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INDC(CCP)-123/L

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NEUTRON CROSS-SECTION CALCULATIONS FOR ^{239}Pu, ^{241}Pu, ^{243}Pu AND ^{235}U, ^{237}U AND ^{239}U IN THE 1-150 keV ENERGY REGION

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(Translation of article published in
Nuclear Constants Vol. 26, 1977, distributed
as INDC(CCP)-116/G, December 1977)

Translated by the IAEA
June 1977

IAEA NUCLEAR DATA SECTION, KÄRNTNER RING 11, A-1010 VIENNA

Reproduced by the IAEA in Austria

June 1977

78-5748

INDC(CCP)-123/L

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Translated by the IAEA
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78-468
Translated from Russian

NEUTRON CROSS-SECTION CALCULATIONS FOR ^{239}Pu, ^{241}Pu, ^{243}Pu AND ^{235}U, ^{237}U AND ^{239}U IN THE 1-150 keV ENERGY REGION

V.E. Marshalkin and V.M. Povyshev

By now we have reached a qualitative understanding of the experimental data on individual nuclear reactions and on nuclear reactions as a whole. It is therefore only natural that there should be increased interest in a more detailed quantitative study and in a self-consistent description of the fullest set of data as a means of improving the existing concepts. Moreover, the development and improvement of methods of calculating cross-sections for neutron-induced nuclear reactions is of great importance to nuclear power engineering.

In the present study an attempt has been made to give a self-consistent description of practically all the available experimental data on the interaction of 1-150 keV neutrons with the ^{239}Pu nucleus. Particular care has been taken to ensure that the behaviour of each cross-section in this energy range is described with the same degree of accuracy as the experimental data. This level of description has been achieved by using the method of coupled channels [1] instead of the ordinary optical model, the statistical model in its most sophisticated variant [2] and also the results of channel analysis by the two-hump fission barrier model of experimental data on ^{239}Pu (d, pf) and ^{238}Pu (t, pf) reactions [1]. Quantities like the level density parameters of the excited states of the compound nucleus Γ_γ were taken as equal to those normally used [3,4].

The description of the experimental data on the interaction of neutrons with ^{239}Pu was used as an example for studying the critical behaviour of the cross-sections of individual reactions in relation to target-nucleus and compound-nucleus properties. This is important in evaluating the accuracy of the calculated reaction cross-sections for the isotopes ^{241}Pu, ^{243}Pu and ^{235}U, ^{237}U and ^{239}U. The calculations for these nuclei were performed by the same method and in the same energy region. Qualitative variations in the behaviour of the calculated cross-sections give a quantitative representation of the differences in the physical characteristics of these target nuclei and their corresponding compound nuclei.

Selection of the optical potential parameters

In Ref. [1] the method of coupled channels is described in considerable detail; the accuracy and reliability of the calculated quantities are explained as a function of the degree of approximations used in the method, and their self-consistent level is recommended. In the present study, the calculations have been performed with all approximations at the level of those recommended in Ref. [1]. The procedure for selecting the optical potential parameters

$$V(z,\vartheta) = -\frac{V_0}{1+\exp\left[\frac{z-R(\vartheta)}{a}\right]} - 4i\cdot W_D \cdot \frac{\exp\left[\frac{z-R(\vartheta)}{b}\right]}{\left(1+\exp\left[\frac{z-R(\vartheta)}{b}\right]\right)^2} - V_{S_0}(\hat{\sigma}\,\hat{\ell})\,\frac{1}{a\,z}\cdot\frac{\exp\left[\frac{z-R_0}{a}\right]}{\left(1+\exp\left[\frac{z-R_0}{a}\right]\right)^2} \qquad (1)$$

consisted in performing numerical calculations with a view to studying the quantitative influence of each parameter on the calculated quantities and in seeking the optimum set of parameters from the point of view of a description of the experimental data and from that of the correspondence between the parameter values and the physical characteristics of the nucleus.

The optical potential parameters were selected on the basis of experimental data on the most fully and reliably studied ^{239}Pu nucleus. The selection criterion was the simultaneous and most accurate description of the total cross-section $\sigma_t(\varepsilon)$, the potential elastic scattering cross-section $\sigma_{sel}(\varepsilon)$ and the compound-nucleus formation cross-section $\sigma_c(\varepsilon)$ at 1 keV-15 MeV energies. The dependence of the cross-sections on the change of parameters was studied in the greatest detail in the 1-3 MeV and 1-100 keV energy regions.

In the 1-3 MeV region, at a neutron energy of ~3 MeV, heavy nuclei exhibit optical resonance in the neutron elastic scattering cross-section and consequently in the total cross-section. As might be expected, the behaviour of these cross-sections in the resonance region is most critical for the geometric potential parameters.

Table 1 shows the cross-sections as a function of parameter R_o, the values of all other parameters being fixed. The value of $R_o = 1.28$ is the most accurate representation of the energy dependence of behaviour in the experiment on total cross-section up to, and in the region of, optical resonance. Table 2 shows the cross-sections as a function of the value of diffusivity of the imaginary part of the potential. The most critical ones for this parameter are the cross-sections for compound-nucleus formation and for direct inelastic scattering. A better agreement with the experimental values is obtained with $b = 0.47$. From the data of Table 3 it follows that the value of 0.65 normally used in other studies for the diffusivity of the real part of the potential agrees best with the experimental data.

The characteristic feature of the 1-100 keV region is the fact that practically up to 10 keV only s-wave neutrons interact with the nucleus, while the p-wave begins to be involved from 10 keV, and at 100 keV the cross-sections are determined largely by the p-wave neutrons. Accordingly, a qualitative change occurs in the behaviour of the cross-section for the formation of a compound nucleus, which diminishes by the $1/\sqrt{\varepsilon}$ law at 1-10 keV and at a higher energy is determined by the relative weights of the s- and p-waves.

The variation in the potential scattering cross-section is comparatively slow. Therefore, the qualitative change in the energy dependence of the cross-section for compound-nucleus formation and consequently of the total cross-section affords a means of selecting the potential parameters successively on s- and p-waves so that the geometric potential parameters remain fixed ($R_o = 1.28$; $a = 0.65$; $b = 0.47$), and a description of the cross-sections in the region above 1 MeV is made possible.

