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Presented by
Heat and Mass-Exchange Institute of the
Byelorussian Academy of Sciences in Minsk,
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Fifth Conference on Neutron Physics

THE DEVELOPMENT OF NUCLEAR DATA EVALUATION METHODS FOR FISSILE NUCLEI

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ABSTRACT

Progress in the development and use of theoretical models for evaluating nuclear constants for fissile nuclei is reviewed briefly.

Over the last few years an independent system of theoretical methods, incorporated in a set of carefully tested computer programs and capable of performing a self-consistent evaluation of nuclear data for fissile nuclei, has been developed at the Laboratory of the Physics of Elementary Processes (Byelorussian Academy of Sciences, Heat and Mass Exchange Institute). Particular attention has been paid to the development of techniques for evaluating neutron cross-sections in the resolved resonance, unresolved resonance and fast-neutron energy regions, to the elaboration of methods of evaluating experimental data, including those taking correlations between different experimental results into account, and to the study of the degree of reliability and the limits of applicability of existing theoretical models and of those developed. These methods were used to draw up complete files of nuclear constants for fissile nuclei which have been included in the national evaluated nuclear data library.

For the evaluation of nuclear data on fissile nuclei in the resonance region, three computer programs, based on the Adler-Adler, Reich-Moore and Bright-Wigner formalisms, have been prepared at our Institute.

The main assumption in the Adler-Adler approach - that of almost constant total widths - is legitimate for heavy nuclei; the radiative capture cross-section σ_γ for these nuclei is comparatively large and thus the Adler-Adler approach provides a good description of all types of neutron cross-section.

With the nuclei of structural materials, for which σ_γ amounts to the small difference between σ_t and σ_n, so that even a slight violation of the unitarity of the collision matrix can have serious consequences, this formalism could in principle give an insufficiently accurate description of σ_γ. The best approach in this case, despite the complexity of taking the Doppler effect into account, is to use the Reich-Moore method.

The Reich-Moore method, which unlike the Adler-Adler method requires us to know the spins of the resonances when performing cross-section analyses, was used by us together with the Adler-Adler method to determine resonance parameters of a complex nucleus like ^{235}U, with strong inter-level interference. For this nucleus multi-level analysis gave a better approximation of σ_f and σ_t in the regions 13.5-18.0, 24.0-26.5 and 32-40 eV. Inter-resonance troughs in the region 32-35 eV cannot be described by a single-level formalism at all.

Analysis of experimental data has shown that important factors in resonance analysis are an exact knowledge of the experimental resolution at each energy point (as a rule, in the experimental results obtained so far, this is not known very exactly), consistent normalization and a consistent energy scale.

In general, for all the actinides examined, the mean resonance parameters obtained for the resolved resonance region are not known sufficiently exactly, and a detailed analysis by the Reich-Moore method is hindered by the lack of experimental data on resonance spins.

In the unresolved resonance region, which extends to 100 keV for odd target nuclei and 150-200 keV for even nuclei, a self-consistent calculation was performed of mean neutron cross-sections (σ_t, σ_f, $\sigma_{n'}$, and σ_γ) and of the errors in them for heavy fissile nuclei. If the mean resonance parameters are determined with sufficient accuracy (preferably they should be tested against experimental values of σ_t and σ_f), the accuracy with which this method can predict, say, σ_γ in the energy region considered is ~5-10%. The minimum experimental information necessary to be able to do this is resolved resonance data and data on σ_t and σ_f for at least a limited energy region (keV region).

In the energy region under consideration, when calculating mean cross-sections of heavy fissile nuclei, account must be taken of the neutron inelastic scattering reaction (the effect of which is ~10% for $\sigma_f(^{239}Pu)$ and $\sigma_\gamma(^{241}Pu)$ at 100 keV), the direct excitation of levels (4% at 100 keV for ^{239}Pu), the energy dependence of the mean level spacing (if this dependence is disregarded, σ_γ will be reduced by ~15% at 100 keV), the energy dependence of the radiative width Γ_γ (at 100 keV the difference between calculated $\langle\sigma_\gamma\rangle$ values with constant $\langle\Gamma_\gamma\rangle$ and with allowance for $\Gamma_\gamma(E)$ is 4% at 100 keV and 8% at 200 keV) and the $(n,\gamma f)$ reaction for nuclei with a negative fission threshold (the contribution of the $(n,\gamma f)$ process cross-section for ^{239}Pu at 1 keV is ~15% on σ_f and ~20% on σ_γ and, at 100 keV, ~5% on σ_f and ~25% on σ_γ).

In calculating the mean cross-sections of odd target nuclei, account need only be taken of the contribution of s- and p-waves, not only to the total cross-section σ_t but to the partial cross-sections as well (the contribution of the d-wave for ^{235}U at 100 keV is ~0.6% σ_t), while for even target nuclei s-, p- and d-waves must be taken into account.

The structure in the neutron cross-sections σ_t and σ_f for ^{239}Pu and ^{235}U were taken into account by variation of the strength function S_o and of the fission widths.

To determine the mean level spacings $\langle D\rangle_J$ in the unresolved resonance region, both the traditional Fermi-gas model and a model allowing for superconducting-type pair correlations and collective degrees of freedom were used [1]. In the energy region under consideration, the traditional Fermi-gas model provides a sufficiently good approximation. Since the energy range studied is small and lies near the normalized value on $\langle D\rangle_{obs}$, it is not necessary to take the energy dependence of the parameter a and the contribution of rotational and vibrational movement modes to the level densities into account. The use of different expressions for the parameter σ^2 in the Fermi-gas model equation does not affect the calculated values of $\langle D\rangle_J(E)$.

contradiction

An important question is the calculation of the width fluctuation factor, for which averaging is performed in accordance with the accepted width distribution laws. In the general case, where we have unequal relative contributions by the different channels to the mean width, a generalized distribution must be used [2]. We have studied [3] the influence of different methods of describing partial width distributions on mean elastic scattering, radiative capture and fission cross-sections for the case of several channels and have obtained simple expressions of the generalized Porter-Thomas distribution for the most important cases of two and three reaction channels; we have shown the possibility of using the generalized Porter-Thomas distribution for an analysis of the experimentally determined fission width distribution, thus allowing a more complete link to be established between the statistical properties of the widths and the structural parameters of the fissioning nucleus. In particular, to describe the fluctuations of the fission widths with a small number of channels (of the Γ_f^{0+} type for ^{239}Pu) it is necessary to use the generalized rather than the traditional Porter-Thomas distribution. The use of ν_{effxr} and the Porter-Thomas distribution for describing fluctuations in Γ_{fr} is justified only when the relative contributions of the channels differ either very little or very greatly, when whole values of ν could be used with equal justification.

In Ref. [3] it is shown that the method used for describing fission width distributions has a considerable influence on the S_{nx} factors. Thus, the difference in S_{nn}^{0+} and $S_{n\gamma}^{0+}$ for ^{239}Pu calculated with the traditional Porter-Thomas distribution and the generalized distribution can be as great as ~18% at 0.1 keV, while in S_{nf}^{0+} it can be ~5% with a difference in channel contributions of ~0.7-0.9. With increasing energy the difference between the traditional method of taking fission width fluctuations into account using ν_{eff} and the method based on a two-channel distribution decreases (at 100 keV for S_{nn}^{0+} and $S_{n\gamma}^{0+}$ it decreases by a factor of 2-3 and for S_{nf}^{0+} by a factor of 1.5-2.0).

