hauser-Feshbach formalism [8]. Bhat et al [9] obtain the mean resonance parameters for ^{235}U used in the files of the ENDF/B-V library and representating the initial data for calculating the recommended mean cross-sections. The present authors aimed to refine these parameters on the basis of additional experimental data on transmission functions. These values are sensitive to the effects of inter-resonance interference, and therefore the calculational model must take fairly strict account of them. Obviously the transmission functions cannot theoretically be calculated using the Hauser-Feshbach formalism. Moreover, only a multilevel formalism is suitable for this purpose. It was decided that the Reich-Moore formalism was here appropriate. It expresses the link between the neutron cross-sections and the S-matrix in the well-known way:

$$\sigma_t(E) = 2\pi\lambda^2 \sum_{J\pi} g(J) \sum_{\ell_j} (1 - Re\, S^{J\pi}_{n\ell_j, n\ell_j}) ;$$

$$\sigma_f(E) = \pi\lambda^2 \sum_{J\pi} g(J) \sum_{\ell_j} \left| S^{J\pi}_{n\ell_j, f\ell_j} \right|^2 ;$$

$$\sigma_{e\ell}(E) = \pi\lambda^2 \sum_{J\pi} g(J) \sum_{\ell_j} \left| 1 - S^{J\pi}_{n\ell_j, n\ell_j} \right|^2 .$$

There is a unique relationship between the collision matrix S and the R-matrix which in the Reich-Moore approximation and has the form.

$$R_{cc'}(E) = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\bar{\Gamma}_\gamma/2},$$

where $\gamma_{\lambda c}$ is the amplitude of the reduced widths in the channel with the set of quantum numbers c; E_λ is the resonance energy; $\bar{\Gamma}_\gamma$ is the mean resonance width. The radiative capture cross-section was defined as the difference between the total cross-section and the fission and scattering cross-sections. This may account for the insignificance of interference effects in the radiative capture. In order to calculate the mean cross-sections and transmission functions using the Reich-Moore formalism, a method of statistical generation (Monte-Carlo method) of neutron cross-sections was developed. The authors describe the method in detail in Ref. [10].

Optimization method. The evaluation of the mean resonance parameters for ^{236}U was based on a combined analysis of the cross-sections in Ref. [2] and the transmission functions averaged in energy groups using the format of the BNAB-78 system of constants [4]. It is used in draft reactor calculations, and therefore the results obtained by the authors of the present work have practical significance. Moreover, the energy intervals (group widths) in this system are fairly large, which results in an averaging of the neutron cross-section fluctuations due to the resonance statistics and thereby ensures the correctness of the theoretical description in terms of the mean resonance parameters. The mean group cross-sections for ^{235}U from ENDF/B-V library file were obtained using the RECENT program. Optimization was performed using Bayes' method [11] which requires the following initial values:

- The initial a priori evaluation of the mean resonance parameters and their a priori error. The ENDF/B-V library evaluation [2] was taken for the values $\overline{D}$, S_o and Γ_γ, and the results in Ref. [12] for the other parameters. The errors were assumed to be 25% (for the parameter R' the error was assumed to be 5%);
- The deviation of the evaluated experimental data for the mean cross-sections and transmission functions from the calculated values;
- The errors in the evaluated experimental values for the mean cross-sections (5% for σ_f and 7% for σ_γ) and the transmission functions (2-3% for thin samples, increasing with the thickness of the sample to 20-30%). All the errors were reduced to the 95% confidence interval;

- sensitivity coefficients, i.e. the values $\frac{\partial \bar{F}_i}{\partial p_k} / \frac{\bar{F}_i}{p_k}$ where $\bar{F}_i$ is the mean cross-section of transmission and P_k is the variable parameter of the model.