The influence of the depth of the real part of the potential is shown in Table 4, where the dependence of $\sigma_{sel}(\varepsilon)$ on the values of V_o and comparison with experimental values indicate that 45-46 MeV are acceptable values for the depth of the real part of the potential. Table 5 shows a sharp reduction in the cross-section for compound-nucleus formation and consequently in the total cross-section with a decrease in the depth of the imaginary part of the potential to 3.8 MeV. With further decreases in depth the criticality of these cross-sections becomes slighter. The most acceptable value of this parameter is 3.6-3.8 MeV.

The dependence of the cross-section for compound-nucleus formation and consequently of the total cross-section on the deformation parameter values is shown in Table 6. The most acceptable deformation parameter values are $\beta = 0.22$–0.24. The value of the spin-orbit coupling parameter and the energy dependence of the magnitude of the real and imaginary parts of the potentials are taken as equal to those normally used [5] and were not studied by us.

Thus, the study showed that the behaviour of the cross-sections in certain regions of incident neutron energy is comparatively critical for the corresponding optical potential parameters. The experimental data on $\sigma_t(\varepsilon)$, $\sigma_c(\varepsilon)$, $\sigma_{sel}(\varepsilon)$ for 1 keV–15 MeV energies are sufficiently complete for determining the practically unique set of the optical potential parameters. The values of parameters $V_o = -45.0 + 0.3E$;

$$W_D = \begin{cases} -3.6 - 1.43\sqrt{\varepsilon} & \text{for } \varepsilon \leq 1 \text{ MeV;} \\ -4.0 - 1.03\sqrt{\varepsilon} & \text{for } \varepsilon \geq 1 \text{ MeV;} \end{cases} \quad R_o = 1.28; \quad a = 0.65; \quad b = 0.47; \quad \beta = 0.22;$$

$V_{so} = 7.5$ enables us to describe the total cross-section with an accuracy of ~3% and the cross-sections for compound-nucleus formation and elastic scattering with an accuracy of ~5% (Table 7). The angular distribution of 1 MeV neutrons scattered from the ground state and accompanied by the excitation of the first levels of the target nucleus, agrees to within ~20% with the experimental value as shown in Fig. 1.

The basic relations of the statistical model

The cross-sections of reactions occurring through the compound nucleus were calculated by the statistical model formulae. The expression for oalculating neutron scattering takes the form

$$\sigma_{nn'}(\varepsilon I \Pi_I;\ \varepsilon' I' \Pi_{I'}) = \frac{\pi}{K^2} \cdot \frac{1}{2(2I+1)} \sum_{J\pi_J} (2J+1) \sum_{\ell j \ell' j'} \times$$
$$\times \left\{ \frac{\Theta^{J\pi_J}_{\ell j I \Pi_I}(\varepsilon, A+1)\ \Theta^{J\pi_J}_{\ell' j' I' \pi_{I'}}(\varepsilon', A+1)\ S^{J\pi_J}_{nn'}}{\Theta^{J\pi_J}} - \right. \tag{2}$$
$$\left. - \frac{1}{4}\ \delta_{\ell\ell'} \delta_{jj'} \delta_{II'} \delta_{\Pi_I \Pi_{I'}} \delta_{\varepsilon\varepsilon'}\ Q\ \left(\Theta^{J\pi_J}_{\ell j I \Pi_I}(\varepsilon, A+1)\right)^2 \right\}.$$

This expression is used to calculate the cross-section for the scattering of neutrons of energy ε by a nucleus in a state with moment I and parity Π_I with subsequent emission of a neutron of energy ε' and transition of the nucleus to a state of energy $E = \varepsilon - \varepsilon'$ with moment I' and parity $\Pi_{I'}$. The energies of the incident ε and outgoing ε' neutrons are measured in the centre-of-mass system and represent energies of relative motion. $\theta^{J\pi_J}_{\ell' j' I' \pi_{I'}}(\varepsilon'; A+1)$ is the coefficient of adhesion of a neutron of energy ε', orbital moment ℓ' and total moment j to a nucleus in a state with moment I' and parity $\Pi_{I'}$, with formation of a compound nucleus A + 1 of moment J and parity π_J. This coefficient is determined, in accordance with Ref. [2], by using the coefficient of adhesion $T^{J\pi_J}_{\ell' j' I' \pi_{I'}}(\varepsilon'; A+1)$ calculated by the coupled channel method from the expression

$$\theta^{J\pi_J}_{\ell j I \pi_I}(\varepsilon) = \frac{2}{Q}\left[1 - \sqrt{1 - Q\, T^{J\pi_J}_{\ell j I \pi_I}(\varepsilon)}\right] \qquad (3)$$

The parameter Q changes from 1 in the region of low neutron energies to 0 with an increase in energy. The denominator in expression (3) is the sum of the θ coefficients of decay of the compound nucleus A + 1 in all the competing channels:

$$\begin{aligned}
\theta^{J\pi_J}(A+1) = {} & \sum_{\varepsilon'', \ell'' j'' I'' \pi_{I''}} \theta^{J\pi_J}_{\ell'' j'' I'' \pi_{I''}}(\varepsilon''; A+1) + \theta^{J\pi_J}_{\gamma}\left[\varepsilon + B_n(A+1); A+1\right] + \\
& + \sum_k \theta^{J\pi_J k}_f \left[\varepsilon + B_n(A+1); A+1\right] + \sum_{\ell'' j'' I'' \pi_{I''}} \int_{E_{min}}^{\varepsilon} \theta^{J\pi_J}_{\ell'' j'' I'' \pi_{I''}}(\varepsilon - E; A+1) \times \\
& \times \rho(E I'' \pi_{I''}, A)\, dE + \int_{V_{min}+\Delta}^{\infty} P_f\left(\varepsilon + B_n(A+1); A+1; E_f^{J\pi_J}\right) \times \\
& \times \rho(E_f^{J\pi_J} J\pi_J, A+1)\, dE_f^{J\pi_J} + F^{J\pi_J}\left[\varepsilon + B_n(A+1); A+1\right],
\end{aligned} \qquad (4)$$

where the first term represents neutron scattering with excitation of discrete levels of the target nucleus, the second term radiation decay, the third term fission through discrete transitional states, the fourth term neutron inelastic scattering with excitation of a continuous target spectrum, the fifth term fission through a continuous spectrum of the transitional states and the sixth term other possible decay channels for the compound nucleus.