When evaluating mean cross-sections of fissile odd target nuclei in the unresolved resonance region, the fluctuation factors S_{nf} for fission widths with a small number of channels (of the $\langle\Gamma_f\rangle^{0+}$ type for ^{239}Pu) must be calculated by means of the generalized Porter-Thomas distribution. For even-even target nuclei, the S_{nf} factor must be calculated with allowance for the fission-width distribution in the sub-barrier region: this gives a convolution of the Porter-Thomas distribution characterizing the distribution of fission widths in relation to their local mean values with a distribution function of mean fission widths. The value of the S_{nf} factor is not calculated analytically in this case, and for this reason it was determined by averaging values of $\frac{\Gamma nr\ \Gamma xr}{\Gamma r}$ obtained through a lottery of the corresponding distributions by means of the Monte-Carlo method.

For evaluating neutron cross-sections in the fast neutron energy range we have developed a technique which can be used in the context of the optical-statistical approach, with allowance for fission and radiation channel competition, to calculate and predict neutron cross-sections for all types of processes, including the cross-sections of cascade reactions, in the energy region 1 keV-15 MeV.

A version of the coupled-channel method and a computer program written for it, possessing distinct physical and mathematical characteristics by comparison with existing approaches, have also been developed. By linking the coupled-channels program with the optimization task of potential parameter search and determining the initial experimental data which should be used as a basis, it was possible to determine optimum potential parameters for even and odd nuclei; this in turn opened the way for theoretical prediction of direct inelastic scattering cross-sections at different levels and angular distributions of elastically and inelastically scattered neutrons.

Both these methods are discussed in greater detail in two other papers presented at this Conference.

We have also studied the possibility of using the Monte-Carlo method in the neutron energy region above 5 MeV for predicting neutron cross-sections of fissile nuclei on the basis of a generalization of the exciton model of pre-equilibrium decay. The discovery by Gudima et al. [4] of a link between the process of transition of a non-equilibrium nuclear system to equilibrium and random Markov processes made it possible to use the Monte-Carlo method to obtain an accurate solution of the generalized kinetic equation describing the development of an excited system in time, including successive emission of particles at the stage where statistical equilibrium is reached. This model has proved useful for evaluating nuclear data on fissile nuclei, since it can be applied for calculating the partial cross-sections of all processes in which neutrons interact with nuclei, and can be generalized for the case of fissile nuclei; i.e. the competition of evaporation and fission processes can be taken into account when calculating the cross-sections of other processes.

The calculations performed with this model took account of the variation in fission barrier height with the increase in excitation energy - for this purpose results obtained earlier with the Hartree-Fock method were used [5] - and of the influence of pre-equilibrium particle emission on the fissionability of nuclei, which reduces the excitation energy of the compound nucleus and consequently the probability of fission.

If the Monte-Carlo method is used for calculating the intranuclear cascade with allowance for pre-equilibrium neutron emission, the inelastic scattering cross-section and the cross-sections of the (n,2n) and (n,3n) reactions for heavy nuclei in the energy region above 5 MeV can be predicted to within ~20-30%. The calculated inelastic scattering cross-sections ($\sigma_{n'}$) are found to be weakly dependent on the fission barrier values (B_f) used in the calculations, and the main factor affecting the $\sigma_{n'}$ calculation is a correct choice of matrix element type in allowing for pre-equilibrium-emitted neutrons.

For calculating the cross-sections of the (n,2n) and (n,3n) reactions for ^{238}U, this method, using fission barriers (B_f) obtained from experimental σ_f values and taking the temperature dependence of B_f into account, provides the closest fit with experimental values of σ_{2n} and σ_{3n} (agreement is to within ~10-20%).

This model can be used for taking fission competition into account when calculating the (n,2n), (n,3n) and (n,n') cross-sections, but it cannot be used to predict the fission cross-section of nuclei for which there are no experimental σ_f values.

One possibility of obtaining a more correct calculation of σ_f, on which work is currently in progress at our Institute, may lie in the use of an up-to-date level density model taking collective effects into account, and in acceptance of the fact that the first barrier has an axially asymmetric form which produces higher level densities than axially symmetric longitudinal deformation; we must also bear in mind that, for actinides heavier than thorium, there are two parallel second humps with a difference of 0.5 MeV and that the first axially asymmetric barrier may fragment into two distinct barriers [6].

Thus, a number of methods for evaluating and predicting neutron cross-sections of fissile nuclei have been developed in the laboratory. The calculated compound nucleus formation cross-sections for heavy nuclei found by various authors using the optical spherical model show a wide spread (~30-50%), depending on the parameters of the optical model used. Our efforts to determine the parameters of both the spherical and non-spherical potentials which can describe all the experimental data have yielded an optimum form of potential for heavy nuclei which makes it possible to calculate compound nucleus formation cross-sections to within ~10%.

When using theoretical calculation models, the radiative capture cross-section depends not only on the compound nucleus formation cross-section but also on the way in which competition between fission and inelastic scattering is taken into account, on the level density of the compound nucleus and on the form of the spectral factor. Our calculations of σ_γ using the statistical model give satisfactory results for ^{238}U, ^{235}U, ^{239}Pu and ^{240}Pu and make it possible to use this approach for other fissile nuclei (^{241}Pu, ^{242}Pu and ^{241}Am) without further fitting of parameters. Agreement with experimental values for σ_γ , where these exist, is no worse than 10-20%. A second method of calculating σ_γ, used in the unresolved resonance region, makes it possible - provided the mean resonance parameters are obtained from evaluated data - to calculate σ_γ to within 5-10% in the energy region up to 200 keV.

Calculated cross-sections for inelastic scattering to excited levels depend on our knowledge of the neutron strength functions in the entrance and exit channels, and the uncertainty in these corresponds to the uncertainty in the compound nucleus formation cross-section (~10-15%). The existence of a direct mechanism for the excitation of rotational states introduces a further uncertainty into theoretical cross-section calculations. Moreover, the possibility of correlations between the neutron widths for the entrance and exit channels may cause $\sigma_{n'}$ to be somewhat underestimated. Thus, it will be seen that the total error in the inelastic scattering cross-section calculations for discrete levels of fissile nuclei for which there are no experimental data can be 20-30%.

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Translated from Russian

THE OPTICAL POTENTIAL FOR HEAVY NUCLEI

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Fifth Conference on Neutron Physics

ABSTRACT

On the basis of coupled-channel calculations the authors obtained a unique set of generalized optical potential parameters which make it possible to describe the experimental data available for ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu.

The coupled-channel method [1] is widely used at present both for analysing experimental data on neutron interaction with nuclei and for predicting neutron cross-sections. As is well known, this method is based on a generalized optical model which describes the process of neutron interaction with a nucleus more adequately than the traditional optical model. As a result, because of the inadequacy of the description of the nucleon interaction process with a nucleus, the isotopic dependence of the optical potential should be weaker for the generalized optical model, particularly since this model takes into account individual nuclear characteristics important to the interaction process such as the energies of the ground rotation band levels and deformations.

The authors present the results of work on the determination of the optical potential parameters for a group of heavy fissile nuclei on the basis of experimental data. A computer program based on the generally accepted coupled-channel algorithm method [1] was used for the calculations and tested in accordance with the norms described in Ref. [2]. The difference between the coupled-channel computer program developed by us and existing programs [2-4] is that our method of computation was modified slightly in order to reduce computer time, thereby enabling the coupled-channel method to be combined with an optimized potential parameter search using χ^2 criteria.

Optimization of the potential parameters on the basis of experimental data was carried out with a search program using the saddle-point method, the parameters being fitted not at separate points but simultaneously over the whole energy range from 1 keV to 15 MeV.