The following values varied: the mean distance [for various states the law of proportionality was assumed $\tilde{D}_J \sim (1/2J+1)^{-1}$], the mean radiation width $\bar{\Gamma}_\gamma$ (common to all states), the neutron strength functions S_o (varied in each group) and S_1 (independent of energy), and the fissile width Γ_f and $\ell = 0$ (varied in each group). The ratio of fission channel contributions also varied for the states with $\ell = 0$. The values Γ_f for $\ell = 1$ were fixed.

Description of the results The optimization results are given in Tables 1 and 2, and the fitting is shown in Table 3 and Fig. 1. Measurement of transmission functions for large thicknesses provides information about the scattering radius R', which in our model is assumed to be the same in all states. The optimization result showed the monotonic dependence of R' on neutron energies (see Table 2).

As is shown in Fig. 1 and Table 3, the parameters obtained provide a good description of the experimental material on mean cross-sections and transmission functions for ^{235}U. Figure 2 (continuous histogram) shows the calculation results for resonance self-shielding factors at room temperature based on optimized mean resonance parameters. The tabular data from the BNAB-78 libfary [7] are also shown there for comparison (broken line). It can be seen that the results of the authors' evaluation show a more pronounced resonance self-shielding effect for all ^{235}U reaction cross-sections.

Reliability of the evaluations. As a result of optimization, a covariation matrix of the D(p) parameters was obtained, which is not given here. Its diagonal elements characterize the a posteriori evaluation error. For the basic parameters such as S_o, $\bar{\Gamma}_\gamma$ and $\bar{\Gamma}_f$ ($\ell = 0$), the a posteriori errors never exceed 10% and the error of R' is less than 1.5%. The

Table I

Evaluation of non-energy dependent mean resonance parameters for ^{235}U (optimization result)

$J\pi$	D, eV	Γ_γ, MeV	$S_n \cdot 10^4$	Γ_f, eV	f_1	f_2
3^-	0,967	30	Var.	Var.	0,5	0,5
4^-	0,801	30	Var.	Var.	0,5	0,5
2^+	1,256	30	1,68	0,468	0,5	0,5
3^+	0,967	30	1,68	0,165	1,0	0,0
4^+	0,801	30	1,68	0,322	0,5	0,5
5^+	0,770	30	1,68	0,130	1,0	0,0

Note: f_1, f_2 - the ratio of fission channel contributions in the given state; Var. means that the parameter is variable in each energy group.

Table 2

Evaluation of the mean resonance parameters which are dependent on the number of the energy group (optimization result).

Number of group	Energy interval, keV	R', fm	$S_0 \cdot 10^{-4}$	$\bar{\Gamma}_f^{3-}$ MeV
11	10,0-21,5	9,1	1,05	153
12	4,65-10,0	9,2	0,964	170
13	2,15-4,65	9,2	0,901	243
14	1,00-2,15	9,2	0,910	170
15	0,465-1,00	9,2	1,05	176
16	0,215-0,465	9,2	0,940	144
17	0,100-0,215	9,5	0,950	120

Note: It is assumed that $\bar{\Gamma}_f^{3-} = \bar{\Gamma}_f^{4-}$.

Table 3

Mean cross-sections for ^{235}U in energy groups, b

Cross-section	Number of group						
	11	12	13	14	15	16	17
σ_t	15,0 / 14,7	16,6 / 16,4	18,5 / 18,9	22,3 / 22,5	28,3 / 28,7	35,9 / 36,0	44,5 / 46,5
σ_γ	1,00 / 1,08	1,42 / 1,38	1,69 / 1,69	3,00 / 2,94	4,69 / 4,61	7,19 / 7,33	11,5 / 11,5
σ_f	2,48 / 2,56	3,49 / 3,45	4,93 / 5,18	7,15 / 7,15	11,3 / 11,5	16,3 / 16,0	20,5 / 21,5

Note: The numerator indicates the calculation from data in the ENDF|B-V library, the denominator indicates the optimized calculation.