The correlation function

$$S^{J n_J}_{\ell j I n_I, \ell' j' I' n_{I'}}(\varepsilon) = \left\langle \frac{\Gamma^{J n_J}_{\ell j I n_I}(\varepsilon)\, \Gamma^{J n_J}_{\ell' j' I' n_{I'}}(\varepsilon) \prod_m P\left(\Gamma^{J n_J}_m(\varepsilon)\right)}{\sum_m \Gamma^{J n_J}_m(\varepsilon)} \right\rangle \frac{\sum_m \bar{\Gamma}^{J n_J}_m(\varepsilon)}{\bar{\Gamma}^{J n_J}_{\ell j I n_I}(\varepsilon)\, \bar{\Gamma}^{J n_J}_{\ell' j' I' n_{I'}}(\varepsilon)} \qquad (5)$$

takes into account the non-equivalence of substitution of the average ratio of $\Gamma^{J n_J}_m$ - widths by the ratio of average $\bar{\Gamma}^{J n_J}_m$ used in the statistical model [6]. The distribution functions of widths $P(\Gamma^{J n_J}_m)$ were taken in the form of the Porter-Thomas distribution with one degree of freedom for neutron channels in the δ-form for the radiation channel and in the form obtained in Ref. [1] for the fission channels.

The density of the excited states of the nucleus is calculated by the formulae of Ref. [7] with parameters from a later study [3]. The same formula from Ref. [7] was used to evaluate the density of the transitional states of the fissionable nucleus. The parameters were selected from the description of experimental data on the interaction of neutrons with the ^{239}Pu nucleus, and the selection is shown below.

The radiation coefficient was calculated in accordance with the definition

$$\theta^{J n_J}_\gamma\left(\varepsilon + Bn(A+1)\right) = 2\pi\, \rho\left(\varepsilon + Bn(A+1), J n_J\right)\, \Gamma^{J n_J}_\gamma\left(\varepsilon + Bn(A+1)\right). \qquad (6)$$

The energy dependence of the radiation width was evaluated in accordance with the assumption of dipole gamma-quanta emission, and its absolute value was determined through using the experimentally known values at neutron binding energy [4]

$$\Gamma^{J n_J}_\gamma(\varepsilon + Bn) = \Gamma^{J n_J}_\gamma(Bn)\, \frac{\rho(Bn, J n_J) \int_0^{Bn+\varepsilon} \varepsilon_\gamma^3 \sum_{J' n_{J'}} \rho(\varepsilon + Bn - \varepsilon_\gamma, J' n_{J'})\, d\varepsilon_\gamma}{\rho(\varepsilon + Bn, J n_J) \int_0^{Bn} \varepsilon_\gamma^3 \sum_{J' n_{J'}} \rho(Bn - \varepsilon_\gamma, J' n_{J'})\, d\varepsilon_\gamma}. \qquad (7)$$

The laws of moment and parity conservation determine the set $J' n_J$, on the basis of $|J - 1| \leq J' \leq J + 1$, $n_J 1 = n_J(-1)$, respectively.

The fission $\vartheta_f^{Jn_JK}$ coefficients of penetrability were calculated by the two-hump barrier model from the formulae of Ref. [8]. The parameters of the barriers of transitional-states of a discrete spectrum were taken as equal to those obtained from the channel analysis of experimental data on the (t, pf) reaction for the corresponding nuclei [9].

The cross-sections of the other competing reactions were calculated by formula (2) by replacing the neutron penetrability factor $\Theta_{\ell' j' I' \Pi_{I'}}^{Jn_J}$ and the $S_{nn'}^{Jn_J}$ function in the exit channel by the corresponding values.

<u>Neutron cross-section calculations</u>

In order to study the possibility of describing the behaviour of two-particle reaction cross-sections and to determine the accuracy of such a description, we performed neutron cross-section calculations for the ^{239}Pu and ^{235}U nuclei, which are the ones which have been the subject of the most thorough experimental study. In the calculations use was made of the results of analyses of experimental data on these nuclei and on their corresponding compound nuclei: $\Gamma_\gamma(Bn)$ has been taken from Ref. [4], the density parameters of the excited states are taken as equal to the values given in Ref. [3] and the parameters of the barriers of the transitional-state bands are from Ref. [9]. Hence there are reasons for trusting that the decay of the compound nucleus, in accordance with expression (2), through the neutron channels, the radiation channel and the fission channels of the discrete spectrum of the transitional states can be described with comparative reliability. However, the existing uncertainties in the quantities used will affect the accuracy of the calculated cross-sections. The extent of this influence varies from nucleus to nucleus, and will be discussed below.

The least studied of the competing decay channels of the compound nucleus is fission through the continuous spectrum of transitional states. The decisive importance of the density behaviour of these states for the energy dependence of the fission cross-section and other competing reaction cross-sections in the case of an increase in neutron energy is qualitatively understandable by analogy with the influence of the level density of the residual nucleus.

Considering the identical nature of the excited states for stable deformation and deformation at the saddle point, the same Fermi gas formula from Ref. [7] was used to describe the density of the transitional states. However, in view of the change in the single-particle spectrum near the Fermi energy during transition from stable deformation to deformation at the saddle point, changes can naturally be expected in the values of shell corrections S(N) and S(Z) and pairing energies P(N) and P(Z) for neutrons and protons, respectively. Therefore, in the calculations parameters a and Δ = P(N) + P(Z) were chosen by varying them within reasonable limits.

In describing fission through the continuous spectrum of the transitional states it is important to give a correct expression not only for the density of these states but also for the energy dependence of their fission barrier penetrability. The most important features of this dependence, namely the rate of its damping in the sub-barrier region with a decrease in the excitation energy and a change in the slope during the transition from a sub-barrier fission to an above-barrier fission, can be expressed in the single-hump fission barrier model on the basis of the normally used Hill and Wheeler formula

$$P_f(E^*, E_f^{Jn_J}) = \frac{1}{1 + \exp\left[-\frac{2\pi\,(E^* - E_f^{Jn_J})}{\hbar\omega}\right]} \qquad (8)$$

It is possible to make the curvature of the barriers identical for different transitional states $\hbar\omega$ and its value approximately equal to that of the curvature of the barrier of the lowest transitional state: 0.4 MeV.