The procedure for the unique potential search was as follows. The first stage was to determine an optimum set of potential parameters for the ^{238}U nucleus, for which the most experimental data are available, and, in addition, the ground state zero spin reduces the amount of work involved in the search. In the low-energy range, the theoretical values were fitted to the evaluated strength functions S_0 and S_1 and to the potential scattering radius R' [5]. At the same time as fitting the parameters throughout the entire energy range, we used experimental values for the total neutron interaction cross-section σ_t with the ^{238}U nucleus and reliable existing data on the angular distributions of elastically and inelastically scattered neutrons in the range of energies where the contribution of the compound mechanism can be disregarded. Experimental data on $\frac{d\sigma}{d\Omega}$ were not taken into account in the fit in the lower energy range but the calculated values were checked against them for consistency.

It was assumed in the parameter search that the optical potential had the following form:

$$U(r) = -V_R f(r,a_R,R_R) + i W_D \cdot 4 a_D \frac{d}{dr} f(r,a_D,R_D) + + \left(\frac{\hbar}{m_\pi c}\right)^2 V_{so} \vec{l}\cdot\vec{\sigma} \frac{1}{r} \frac{d}{dr} f(r,a_R,R_R) , \qquad (1)$$

where

$$f(r,a,R) = [1 + \exp(r-R)/a]^{-1} .$$

For the deformed terms V_R and W_D, the radius was taken as:

$$R = R^0 A^{1/3} [1 + \beta_2 Y_{20}(\theta) + \beta_4 Y_{40}(\theta)] ; \qquad (2)$$

the spin-orbit potential V_{SO} was not deformed and its radius was taken as: $R_R = R_R^0 A^{1/3}$.

The coupling of the first three levels only of the ground rotation band - 0^+, 2^+, 4^+ - was taken into account in the calculations, as the inclusion of the next level, 6^+, alters the calculation results within the experimental data error limits (except the excitation cross-section of level 4^+). It was assumed in the fit that the parameters V_R, W_D, a_R and a_D are linearly dependent on energy, but as results showed it is not necessary to include the energy dependence of the diffuse real part of the potential to describe the experimental data. However, the introduction of the energy dependence of the parameter a_D significantly improves the description. The following potential parameters were obtained for a ^{238}U nucleus as a result of the optimization using experimental and evaluated data:

$$V_R = 45{,}87 - 0{,}3E \qquad R_R^0 = \text{I}{,}256 \qquad a_R = 0{,}626$$

$$W_D = \begin{cases} 2{,}95 + 0{,}4E & (E \leqslant \text{IO МэВ}) \\ 6{,}95 & (E > \text{IO МэВ}) \end{cases} \qquad R_D = \text{I}{,}260 \qquad a_D = 0{,}555 + 0{,}0045E$$

$$V_{SO} = 7{,}5\ ; \qquad \beta_2 = 0{,}2\text{I}6\ ; \qquad \beta_4 = 0{,}080.$$

Calculations using these parameters allow existing data for ^{238}U to be described in the energy range from 1 keV to 15 MeV almost within the experimental error limits. Figure 1 compares the theoretical values for the total interaction cross-section with the experimental values in the 0.1-15 MeV energy range.

Figures 2-4 show the differential elastic and inelastic neutron scattering cross-sections for the energies 3.4, 8.56 and 15.2 MeV, respectively. The table compares the theoretical values and the data evaluated on the basis of experimental values for the strength functions S_0 and S_1 and the potential scattering radius R'.

Table: Theoretical and evaluated data for S_0, S_1 and R'

Quantity	$S_0 \cdot 10^4$, $(eV)^{-1/2}$		$S_1 \cdot 10^4$, $(eV)^{-1/2}$		R', φ	
Nucleus	Theory	Evaluation	Theory	Evaluation	Theory	Evaluation
^{238}U	I,I6	I,I68±0,05	I,95	I,93±0,5	9,48	9,44±0,25
^{235}U	I,05	I,07±0,07	2,4	2,0 ±0,5	9,I4	9,I5±0,25
^{239}Pu	I,I5	I,I9±0,I7	2,2	2,3 ±0,4	9,05	9,I0±0,25
^{240}Pu	0,96	I,I ±0,I6	2,0	2,8 ±0,8	9,00	8,56±0,6

The second stage in obtaining the unique potential for heavy nuclei was to attempt to describe experimental data available for ^{235}U, ^{239}Pu and ^{240}Pu nuclei using the geometrical parameters derived for ^{238}U. The same spin-orbit potential value V_{SO} was also used. The following data were utilized: in the case of ^{239}Pu and ^{235}U, our own evaluated data for $\sigma_t(E)$ in the energy range up to 15 MeV, evaluated data for S_0, S_1 and R', and experimental data on angular distributions; in the case of ^{240}Pu, only evaluated data for S_0, S_1 and R' and σ_t in the energy range up to 3.5 MeV. The calculations were performed assuming the following level coupling systems:

^{235}U - $7/2^-$, $9/2^-$, $11/2^-$, $13/2^-$, $15/2^-$;

^{239}Pu - $1/2^+$, $3/2^+$, $5/2^+$, $7/2^+$, $9/2^+$;

^{240}Pu - 0^+, 2^+, 4^+.

To describe the experimental data, it proved sufficient to include in the potential obtained for ^{238}U, the isotopic dependence of the depths of the real and imaginary parts and to fit the deformation parameters β_2 and β_4. It was found that the depths of the real and imaginary parts of the potential, including the isotopic dependence obtained in the fit process can be described as follows:

$$V_R = 49.72 - 17 \frac{N - Z}{A} - 0.3\ E;$$

$$W_D = 5.22 - 10 \frac{N - Z}{A} + 0.4\ E.$$

The deformation parameters of the ^{235}U, ^{239}Pu and ^{240}Pu nuclei for the potential with the above-mentioned values of V_R and W_D are $\beta_2 = 0.201$, $\beta_4 = 0.072$; $\beta_2 = 0.217$; $\beta_4 = 0.082$; $\beta_2 = 0.191$ and $\beta_4 = 0.094$, respectively. The set of parameters given makes it possible to describe existing experimental data for the nuclei mentioned virtually within the limits of the error in it. Some examples of this description are given in Figs 5-7.

Certain difficulties arise with this version of the coupled channel method when attempting to reproduce a detailed structure in the angular distribution of inelastically scattered neutrons at the 2^+ level - the structure obtained in the calculations is less marked than in the experiment. Similar problems occur when describing the shape of the angular distribution of the levels ($5/2^+$, $7/2^+$) for ^{239}Pu. However, it should be pointed out that the reliability of measurements for the first level is very poor (it should be recalled that the recoil nucleus energy is similar to that of the first level).

The values obtained by us for the depths of the real and imaginary parts of the potential for ^{238}U are 0.6% and 20% lower, respectively, than the parameters given in Ref. /̄6_/, which were determined by attributing considerable weight to the experimental data on the angular distributions of elastically and inelastically scattered neutrons obtained in the same paper. The difference between our own potential and that obtained by others is also that ours includes the energy dependence of the geometrical parameter a_D, which allows the competition between surface adsorption and volume absorption to be taken into account effectively (this is particularly significant in the energy range above 10 MeV).