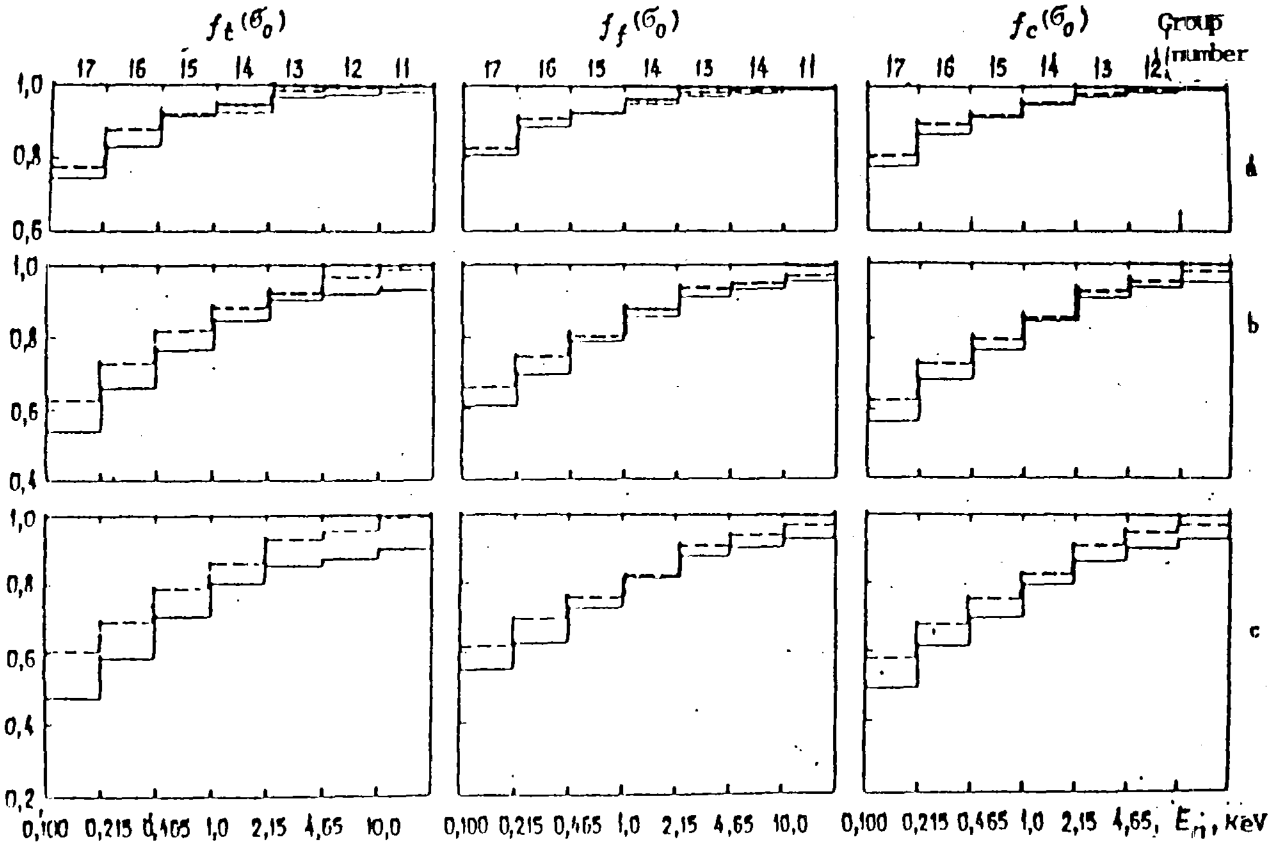

Fig. 2. Resonance self-shielding factors of total cross-section and of fission and capture cross-sections for ^{235}U at room temperature for dilution cross-sections σ_0, equal 100 b (a), 10 b (b) and 0 (c)

Table 4

Comparison of the discrepancies between the experimental (e) and optimized calculated (c) values of mean cross-sections with their a posteriori errors.