The effective number of fission channels in the continuous spectrum of the transitional states with definite Jn_J was calculated by the formula

$$T_f^{Jn_J}(E^*) = \int_{V_{min}+\Delta}^{\infty} \rho(E_f^{Jn_J}, Jn_J)\, P_f(\varepsilon + Bn(A+1), E_f^{Jn_J})\, dE_f^{Jn_J}, \qquad (9)$$

where the lower limit of the integral is the beginning of the continuous spectrum of the transitional states and is determined by the height of the barriers of the lowest 0^+ transitional state V_{min} and by the value of the energy gap Δ.

It was the description of the energy dependence of the fission and radiative capture cross-sections for the ^{239}Pu nucleus at 1-150 keV neutron energies which also determined the values of parameters $\Delta = 1.34$ MeV, $\hbar\omega = 0.35$ MeV and $a/A = 0.150$. The variation in the cross-sections was found to be fairly critical with respect to the value of $\hbar\omega = 0.35$ MeV and the value of the fission cross-section determined the value of $\Delta = 1.34$ MeV. It should be noted that the energy dependence of the fission and radiative capture cross-sections indicates that fission from the $J^{\pi_J} = I^+$ state occurs to a greater extent through the transitional states of the continuous spectrum than through the transitional state of a collective nature. The behaviour of the cross-sections in this energy region was only slightly dependent on the values of parameter a. For this reason, it can be determined with greater accuracy by the description of the cross-sections in the region of higher energy values.

In the fissionable ^{240}Pu nucleus the neutron binding energy appreciably exceeds the energy of the barriers of the lower transitional-state bands. Moreover, the curvature of the barriers of states with negative parity is comparatively greater and consequently the penetrability of the fission barrier is damped comparatively slowly in the sub-barrier region. This being so, there is a possibility of fission after the emission of low-energy gamma quanta. In Ref. [1] we pointed out the commensurability of widths Γ_f and $\Gamma_{\gamma f}$ for a number of resonances of the ^{240}Pu compound nucleus in the resonance energy region.

Therefore the cross-section of the $(n,\gamma f)$ reaction was evaluated by the formula

$$\sigma_{n,\gamma f}(\varepsilon I\Pi_I;\gamma;f) = \frac{\pi}{k^2}\cdot\frac{1}{2(2I+1)}\sum_{J\pi_J}(2J+1)\cdot\frac{\sum_{\ell j}\theta^{J\pi_J}_{\ell j I\Pi_I}(\varepsilon)\,S^{J\pi_J}_{n\gamma}(\varepsilon)}{\theta^{J\pi_J}} \times$$

$$\times\, 2\pi\,\rho(Bn(A+1), J\pi_J)\cdot\Gamma_\gamma^{J\pi_J}(Bn)\,\times \tag{10}$$

$$\times\frac{\displaystyle\int_0^{\varepsilon+Bn-V_{min}+0.3} d\varepsilon_\gamma\cdot\varepsilon_\gamma^3\cdot\sum_{J'\pi_{J'}}\rho(Bn+\varepsilon-\varepsilon_\gamma, J'\pi_{J'})\cdot\frac{\sum_k\theta_f^{J'\pi_{J'}k}(Bn+\varepsilon-\varepsilon_\gamma)}{\sum_k\theta_f^{J'\pi_{J'}k}(Bn+\varepsilon-\varepsilon_\gamma)+\theta_\gamma^{J'\pi_{J'}}(Bn+\varepsilon-\varepsilon_\gamma)}}{\displaystyle\int_0^{Bn} d\varepsilon_\gamma\cdot\varepsilon_\gamma^3\sum_{J'\pi_{J'}}\rho(J'\pi_{J'}, Bn-\varepsilon_\gamma)},$$

where, in accordance with the assumption of the most probable emission of electric dipole gamma quanta, the set $J'n_{J'}$ is determined by the relations $|J - 1| \leq J' \leq J + 1$ and $n_{J'} = -n_J$. The share of the (n, γf) reaction in the (nγ) reaction cross-section was ~10% at 1 keV and this decreased with increasing neutron energy, owing to the relatively large probability of fission by p-wave neutrons.

After the input information was thus defined, calculations were made of the cross-sections of all reactions occurring in the interaction of low-energy neutrons with the ^{239}Pu nucleus. The calculation results are given in Table 8. The decomposition of the cross-section for the compound nucleus formation at a neutron energy of 1 keV into the competing channels of fission and the emission of gamma quanta and neutrons, was determined by the ratio of their corresponding penetrability coefficients from the J^{π_J} states equal to 0^+ and I^+. When $\vartheta^{0+}_{0\frac{1}{2}\frac{1}{2}+} = 0.021$, $\vartheta^{0+}_{\gamma} = 0.033$ and $\vartheta^{0+0}_{f} = 0.91$, the compound nucleus from the 0^+ state will undergo fission with overwhelming probability. When $\vartheta^{1+}_{0\frac{1}{2}\frac{1}{2}+} = 0.020$, $\vartheta^{1+}_{\gamma} = 0.098$ and $\vartheta^{1+1}_{f} = 0.04$, the compound nucleus will more probably decay with the emission of gamma quanta, less probably undergo fission and even less probably emit neutrons. The S function has a substantial effect on the distribution of decay probability along the channels [4]. As neutron energy increases, there is a decrease in the cross-sections of all reactions parallel with the reduction in the cross-section for compound-nucleus formation and the share of neutron emission increases with relatively rapid growth of the $\theta^{J n_J}_{\ell j I n_I}(\varepsilon)$ coefficients.

A comparison of neutron reaction cross-sections for ^{235}U calculated by the same principle (Table 9) with the cross-sections evaluated in other studies shows satisfactory agreement: the fission cross-section agrees with an accuracy of not less than 10% and the radiative capture cross-section to within ~20%.