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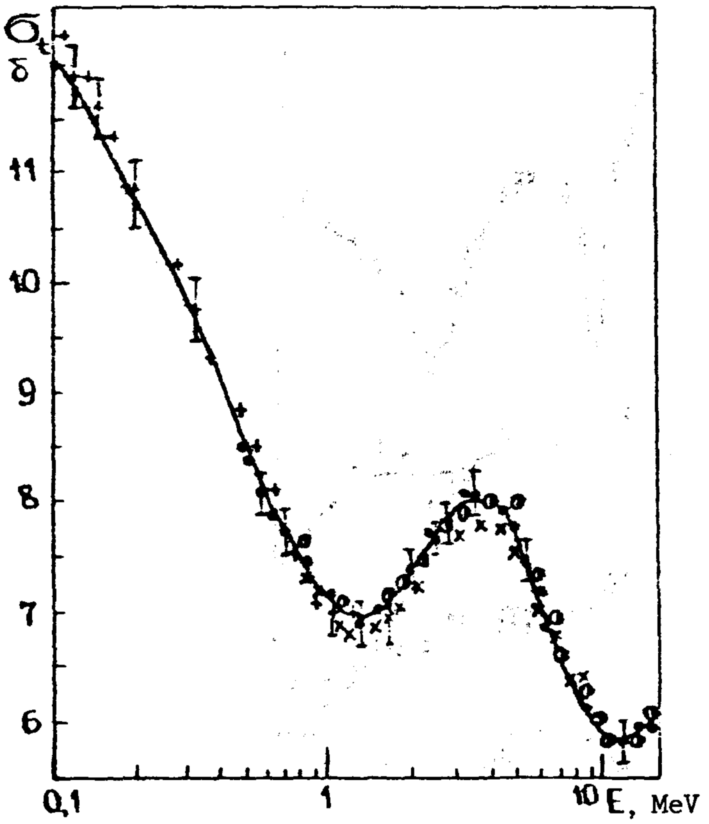

Fig. 1. Comparison of experimental and theoretical data on σ_t (^{238}U) in the 0.1-15 MeV energy range

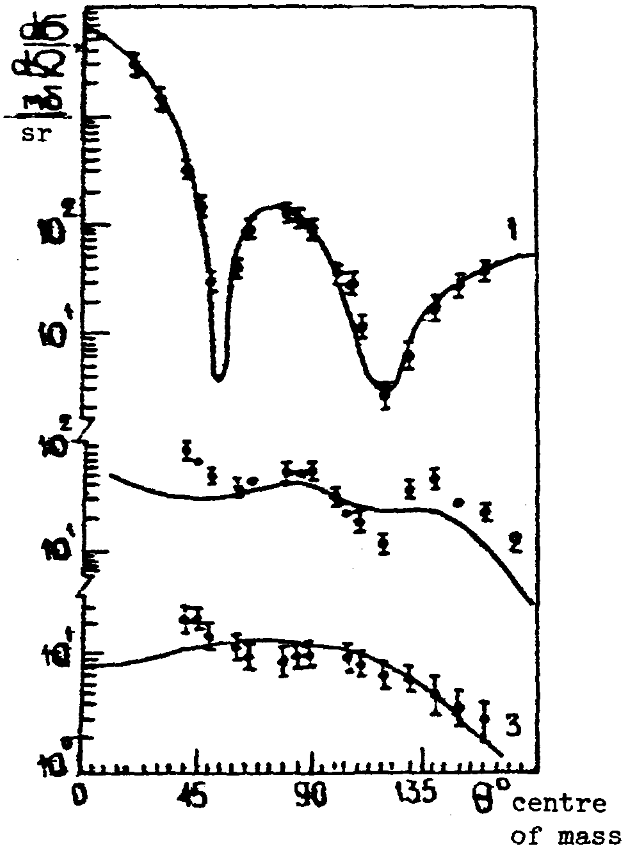

Fig. 2. Differential cross-sections for 3.4 MeV neutron scattering by a nucleus at:

1 - ground state (0^+)

2 - first excitation level (2^+, 44 keV)

3 - second excitation level (4^+, 148 keV)

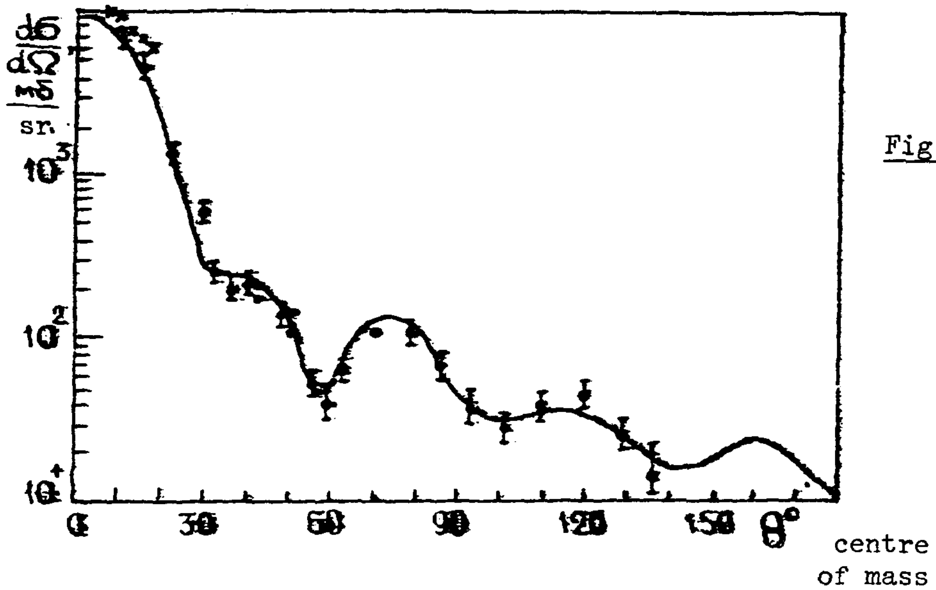

Fig. 3. Differential cross-sections for 8.56 MeV neutron scattering by a ^{238}U nucleus. The sum of three levels ($0^+ + 2^+ + 4^+$)

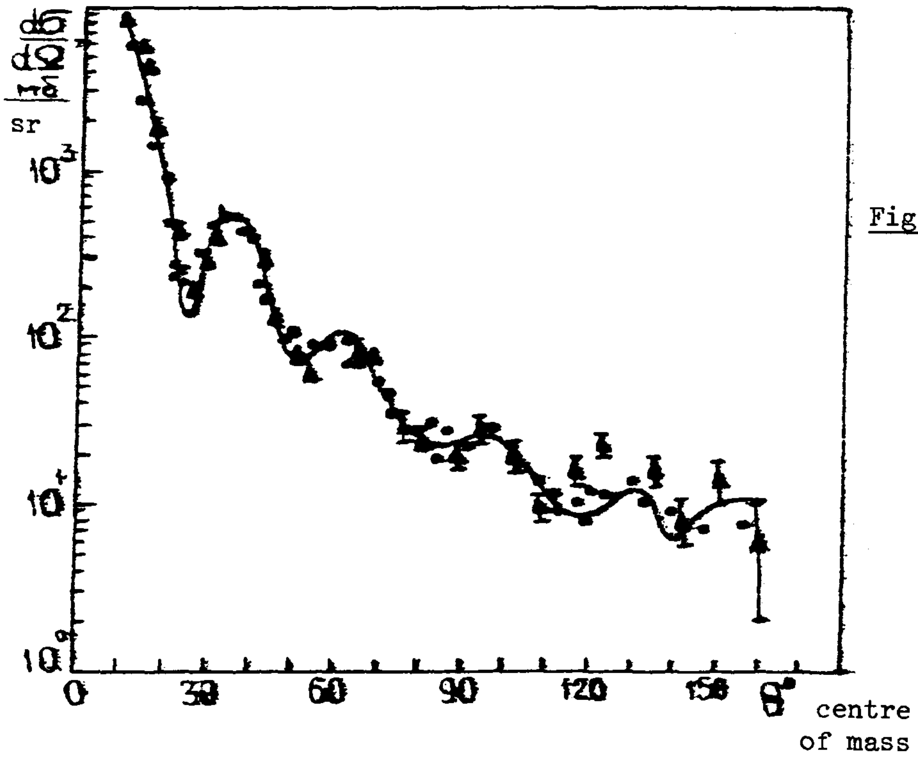

Fig. 4. Differential cross-sections for 15.2 MeV neutron scattering by a ^{238}U nucleus. The sum of three levels $(0^+ + 2^+ + 4^+)$