Energy Interval keV	$\bar{\sigma}_t$	$\bar{\sigma}_f$	$\bar{\sigma}_\gamma$
10-21,5	2,3	-3,1	-7,4
	1,9	5,7	5,7
4,65-10	1,4	1,2	2,9
	1,9	5,6	6,0
2,15-4,65	-2,3	-4,8	0,0
	1,9	5,2	5,8
1,00-2,15	-0,9	0,0	2,0
	2,0	5,1	5,7
0,465-1,00	-1,5	-2,2	1,7
	2,0	4,7	5,6
0,215-0,465	-0,3	2,3	-1,9
	2,0	4,1	5,6
0,100-0,215	-4,5	-4,9	0,4
	2,1	4,5	5,1

Note: The numerator indicates the discrepancy [(e-c)], %; the denominator indicates the a posteriori error, %.

Table 5

Comparison of the discrepancies between the experimental (e) and optimized calculated (c) transmission functions with their a posteriori errors.

Energy interval keV	0,02145	0,0858	0,1716
10-21,5	-0,6	-4,4	-2,1
	0,6	2,2	4,0
4,65-10,0	0,3	-2,3	-1,3
	0,6	2,3	4,1
2,15-4,65	1,5	-4,1	-1,8
	0,7	2,6	4,6
1,00-2,15	0,5	-6,2	-2,6
	0,8	2,6	4,4
0,465-1,00	0,0	-6,6	3,4
	1,0	2,8	4,5
0,215-0,465	1,0	-9,5	-4,0
	1,2	2,9	4,5
0,100-0,215	1,7	-5,2	17,7
	1,1	2,9	48

Note: The numerator indicates the discrepancy [(e-c)/c], %; the denominator indicates the a posteriori error, %.

reliability of the evaluation can be judged by comparing the a posteriori errors with the discrepancy between the results of the optimized calculation and the experimental evaluations (Tables 4 and 5). The a posteriori errors of F are obtained from the diagonal elements of the covariation matrix

$$D(p) : D(F) = K^T D(p) K,$$

where

$$K_{ij} = \frac{\partial F_i}{\partial p_j} \Big/ \frac{F_i}{p_j} .$$

The sensitivity coefficients were calculated using the perturbation method (in Monte Carlo calculations). Tables 4 and 5 show that the a posteriori errors obtained are comparable with the discrepancies in the experimental and optimized cross-sections and transmission functions. As the thickness of the sample increases, the tranmission measurement error significantly increases, and hence at specific points the discrepancy (e - c)/p may be 2-3 times greater than the a posteriori error. This is in agreement with the evaluations of the measurement errors, which exceed 10% for large thicknesses. On the whole, the data in Tables 4 and 5 demonstrate the self-consistency of the statistical errors and the reliability of the established confidence limits for the final results.

A high degree of accuracy was obtained a posteriori for the evaluation of resonance self-shielding factors: when σ_0 = 10 b, the relative error f_f and f_γ in the 17th group is 1.2%, further, the monotonic error falls as the energy increases, reaching 0.2% in the 11th group. When σ_0 = 100 b, the corresponding errors are 2-3 times less and have a similar dependence on energy.

When judging the evaluation errors, one has to take into account the fluctuation error in the mean functionals, caused by the natural statistics and the final number of resonances in the group. This error was evaluated in calculations using the Monte-Carlo method. At low energies (groups 16-17), it exceeds 10% for mean cross-sections, and for resonance self-shielding factors (where σ_o is 10 and 100 b) it is 4-8%. At higher energies, the fluctuation error becomes comparable to or less than the a posteriori error. The fluctuation error obviously does not play a role in the averaging of functionals over a wide spectrum. However, in the individual groups, it should be remembered that this error exists, and if it is to be removed, individual fitting must be made in each group permitting local (not physical) fluctuations of the mean resonance parameters.