The basis for this agreement of the fission cross-section is the above-barrier mode of fission by S-wave neutrons, owing to the comparatively high neutron binding energy ~6.545 MeV. In this case, the uncertainties in fission barrier magnitudes do not substantially change the fission cross-sections. The accuracy of the radiative capture calculation is determined by the uncertainty of Γ_γ and also by the uncertainty of the level density of the compound nucleus, and should amount to 20%. Because of the difficulty of making a quantitative evaluation of the accuracy of the calculated cross-sections, it is probably the above comparison which characterizes its level. A noteworthy fact is the large share (25%) of the $(n,\gamma f)$ reaction in the general process with the emission of gamma quanta. This is a consequence of the neutron binding energy being comparatively much greater (1 MeV) than the barrier energy of the lowest transitional-state 0^+ band.

The cross-sections for the ^{241}Pu, ^{243}Pu, ^{237}U and ^{239}U were calculated in a similar manner and in the same energy range of incident neutrons. The calculation results are shown in Tables 10-13. A comparison of the calculated fission cross-sections for the ^{241}Pu nucleus with those given in Ref. [10] also confirms what has been said above concerning the calculation accuracy.

It should be noted that the agreement between the calculated fission cross-section for ^{237}U and the experimental data of Ref. [11] in the energy region below 1 keV and above 100 keV is much less satisfactory. At neutron energies below 1 keV the experimental fission cross-section has a very pronounced resonance character; it is therefore difficult to compare the results with experimental data. However, the averaged experimental fission cross-section in a wider energy range (0.7-1 keV) fully corresponds to the calculated value of $\sigma_f = 2.6$ V. At neutron energies above 100 keV the calculated fission values are reduced by a factor of nearly two in comparison with the experimental data. This is due to the fact that in the calculations, fission by the p-wave neutrons is strongly inhibited by the high barriers of the transitional-state bands of negative parity in comparison with the binding energy. A reduction in the magnitudes of these barriers by 200 keV, which is still within the limits of uncertainties of the channel analysis of (t,p,f) reactions [9], leads to satisfactory agreement between the calculated and experimental fission cross-section values. A comparison of the calculated reaction cross-sections in Tables 12 and 14 shows that the radiative capture cross-section changes little with such a change in parameters.

Discussion of results

The agreement between the calculated results of the cross-sections $\sigma_t(\varepsilon)$, $\sigma_c(\varepsilon)$ and $\sigma_{sel}(\varepsilon)$ for ^{239}Pu and their estimated values when the neutron energy was varied from 1 keV to 15 MeV for the purpose of selecting the optical potential parameters showed that the potential parameters obtained were practically unique and consequently the experimental data on the cross-sections used in the above energy range were sufficiently complete for selecting the parameters by experiment. The reduction in the accuracy of description of the total cross-section to 6% in the low-energy region for ^{235}U may be due to a possible difference between the stable deformation parameter from the value of $\beta = 0.22$ selected for describing the ^{239}U data and used for ^{235}U. However, it should also be noted that the calculated total cross-section values lie between the experimental values obtained by different authors.

In the case of the nuclei considered, with the exception of ^{237}U, at a neutron energy of 1 keV the compound nucleus decays predominantly by fission. The high probability of fission is a consequence of the neutron binding energy exceeding or being approximately equal to the barrier energy of the transitional states through which fission is allowed by the conditions of moment and parity conservation. In the fission of the ^{239}U and ^{241}Pu nuclei which in the ground state have the moment and parity values $I^{\Pi_I} = \frac{5}{2}^+$, the process occurs through the transitional states $J^{\Pi_J} = 2^+$ of the first and second bands $K^{\Pi_J} = 0^+$ and 2^- and the state $J^{\Pi_J} = 3^+$ of the second band $K^{\Pi_J} = 2^+$. The fission of ^{243}Pu, which in the ground state has $I^{\Pi_I} = \frac{7}{2}^+$ [12], takes place through the transitional states $J^{\Pi_J} = 4^+$ of the first and second bands $K^{\Pi_J} = 0^+$ and 2^+ and the transitional state $J^{\Pi_J} = 3^+$ of the second band $K^{\Pi_J} = 2^+$. The ^{239}Pu and ^{237}U nuclei in the ground state have $I^{\Pi_I} = \frac{1}{2}^+$ and undergo fission through the transitional state with $J^{\Pi_J} = 0^+$ of the first band and states $J^{\Pi_J} = I^+$, which are formed as a result of pair break-up ($\Delta = 1.34$ MeV). Whereas in the case of ^{239}Pu at a binding energy of 6.533 MeV the fission through state $J^{\Pi_J} = I^+$ occurs with an appreciable probability ($T_f^{1+} = 0.046$), in the case of ^{237}U at a binding energy of 6.143 MeV the fission through this state occurs deep under the barrier and is negligibly small. The ^{235}U nucleus is of interest in that it has $I^{\Pi_I} = \frac{7}{2}^-$ in the ground state. Therefore, fission occurs through the transitional state $J^{\Pi_J} = 4^-$ of bands $K^{\Pi_J} = 1^-$, 2^- and through the transitional state $J^{\Pi_J} = 3^-$ of bands $K^{\Pi_J} = 0^-$, 1^-, 2^-. The agreement between the cross-section calculation results in this case and the experimental values is an important confirmation of the correct determination of the barrier magnitude of transitional states of negative parity. Thus, the good agreement between the calculated fission cross-section and the evaluated or experimental data at 1 keV neutron energy is the result of using a sufficiently correctly determined set of barrier parameters of lower transitional state bands [9]. In evaluating the reliability and accuracy of the fission cross-section calculations it is important to note that in the even-even fissionable nuclei considered, with the exception of ^{238}U, the neutron binding energy exceeds the barrier energy of one or more transitional-state bands and that fission by s-wave neutrons is above the barrier. In this case, the ϑ_f coefficients considerably exceed the ϑ coefficients of the competing processes and the relative fission probability $\sim \vartheta_f/(\vartheta_f + \vartheta)$ is therefore much less inaccurate than ϑ_f. Even the uncertainty of ϑ_f between 0.5 and 1 leads to ~10% inaccuracy in the relative fission probability. Therefore, with ~5% accuracy for the total cross-section calculation and ~10% accuracy for the elastic scattering and compound-nucleus formation cross-sections the fission cross-section can be calculated with an accuracy not lower than 20%.