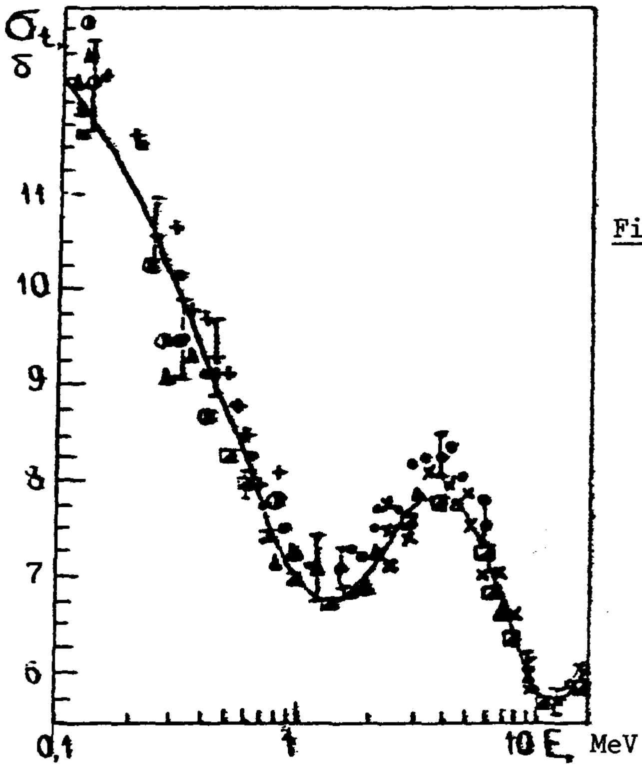

Fig. 5. Comparison of experimental and theoretical data on σ_t (^{239}Pu) in the 0.1-15 MeV range

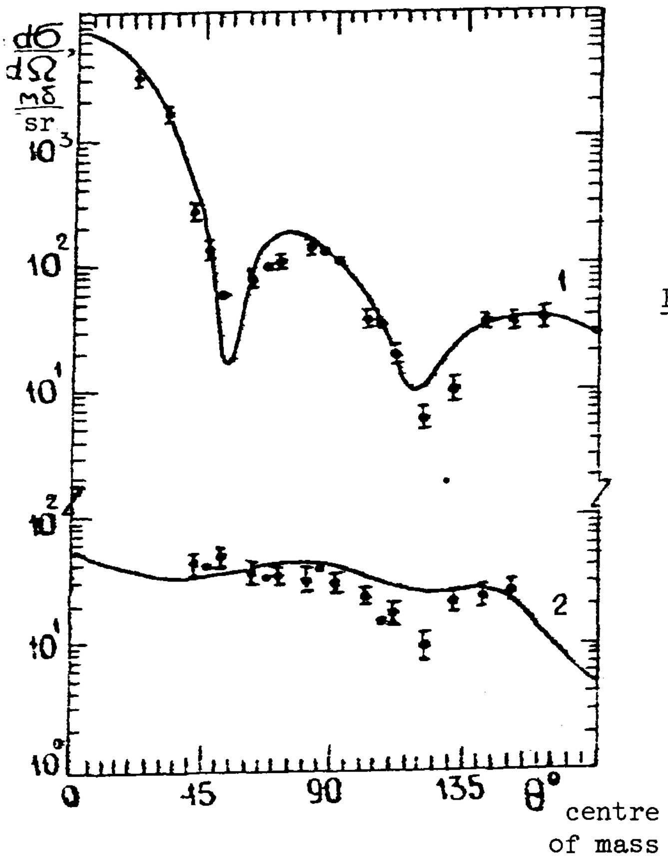

Fig. 6. Differential cross-sections for 3.4 MeV neutron scattering by a ^{239}Pu nucleus:

1 - the sum of the levels $1/2^+$ and $3/2^+$ (8 keV);

2 - the sum of the levels $5/2^+$ (57 keV) and $7/2^+$ (76 keV)

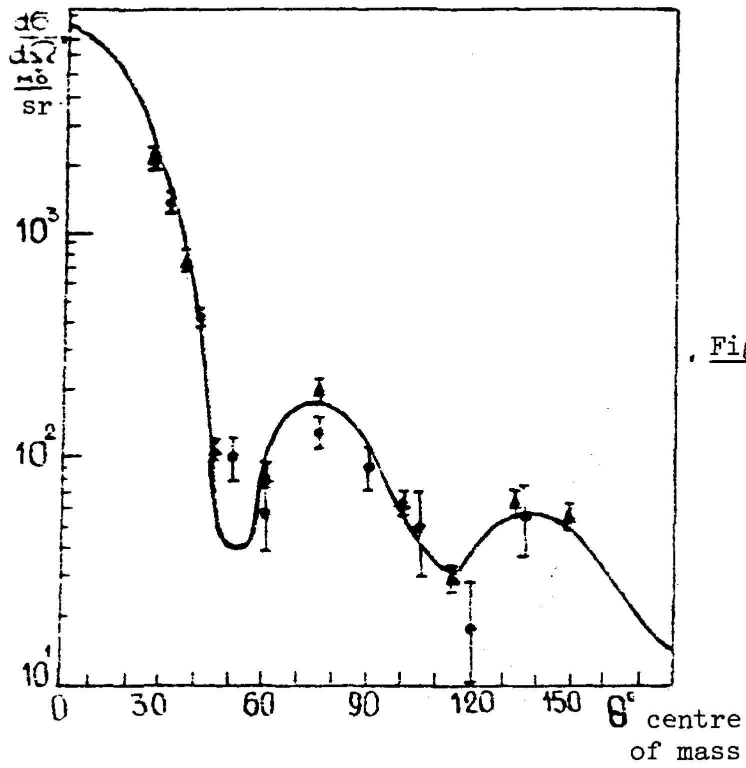

Fig. 7. Differential cross-sections for 4.0 MeV scattering by a ^{239}Pu nucleus. The sum of 5 levels.

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CALCULATION OF CROSS-SECTIONS FOR HEAVY DEFORMED NUCLEI USING A STATISTICAL MODEL

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ABSTRACT

A method for simultaneous calculation of the neutron cross-sections for processes of all types, including cross-sections of cascade reactions, in the neutron energy range 1 keV-15 MeV, using an optical-statistical approach taking fission and radiation channel competition into account, is described.

Neutron cross-section evaluations for heavy fissile nuclei rely to a large extent - and for some nuclei almost entirely - on theoretical models. Many years of work on nuclear data evaluations have resulted in the elaboration at our Institute of a complex statistical model which can be used for simultaneous self-consistent calculation of all types of neutron cross-section for fissile nuclei in the energy range 1 keV-15 MeV.