On the basis of this analysis, the following conclusions can be drawn:

1. In comparison with the evaluations of the ENDF/B-V library, we obtained lower values for the radiation width $\bar{\Gamma}_\gamma$ (30 MeV instead of 35 MeV). For the p strength function, a single evaluation was obtained $S_1 = 1.667 \times 10^{-4}$. In the ENDF/B-V library the values quoted are $S_1 = 1.45 \times 10^{-4}$ ($J^\pi = 2^+, 5^+$) and $S_1 = 1.25 \times 10^{-4}$ ($J^\pi = 3^+, 4^+$). For a satisfactory description of the experimental material, the values S_o and Γ_f have to be varied separately in each group;

2. The best description is obtained by selecting the following fission channel contributions to the total fission width in the states 3^-, 4^-: $f_2 = 0.5$; $f_2 = 0.5$. We do not have any information on fission cross-sections in states with total momentum 3^-, 4^- and so the condition $\bar{\Gamma}_f^{3-} = \bar{\Gamma}_f^{4-}$ was adopted. Since there is only a slight difference in the momenta, this assumption seems reasonable. The selection of fission channel contributions and of the values of Γ_f for $\ell = 1$ has little effect on the optimization results;

3. From the experimental data on transmission functions, it follows that the scattering radius R' is monotonically dependent on neutron energy. If this effect is extracted from data only using $< \sigma_t >$, it is quite small;

4. The new evaluation obtained for mean resonance parameters for ^{235}U offers a good description of all the experimental data on mean cross-sections and transmission functions. Its reliability is characterized by the a posteriori covariation matrix from which the errors in the calculated group constants are obtained. It is recommended that practical use be made of the results when compiling more precise group constants.

REFERENCES

[1] VAN'KOV, A.A., Voprosi atomnoj nauki i tekhniki, Ser. Yadernye konstanty, 4, 53 (1983) 3-8.

[2] GARBER, D., ENDF-102; BNL-NCS-50496 Upton (1979).

[3] HEYWORTH, G.A., MOORE, M.S., In: Proc. of the intern. conf. Harwell (1979) 241-255.

[4] ABAGYAN, L.P., BAZAZYANTS, N.O., NIKOLAEV, M.N. et al, Gruppovye konstanty dlya rascheta reaktorov i zashchity. M.: Ehnergoizdat (1981).

[5] VAN'KOV, A.A., GRIGOR'EV, Yu.V., UKRAINTSEV, V.F., et al, Voprosy atomnoj nauki i tekhniki, Ser. Yadernye konstanty 4 35 (1979) 48-52.

[6] BAKALOV, T., ILCHEV, G., TOSHKOV, S. et al. Transmission and self-indication measurements with ^{235}U and ^{239}Pu in the 2 eV-20 keV energy region. NBS special publ. N.594, Washington (1980) 692-694.

[7] CZIRR, G.B., Nucl. Sci. and Engng 70 3 (1979) 307-308.

[8] HAUSER, W., FESHBACH, H., Phys. Rev. 87 (1952) 366-370.

[9] BHAT, M.R., Evaluation of ^{235}U neutron cross-sections and gamma-ray production data for ENDF/B-V: BNL-NCS-51184 (1980).

[10] VAN'KOV, A.A., TOSHKOV, S., UKRAINTSEV, V.F., et al. Voprosy atomnoj nauki i tekhniki. Ser. Yadernye konstanty 4 53 (1983) 18-25.

[11] VAN'KOV, A.A., Yadernye konstanty (1974) M: Atomizdat 16 (1974) 11-19.

[12] AMTSIPOV, G.V., KON'SHIN, V.A., SUKHOVITSKIJ, E.Sh., In: Nejtronnaya fizika (Proceedings of III All-Union Conference on Neutron Physics, Kiev 9-13 June 1975). M: TsNIIatominform (1976) 15-20.

Article submitted 27 August 1984.