The next in order of probability is radiative decay. The accuracy with which its cross-section can be calculated depends mainly on the accuracy of the $\Gamma_\gamma(B_n)$ values determined in Ref. [4], on the accuracy of the level density parameters of the compound nucleus [4] and also on the correct description of decay through the most probable fission channel; it appears to be at a level of 20%.

The neutron ϑ-coefficients for the s-wave are calculated with an accuracy of 5%; however, the uncertainties in the competing fission and radiation processes can considerably reduce the accuracy of the calculated neutron decay cross-section.

With the increase of the incident neutron energy, the connection of fission channels of opposite parity for the p-wave, in comparison with the s-wave, has different effects for different nuclei on the accuracy of calculating the fission cross-section and consequently of the other processes. If fission by the p-wave is above the barrier, as in the case of ^{235}U and ^{239}Pu, there is no reason to expect a reduction in the accuracy of the calculation. In sub-barrier fission by p-wave neutrons, as in the case of the ^{237}U, ^{239}U and ^{243}Pu nuclei, the uncertainty in the fission barrier magnitudes and curvatures of the transitional-state bands of negative parity can lead to a noticeable decrease in the accuracy of the calculated cross-sections. For this reason further refinement of the barrier parameters of the lower transitional-state bands is a very important problem. Especially large errors in the fission cross-section will be found in the comparatively improbable case of fission by the s-wave neutrons. This is illustrated in the case of the ^{237}U nucleus in which a decrease in the barrier energy of bands $K^{\pi J} = 0^-, 1^-$ by 200 keV resulted at 100 keV neutron energy in an increase in the fission cross-section by a factor of ~1.5. However, in this case too, at neutron energies ≤ 20 keV, where the p-wave neutrons are absorbed by the nucleus with a lower probability than s-wave neutrons, the fission cross-section can be calculated with an accuracy of ~20%.

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Table 1

Dependence of the cross-sections $\sigma_t(\varepsilon)$, $\sigma_c(\varepsilon)$, $\sigma_{sel}(\varepsilon)$, $\sigma^{rot}_{inel}(\varepsilon)$ on the values of parameter R_0 for the following values of the parameters: $V_0 = -45 + 0.3E$; $W_D = -4.27 - 1.03\sqrt{\varepsilon}$; $a = 0.65$; $b = 0.47$; $\beta = 0.24$; $V_{SO} = 7.5$

R_0	ε = I MeV				ε = I,5 MeV				ε = 3 MeV			
	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}
I,25	7,58	3,0I	4,I9	0,38	7,27	2,94	3,88	0,45	7,53	2,99	4,0	0,60
I,28	7,47	3,II	3,93	0,43					7,77	3,I9	3,95	0,63
I,30	7,82	3,59	3,94	0,29					7,8I	3,3I	3,83	0,67

Table 2

Dependence of cross-sections on the values of the diffusivity parameter of the imaginary part of the potential for the following values of the parameters: $V_0 = -46.53 + 0.3E$; $W_D = -4.27 - 1.03\sqrt{\varepsilon}$; $a = 0.65$; $R_0 = 1.25$; $\beta = 0.2$; $V_{SO} = 7.5$

b	ε = I MeV				ε = I,5 MeV				ε = 3 MeV			
	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}
0,65	7,76	3,40	4,I4	0,22	7,36	3,50	3,58	0,28	7,52	3,45	3,76	0,3I
0,47	7,I4	2,93	3,87	0,34					7,3I	3,06	3,7I	0,54

Table 3

Dependence of cross-sections on the values of the diffusivity parameter of the real part of the potential for the following values of the parameters: $V_0 = -45 + 0.3E$; $W_D = -4.27 - 1.03\sqrt{\varepsilon}$; $R_0 = 1.28$; $b = 0.47$; $\beta = 0.24$; $V_{SO} = 7.5$

a	ε = I MeV				ε = I,5 MeV				ε = 3 MeV			
	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}	σ_t	σ_c	σ_{sel}	σ^{zot}_{inel}
0,7	7,66	3,50	3,65	0,5I	7,52	3,58	3,28	0,66	7,93	3,39	3,83	0,7I
0,65	7,47	3,II	3,93	0,43					7,77	3,I9	3,95	0,63

Table 4

Dependence of cross-sections on the value of the depth parameter of the real part of the potential for the following values of the parameters: $W_D = -4 - 1.03\sqrt{\varepsilon}$; $a = 0.65$; $b = 0.47$; $\beta = 0.24$; $V_{SO} = 7.5$; $R_0 = 1.28$

V_0	ε = I keV			ε = 5 keV			ε = I0 keV			ε = I00 keV		
	σ_t	σ_c	σ_{sel}	σ_t	σ_c	σ_{sel}	σ_t	σ_c	σ_{sel}	σ_t	σ_c	σ_{sel}
-45	3I,26	20,04	II,22	20,07	9,I6	I0,9I	I7,37	6,70	I0,67	II,80	3,27	8,49
-46	30,08	I9,97	I0,I	I8,99	9,I6	9,83	I6,34	6,73	9,63			
-48	35,62	27,22	8,43									

Table 5

Dependence of cross-sections on the value of the depth parameter of the imaginary part of the potential at 1 keV neutron energy; $V_0 = -46$, $R_0 = 1.28$; $a = 0.65$; $b = 0.47$; $\beta = 0.24$, $V_{SO} = 7.5$

σ	W_D=-4,0	W_D=-3,8	W_D=-3,7	W_D=-3,6
σ_t	30,08	25,28	24,99	24,70
σ_c	I9,97	I5,27	I4,98	I4,68
σ_{sel}	I0,II	I0,0I	I0,0I	I0,02

Table 6

Dependence of cross-sections on the value of the deformation parameter of the nucleus at 1 keV neutron energy; $V_0 = -46$, $R_0 = 1.28$, $W_D = -3.8$; $a = 0.65$; $b = 0.47$; $V_{SO} = 7.5$

σ	β=0,24	β=0,23
σ_t	25,28	23,99
σ_c	I5,27	I3,98
σ_{sel}	I0,0I	I0,0I

Table 7

Energy dependence of cross-sections for the following parameters of the optical potential: $V_0 = -45 + 0.3E$;

$$W_D = \begin{cases} -3.6 - 1.43\sqrt{\varepsilon} & \text{when } \varepsilon \leq 1 \text{ MeV;} \\ -4.0 - 1.03\sqrt{\varepsilon} & \text{when } \varepsilon \geq 1 \text{ MeV;} \end{cases}$$