Comparative analysis of different statistical models of nuclear reactions led us to the conclusion that the Tepel-Hoffman-Weidenmüller approximation [1] should not be used for calculating neutron cross-sections of fissile nuclei in the energy region up to 1 MeV both because of the small number of decay channels and because of the presence of a strong competing fission channel with small ν_f. However, at an energy of 1.1 MeV, neutron cross-sections calculated by the Hauser-Feshbach method involving the S-factor and the method of Tepel et al. agree to within 10% for σ_γ, ~10% for σ_f and ~2% for $\sigma_{n'}$. It should be mentioned that, when the formalism of Tepel et al. is used in the energy region below 1 MeV, the sum of the cross-sections of reactions occurring through a compound nucleus differs from the compound nucleus formation cross-section calculated by the optical model. However, this difference, which is caused by modification of the neutron penetrabilities for the entrance channel, diminishes with increasing energy, and at $E_n > 1.1$ MeV it practically disappears. The formalism of Tepel et al., which takes into account the correlation of entrance and exit elastic channels, describes the cross-section of elastic scattering through the compound nucleus more correctly than the Hauser-Feshbach formalism, which means that it also gives a better fit to the inelastic scattering cross-section in the energy region above 1.1 MeV. Above 2 MeV both formalisms produce the same results.

A number of difficulties arise when using the optical-statistical model for calculating the neutron cross-sections of fissile nuclei, and the evaluation of neutron cross-sections for these nuclei is comparatively complicated.

Our complex statistical model and the computer program written on the basis of it have certain characteristic features: they take neutron penetrabilities correctly into account; up-to-date theories about level densities are used; account is taken of fission competition; and multi-cascade cross-sections can be calculated.

The neutron penetrability coefficients for the entrance channels were calculated using a generalized optical model (the coupled-channel method). The exactness with which these coefficients are calculated affects, in the first place, the compound nucleus formation cross-section and consequently also the reliability with which the total inelastic scattering cross-section is calculated. Although errors in the calculation of partial cross-sections with the statistical model caused by the use of a spherical optical potential may to a certain extent be offset by renormalizing on the compound nucleus formation cross-section calculated by the coupled-channel method, for deformed nuclei the most correct approximation of neutron penetrabilities is given by the coupled-channel method with careful optimization of the non-spherical potential parameters in order to obtain the best approximation of the optical cross-sections of the nucleus involved. For calculating the exit neutron penetrabilities, use of the spherical optical potential appears justified, since even for the fundamental rotational band it is not obvious that the link between channels is preserved when there is interaction of a neutron with an excited nucleus.

In addition to the neutron penetrabilities used, the level density model chosen exercises a considerable influence on neutron cross-sections calculated with the statistical model. The most correct approach is the microscopic method involving direct modelling of the structure of excited states of nuclei [2]; it enables us to understand questions such as the difference between collective movements of nuclei with different excitation energies, the mixing of collective modes with single-particle modes, and so on. However, these methods of calculating level densities are very cumbersome, especially in the high-energy region, which limits their value for nuclear data evaluations.

To demonstrate the influence of collective level density effects on neutron cross-section calculations for heavy nuclei, we used a statistical method which relies on the averaged characteristics of excited nuclei [3]. With this method it is possible to take into account correlation effects of the superconducting type and coherent effects of a collective nature.

Fission competition was taken into account, in calculating the cross-sections of other processes, by using information on the transient states of the fissioning nucleus obtained by theoretical means and corrected with the help of calculations in the unresolved resonance region, to which was added information on the continuous density of the transitional states - similar to the level densities in the constant-temperature model. This approach makes it possible to parametrize fission penetrabilities and at the same time to describe experimental fission cross-sections and angular distributions of fission fragments. It should be emphasized that this approach takes fission competition into account with sufficient accuracy when one is calculating the neutron cross-sections of other processes; however, it cannot be used to predict the fission cross-sections of nuclei for which there are no experimental data.

The complex statistical model developed at our Institute was generalized for the case of many-particle nuclear reactions, which made it possible to calculate the cross-sections of the cascade reactions (n,2n), (n,n'f), (n,3n) and (n,2n'f) occurring in the region above 5 MeV with conservation laws taken precisely into account for successive emissions of neutrons. These calculations were performed on the assumption that there are a large number of compound nucleus decay channels available and that there is no elastic scattering through the compound nucleus which can occur only via a single channel. The cascade reaction cross-sections are calculated by considering step by step the chain of decay events resulting in a particle and an excited nucleus which in turn can decay further, i.e. can (a) undergo fission, in the (n,n'f) reaction, (b) become de-excited by the emission of a gamma quantum (inelastic scattering) or (c) emit another neutron. In the subsequent cascade, the cross-section for the emission of two neutrons in each channel is multiplied by the probability of gamma discharge, fission and neutron escape, giving the cross-sections of the reactions (n,2n), (n,2nf) and (n,3n) respectively. For this calculation it is assumed that all prohibitions on decay are associated with energy, momentum and parity conservation laws.

The calculations performed on the basis of the complex statistical model described above were used for drawing up and renewing whole files of nuclear data for ^{235}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu.

Figure 1 shows, for purposes of illustration, calculated neutron inelastic scattering cross-sections at different levels for ^{238}U and ^{239}Pu.

By using the neutron penetrabilities from the generalized optical model and taking direct excitation of lower levels into account, one can obtain satisfactory agreement between experimental and theoretical excitation cross-sections not only for the lower levels but also for levels whose excitation cross-sections are determined entirely by compound nucleus decay.

The choice of level density model has practically no influence on the total inelastic scattering cross-section. The differences in the target nucleus level densities found with different models mean that there are different ratios between the scattering cross-sections for discrete and continuous level spectra and different excitation cross-sections for discrete levels.

As can be seen from Fig. 2, the best agreement between theoretical and experimental data on the excitation cross-sections of ^{239}Pu levels is obtained when level densities from the Fermi-gas model are used with collective modes taken into account.

Employing neutron penetrabilities obtained from the generalized optical model, one can, with a single set of parameters in the statistical approach, simultaneously calculate the cross-sections of all types of reaction with accuracies in σ_t and σ_{nx} of ~5%, in σ_γ of ~10-15%, in $\sigma_{n'}$(Eq) of ~20-30% and in σ_{2n} of ~20%, while σ_f can be parametrized to within ~10%. When there are no experimental data at all on σ_γ and $\sigma_{n'}$ for transactinides, they can be calculated to the accuracies quoted above by means of the method we have developed. The minimum information necessary for calculating σ_n, and σ_γ is experimental σ_f values, mean $<\Gamma_\gamma>$ and $< D >$ parameters and an energy-level scheme.

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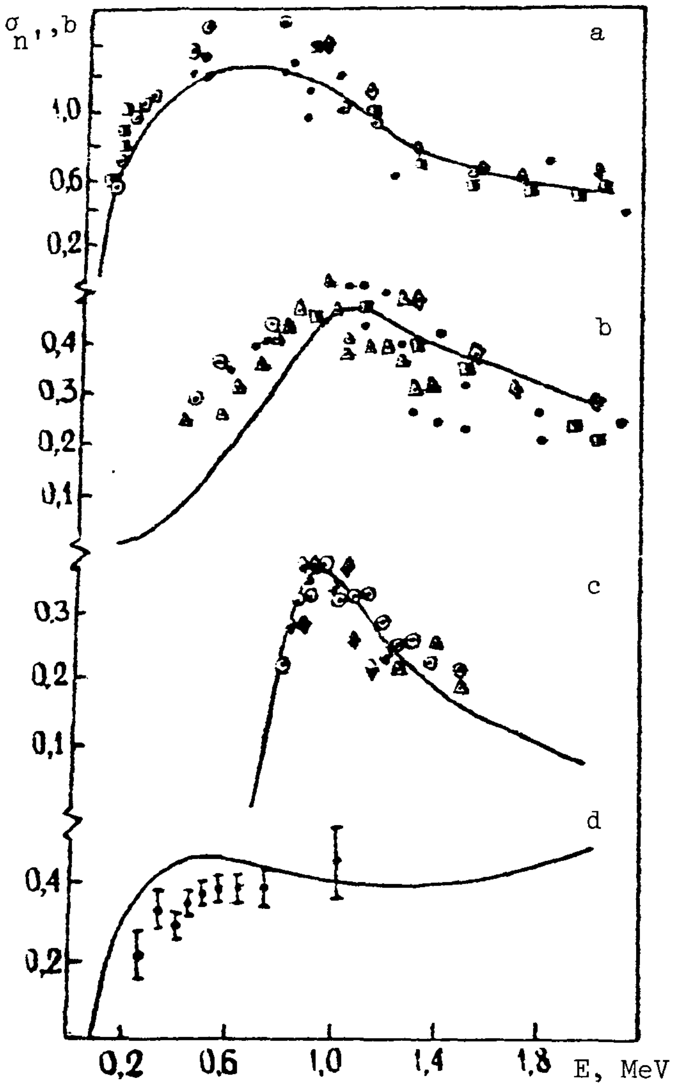

Fig. 1. Excitation cross-sections for various levels of ^{238}U and ^{239}Pu.

(a) ^{238}U, Eq = 44 keV

(b) ^{238}U, Eq = 148 keV

(c) ^{238}U, Eq = 680 keV

(d) ^{239}Pu, 57 keV ≤ Eq ≤ 76 keV

Level densities from the Fermi-gas model, taking collective modes into account, were used for the calculations.

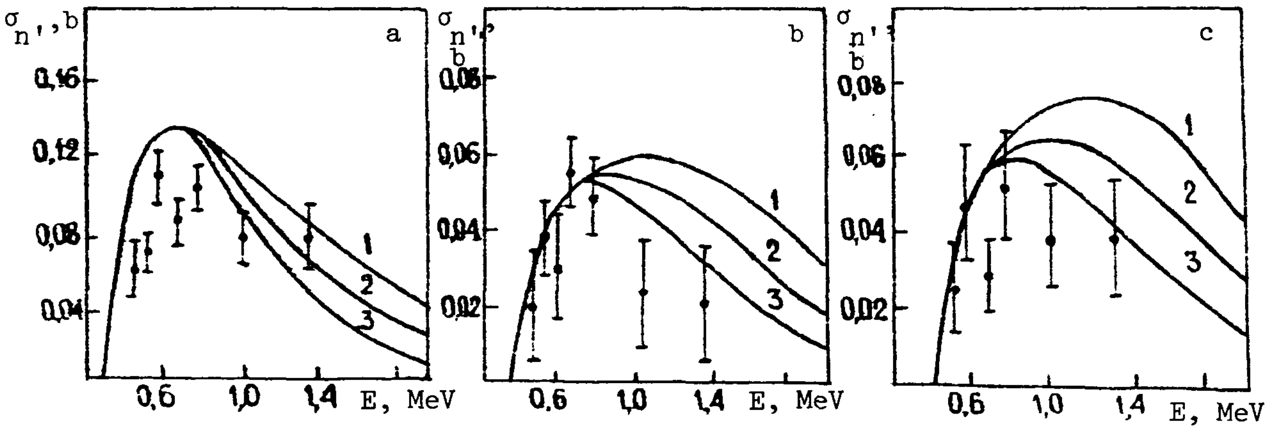

Fig. 2. Excitation cross-sections for various levels of ^{239}Pu using different level density models.

(a) Eq = 285 keV

(b) Eq = 330 keV

(c) 387 keV ≤ Eq ≤ 392 keV

1 - Fermi-gas model

2 - Superfluid-nucleus model

3 - Fermi-gas model taking collective modes into account.

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ON THE POSSIBILITY OF PREDICTING CROSS-SECTIONS FOR THE RADIATIVE CAPTURE OF NEUTRONS BY FISSIONABLE NUCLEI

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ABSTRACT

By comparing theoretical calculations with experimental data, the authors conclude that it is possible to obtain a self-consistent description of σ_γ over a wide energy range by using the non-spherical optical potential, the Lorentz-type spectral factor and the level density from the Fermi-gas model with an adjustment for collective modes and correct allowance for the contribution from the (n, γf) and (n, γn') processes to radiative capture.

Several factors must be taken into account in attempting to predict theoretically the cross-sections for the radiative capture of neutrons by fissionable nuclei. The correct level density model must be used, together with a physically appropriate type of spectral factor and neutron transparency factors derived from the generalized optical model. Furthermore, correct allowance must be made for the contribution from fission and from the (n, γ f) and (n, γn') processes to radiative capture.

The traditional Fermi-gas model is widely used for the level density but it does not fit the conclusions of the microscopic theory, nor does it agree with certain experimental data [1]. The statistical method for describing the averaged characteristics of excited nuclei, as developed by Ignatyuk and co-authors in Refs [2, 3], incorporates the main results of the microscopic theory and allows collective effects and pair correlations in the level density to be taken into account. Since the theoretical fission cross-sections usually fit the experimental data, the radiative capture cross-section is very sensitive to the level-density model used in statistical theory calculations. Our calculations show that there is a considerable difference between the theoretical σ_γ values and experimental data for both types of spectral factor if the traditional Fermi-gas model is used for the level density. This difference cannot be attributed to a poor definition of the parameters used (Fig. 1).

The best fit with the experimental data throughout the energy range is achieved by using the level density from the Fermi-gas model and allowing for collective modes. The Weisskopf spectral factor (curve 4 in Fig. 1) does not provide a better fit with the experimental $\sigma\gamma$ than that obtained by using the Lorentz spectral factor and the level density from the Fermi-gas model, allowing for collective modes. Given the stronger physics justification for using the Lorentz factor, as demonstrated by the results from the description of radiative strength functions [6] and the experimental data on the widths of the (n, γf) process [5], we considered it appropriate to use that factor in our statistical theory calculations.

The coupled-channel method provides the most accurate description of neutron transparency for the actinides. Fig. 2 shows how the calculation of $\sigma\gamma$ is affected by the neutron transparency factors, as derived from the spherical and non-spherical optical model. In both cases the variation in $\sigma\gamma$ is energy-dependent and ranges from 5 to 20%.

In order to predict the cross-sections for radiative neutron capture on the basis of the statistical model, we need to know not only the transparency of radiative capture and of the incident neutrons but also the probability of competing processes.

The authors of Ref. [5] referred to the need to allow for competition from the (n, γf) reaction in calculating the radiative capture cross-sections. Hitherto, calculations of the width of the (n, γf) and (n, γn') processes allowed for contributions from fission and inelastic scattering to the γ-discharge process only after emission of the first γ-ray. However, the studies show that, for nuclei with a negative fission threshold this approach is valid only at low incident neutron energies ($E_n \lesssim 0.5$ MeV): at higher incident neutron energies, there is a definite probability that the nucleus will fission also after the emission of two successive γ-rays.