$R_0 = 1.28$; $a = 0.65$; $b = 0.47$; $\beta = 0.22$; $V_{SO} = 7.5$

σ	ε = I MeV	ε =I0 keV	ε =I00 keV	ε = I MeV	ε =3 MeV	ε = 8 MeV
σ_t	24,62	I6,56	II,78	7,34	7,68	6,36
σ_c	I3,60	4,93	2,98	3,05	3,I9	2,8I
σ_{sel}	II,02	I0,63	8,78	3,87	3,84	3,05
σ_{inel}^{zot}	0	0	0,02	0,42	0,65	0,50

Table 8

Calculated neutron reaction cross-sections for the ^{239}Pu nucleus (cross-sections, b; energy, keV)

ε	σ_t	σ_c	σ_{sel}	σ_{inel}^{zot}			σ_{cel}	σ_{inel}^{c}			σ_{el}	σ_{nf}	$\sigma_{nf}+\sigma_{n\gamma f}$	$\sigma_{n\gamma f}$	$\sigma_{nf}+\sigma_{n\gamma f}$
				$I'=3/2$	$I'=5/2$	$I'=7/2$		$I'=3/2$	$I'=5/2$	$I'=7/2$					
I	24,62	I3,60	II,02				2,97				I3,99	5,34	5,28	0,65	5,99
5	I7,09	6,28	I0,8I				2,04				I2,85	2,33	I,90	0,24	2,57
I0	I5,56	4,93	I0,62	$I.I0^{-5}$			I,63	0,2I			I2,25	I,85	I,23	0,I7	2,02
I5	I4,77	4,30	I0,47	$7.I0^{-5}$			I,43	0,28			II,90	I,63	0,96	0,I4	I,77
20	I4,28	3,96	I0,32	$2.I0^{-4}$			I,3I	0,29			II,63	I,53	0,8I	0,I2	I,65
50	I2,90	3,25	9,64	$I.I0^{-3}$			I,03	0,3I			I0,67	I,4I	0,50	0,09	I,50
70	I2,33	3,07	9,26	$2.I0^{-3}$	$3,4.I0^{-3}$		0,94	0,3I	0,03		I0,20	I,37	0,4I	0,08	I,45
I00	II,78	2,98	8,78	$4.I0^{-3}$	$I,8.I0^{-2}$		0,85	0,32	0,II	0,02	9,63	I,35	0,32	0,07	I,42
I50	II,08	2,9I	8,II	$8.I0^{-3}$	$4,8.I0^{-2}$	$6.I0^{-4}$	0,72	0,32	0,20	0,05	8,83	I,37	0,25	0,06	I,43

Table 9

Calculated neutron reaction cross-sections for the ^{235}U nucleus (cross-sections, b; energy, keV)

ε	σ_t	σ_c	σ_{sel}	σ_{cel}	σ_{el}	σ_{nf}	$\sigma_{nf}+\sigma_{n\gamma f}$	$\sigma_{n\gamma f}$	$\sigma_{nf}+\sigma_{n\gamma f}$
I	27,55	I6,09	II,45	I,75	I3,20	7,67	6,67	I,76	9,43
5	I8,90	7,70	II,20	I,39	I2,59	3,54	2,77	0,70	4,24
I0	I6,87	5,89	I0,98	I,22	I2,I9	2,7I	I,96	0,46	3,I7
20	I5,40	4,76	I0,64	I,07	II,7I	2,24	I,45	0,3I	2,55

Table 10

Calculated neutron reaction cross-sections for the ^{241}Pu nucleus
(cross-sections, b; energy, keV)

ε	σ_t	σ_c	σ_{sel}	σ_{inel}^{zot} $I'=7/2$	σ_{inel}^{zot} $I'=9/2$	σ_{cel}	σ_{inel}^{c} $I'=7/2$	σ_{inel}^{c} $I'=9/2$	σ_{el}	σ_{nf}	$\sigma_{n\gamma}+\sigma_{n\gamma f}$	$\sigma_{n\gamma f}$	$\sigma_{nf}+\sigma_{n\gamma f}$
I	24,99	I4,I5	I0,84			I,40			I2,24	9,79	2,96	0,40	I0,I9
5	I7,42	6,79	I0,63			I,09			II,72	4,39	I,3I	0,20	4,59
I0	I5,65	5,2I	I0,44			0,98			II,42	3,23	I,0	0,I8	3,4I
20	I4,36	4,22	I0,I4			0,92			II,06	2,49	0,8I	0,I6	2,65
50	I3,00	3,54	9,46	2·I0^{-4}		0,96	0,08		I0,42	I,89	0,6I	0,I0	I,99
I00	II,96	3,33	8,63	3·I0^{-3}	2·I0^{-4}	I,03	0,23	8·I0^{-3}	9,65	I,60	0,46	0,08	I,69
I50	II,28	3,27	7,99	6·I0^{-3}	4·I0^{-3}	I,03	0,29	0,I2	8,99	I,46	0,37	0,05	I,5I

Table 11

Calculated neutron reaction cross-sections for the ^{243}Pu nucleus
(cross-sections, b; energy, keV)

ε	σ_t	σ_c	σ_{sel}	σ_{inel}^{zot} $I'=9/2$	σ_{inel}^{zot} $I'=11/2$	σ_{cel}	σ_{inel}^{c} $I'=9/2$	σ_{el}	σ_{nf}	$\sigma_{n\gamma}+\sigma_{n\gamma f}$	$\sigma_{n\gamma f}$	$\sigma_{nf}+\sigma_{n\gamma f}$
I	24,56	I3,92	I0,65			I,55		I2,20	I0,46	I,9I	0,I8	I0,64
5	I7,I3	6,69	I0,44			I,I8		II,62	4,52	0,99	0,I5	4,67
I0	I5,39	5,I3	I0,26			I,09		II,35	3,I8	0,86	0,I6	3,34
I5	I4,62	4,5I	I0,II			I,08		II,I9	2,63	0,80	0,I7	2,80
20	I4,I4	4,I7	9,97			I,I2		II,07	2,29	0,76	0,I7	2,46
50	I2,86	3,54	9,32			I,40		I0,72	I,53	0,60	0,I2	I,65
70	I2,38	3,42	8,96	5.I0^{-4}		I,49	0,II	I0,45	I,3I	0,5I	0,I0	I,4I
I00	II,87	3,36	8,5I	2.I0^{-3}		I,56	0,25	I0,07	I,II	0,42	0,07	I,I8
I50	II,I9	3,30	7,88	5.I0^{-3}	I.I0^{-3}							