In calculating the radiative capture width, we in this paper allow for contributions by fission and inelastic scattering to γ emission after a second cascade. It is thus possible to calculate the width of radiative capture and of the (n, γf) and (n, γn') reactions with sufficient accuracy. The γ-rays in the second cascade are mainly emitted at a nuclear excitation energy not exceeding B_n + 0.5 MeV since inelastic scattering and fission dominate at higher energies. Given that the average γ-ray energy is $E\gamma \gtrsim 1$ MeV, after two successive cascade emissions the excitation energy of the nucleus becomes less than the fission thresholds, and other processes apart from γ emission cannot occur. In Fig. 3 the radiative capture widths we obtain in this paper for ^{238}U and ^{239}Pu nuclei are compared with the results of calculations which allow for competition from fission and inelastic scattering only after the first γ-ray cascade. Fig. 3 shows that at low incident neutron energies the values virtually coincide.

At higher energies, $\Gamma\gamma$ behaves differently. ^{238}U has a positive fission threshold, and the radiative capture width is only slightly reduced when allowance is made for competition from fission and inelastic scattering in the second γ-ray cascade, whereas for ^{239}Pu $\Gamma\gamma$ drops considerably. It is also important to make correct allowance for competition from fission and inelastic scattering at nuclear excitation energies exceeding B_n. This can be seen from Fig. 3 where our results are compared with the results from Ref. [5], whose authors did not allow for the contribution to the radiative capture width by γ-rays from the second cascade emitted at nuclear excitation energies greater than B_n.

The present theoretical analysis thus shows that in order reliably to predict the energy dependence of $\sigma\gamma$ for fissionable nuclei in the energy region up to 4 MeV:

(a) The generalized optical model must be used to derive neutron transparency;

(b) Correct allowance must be made for the contributions from the $(n, \gamma f)$ and $(n, \gamma n')$ reactions to the radiative capture process;

(c) The calculations must be based on the Lorentz-type spectral factor and the level density from the Fermi-gas model, allowing for collective effects.

Figure captions

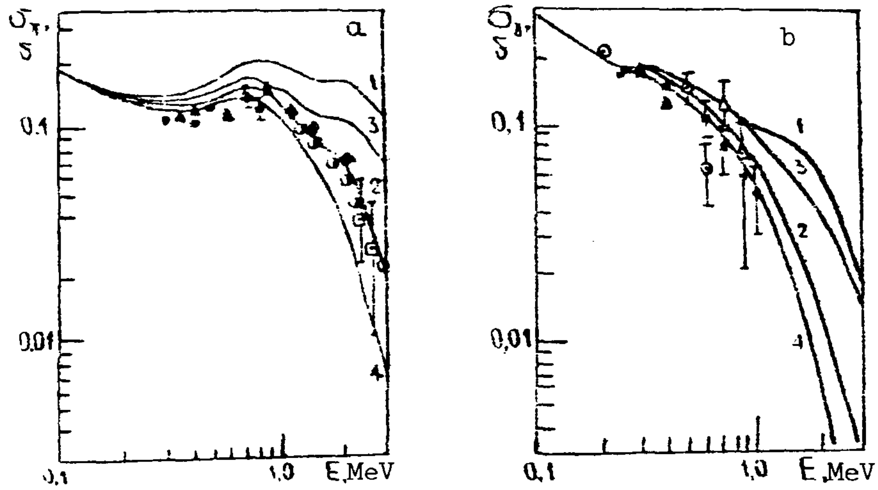

Figure 1. A comparison of experimental data on σ_γ(a - ^{238}U, b - ^{239}Pu) and theoretical results obtained by using different level-density models:

1 - the Fermi-gas model and the Lorentz spectral factor,

2 - the Fermi-gas model allowing for collective effects and the Lorentz spectral factor,

3 - the superfluid model, allowing for collective effects, and the Lorentz spectral factor,

4 - the same as curve 2 but with a Weisskopf-type spectral factor

(^{238}U : $\langle D \rangle_{observ.}$ = 24.8 eV [4],
$\langle \Gamma_\gamma \rangle_{observ.}$ = 23.5 MeV (ENDF-B/IV);
^{239}Pu : $\langle D \rangle_{observ.}$ = 2.38 eV [5],
$\langle \Gamma_\gamma \rangle_{observ.}$ = 43.3 MeV [5] ; T_n values determined by the coupled-channel method).

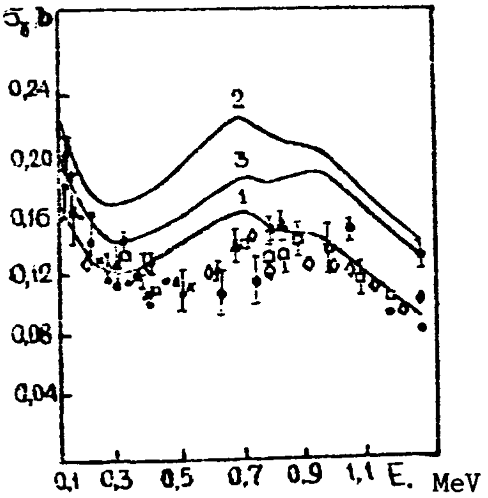

Figure 2

Theoretical σ_γ values (for ^{238}U) as a function of $<D>_{\text{observ.}}$ and of the neutron transparency factor T_n. The calculation was based on the Fermi-gas model, with allowance for collective effects, on the Lorentz spectral factor and on a $<\Gamma_\gamma>_{\text{observ.}}$ value of 23.5 MeV.

1 - $<D>_{\text{observ.}}$ = 24.8 eV [4], with a non-spherical potential;
2 - $<D>_{\text{observ.}}$ = 17.7 eV [7], with a non-spherical potential;
3 - $<D>_{\text{observ.}}$ = 17.7 eV, with a spherical potential.

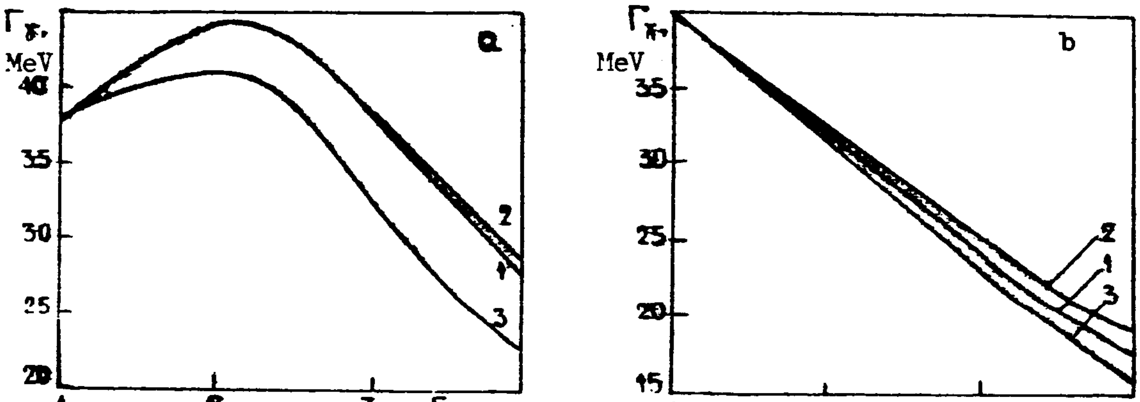

Figure 3. A comparison of various ways of calculating radiative capture widths:

a) $\Gamma_\gamma^{3/2-}$ for a ^{238}U target nucleus;

b) Γ_γ^{0+} for a ^{239}Pu target nucleus;

1 - this paper;

2 - this paper, allowing for competition from fission and inelastic scattering only after the first γ-ray cascade;

3 - curve allowing for the (n, γf) and (n, γn') processes according to the method proposed by the authors of Ref. [5].

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