Table 12

Calculated neutron reaction cross-sections for the ^{237}U nucleus
(cross-sections, b; energy, keV)

ε	σ_t	σ_c	σ_{sel}	σ_{inel}^{zot} $I'=3/2$	σ_{inel}^{zot} $I'=5/2$	σ_{cel}	σ_{inel}^{c} $I'=3/2$	σ_{inel}^{c} $I'=5/2$	σ_{inel}^{c} $I'=7/2$	σ_{el}	σ_{nf}	$\sigma_{n\gamma}+\sigma_{n\gamma f}$	$\sigma_{n\gamma f}$	$\sigma_{nf}+\sigma_{n\gamma f}$
I	25,37	I4,I4	II,22			4,I7				I5,39	2,47	7,50	0,I3	2,6
5	I7,73	6,73	II,0			2,78				I3,78	I,08	2,87	0,07	I,I5
I0	I5,9I	5,I0	I0,8I	I·I0^{-5}		2,I5	0,29			I2,96	0,78	I,88	0,06	0,84
I5	I5,09	4,45	I0,64	8·I0^{-5}		I,87	0,38			I2,5I	0,66	I,53	0,06	0,72
20	I4,58	4,09	I0,49	2·I0^{-4}		I,74	0,4I			I2,23	0,59	I,35	0,06	0,65
50	I3,I2	3,34	9,78	2·I0^{-3}		I,52	0,50			II,30	0,42	0,90	0,05	0,47
70	I2,54	3,I5	9,39	2·I0^{-3}	3·I0^{-3}	I,44	0,53	0,07		I0,83	0,37	0,74	0,05	0,42
I00	II,95	3,04	8,89	4·I0^{-3}	2·I0^{-2}	I,35	0,55	0,2I	0,04	I0,24	0,32	0,57	0,04	0,36
I50	II,22	2,95	8,2I	8·I0^{-3}	5·I0^{-2}	I,22	0,56	0,34	0,09	9,43	0,30	0,44	0,03	0,33

Table 13

Calculated neutron reaction cross-sections for the ^{239}U nucleus
(cross-sections, b; energy, keV)

ε	σ_t	σ_c	σ_{sel}	σ_{inel}^{rot}		σ_{cel}	σ_{inel}^{c}		σ_{el}	σ_{nf}	$\sigma_{n\gamma}+\sigma_{n\gamma f}$	$\sigma_{n\gamma}$	$\sigma_{nf}+\sigma_{n\gamma f}$
				$I'=7/2$	$I'=9/2$		$I'=7/2$	$I'=9/2$					
I	25,66	I4,62	II,04			I,94			I2,98	9,53	3,I5	0,02	9,55
5	I7,83	7,0I	I0,82			I,46			I2,28	4,0I	I,54	0,02	4,03
I0	I5,99	5,37	I0,62			I,32			II,94	2,78	I,27	0,03	2,8I
20	I4,66	4,35	I0,3I			2,30			II,6I	I,95	I,I0	0,04	I,99
50	I3,23	3,62	9,6I			I,48	0,II		II,09	I,20	0,83	0,04	I,24
I00	I2,I4	3,38	8,75	$3\cdot I0^{-3}$		I,60	0,36	0,0I	I0,35	0,83	0,58	0,03	0,86
I50	II,4I	3,3I	8,09	$6\cdot I0^{-3}$	$4\cdot I0^{-3}$	I,55	0,43	0,I9	9,64	0,70	0,44	0,03	0,73

Table 14

Calculated neutron reaction cross-sections for the ^{237}U nucleus.
The parameters of barrier magnitudes of the transitional-state bands of negative parity are reduced by 200 keV
(cross-sections, b; energy, keV)

ε	σ_t	σ_c	σ_{sel}	σ_{inel}^{rot}		σ_{cel}	σ_{inel}^{c}			σ_{el}	σ_{nf}	$\sigma_{n\gamma}+\sigma_{n\gamma f}$	$\sigma_{n\gamma f}$	$\sigma_{nf}+\sigma_{n\gamma f}$
				$I'=3/2$	$I'=5/2$		$I'=3/2$	$I'=5/2$	$I'=7/2$					
I	25,37	I4,I4	II,22			4,I7				I5,39	2,50	7,47	0,29	2,79
5	I7,73	6,73	II,0			2,78				I3,78	I,I5	2,80	0,I2	I,27
I0	I5,9I	5,I0	I0,8I	$I\cdot I0^{-5}$		2,I4	0,29			I2,95	0,88	I,79	0,08	0,96
I5	I5,09	4,45	I0,64	$8\cdot I0^{-5}$		I,85	0,38			I2,49	0,78	I,44	0,07	0,85
20	I4,58	4,09	I0,49	$2\cdot I0^{-4}$		I,72	0,40			I2,2I	0,72	I,25	0,07	0,79
50	I3,I2	3,34	9,78	$2\cdot I0^{-3}$		I,46	0,47			II,24	0,59	0,82	0,05	0,64
70	I2,54	3,I5	9,39	$2\cdot I0^{-3}$	$3\cdot I0^{-3}$	I,38	0,49	0,06		I0,77	0,55	0,67	0,05	0,60
I00	II,95	3,04	8,89	$4\cdot I0^{-3}$	$2\cdot I0^{-2}$	I,29	0,50	0,I9	0,03	I0,I8	0,5I	0,52	0,04	0,55
I50	II,22	2,95	8,2	$8\cdot I0^{-3}$	$5\cdot I0^{-2}$									

Fig. 1. Angular distribution of elastically scattered neutrons for $\varepsilon = 1$ MeV: — - calculated curve; experimental data: • - Cranberg. - A-2177, 1959; ⊙ - Cavanagh et al., - AERE-R-5972, 1969.