International Atomic Energy Agency

INDC(CUB)-007
Distrib.: G

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

FISSION CROSS SECTION CALCULATION FOR $^{239}Pu(n,f)$, $^{241}Am(n,f)$ REACTIONS USING THE SEMIMICROSCOPICAL COMBINED METHOD IN LEVEL DENSITY FORMALISM

V.F. García, P.E. Garrote, T.E. López
CEADEN
P.O. Box 6122, Havana, Cuba

and

H.O. Rodriguez
ISCTN
P.O. Box 6122, Havana, Cuba

September 1992

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

Reproduced by the IAEA in Austria
September 1992

INDC(CUB)-007
Distrib.: G

FISSION CROSS SECTION CALCULATION FOR $^{239}Pu(n,f)$, $^{241}Am(n,f)$ REACTIONS USING THE SEMIMICROSCOPICAL COMBINED METHOD IN LEVEL DENSITY FORMALISM

V.F. García, P.E. Garrote, T.E. López
CEADEN
P.O. Box 6122, Havana, Cuba

and

H.O. Rodriguez
ISCTN
P.O. Box 6122, Havana, Cuba

September 1992

"Fission Cross Section Calculation for $^{239}Pu(n,f)$, $^{241}Am(n,f)$ reactions using the semimicroscopical Combined Method in level density formalism".

Garcia V.F*, Rodriguez H.C**, Garrote P.E* and Lopez T.E*

* CEADEN, P. O. BOX 6122 Havana, Cuba

** ISCTN, P. O. Box 6122 Havana, Cuba

Abstract

The energy dependence of the fission cross section for $^{239}Pu(n,f)$ and $^{241}Am(n,f)$ is analyzed in terms of the double humped fission barrier model to deduce the barrier heights. Good fits were obtained by assuming that the first barrier is axially-asymmetric, while the second one is mass asymmetric. Obtained height barriers parameters are compared with others works results. The level density was calculated in the frame of the semimicroscopical Combined Method, and compared with anothers used methods.

I. Introduction

Fission Cross Section of actinide nuclei is included among the most important and necessary nuclear data for energetic and technology. To complete accurately and reliably the available data further development of evaluation methods is needed.

The calculation of the fission cross section energy dependence is one of the main sources of information of the fission barrier structure. The used approach on level density part of calculation is very important and in fact level density values for low energies determines the barrier height.

For deformed nuclei and especially for extreme points of fission path the phenomenological method in level density calculations have many disadvantages. Phenomenological approaches have been developed in several works taking into

consideration the shell, pairing and collective effects. To take into account these effects, a great amount of experimental information about level densities in a broad energy interval is needed. Therefore, the application of phenomenological formulae for the deformed states in fission or for nuclei far from nuclear stability line is under question.

The disadvantages of the phenomenological models lead to the development of semimicrbscopical models for level density calculations. The quantum-statistical model of nuclear level density calculations has been proposed and investigated by many authors [1-4] taking into account shell and pairing effects in the framework of the nuclei superfluid model. But the quantum statistical model does not give adequate description of level densities at low energies, where is necessary to take into account the discrete structure of spectrum. At low excitation energy the combinatorial method in the frame of BCS model is more preferable.

In this work the semimicroscopical Combined Method for level density calculations is used [5,6,7], and the aim of the paper is to test it in practical fission cross section calculations. It is assumed in the present analysis that all the reactions proceed via compound nucleus and the Hauser-Feshbach formalism is used. For this purpose, two representative nuclei ^{240}Pu (even-even) and ^{242}Am (odd-odd) were taken. As is well known, the energy dependence of fission cross section is governed mainly by level density correlation of gamma, neutron and fission channels. The use of only this method allow us to evaluate its descriptive capability in dependence of nuclear deformation.

Chapter II describes the so call Combined Method and presents a detailed analysis of results and comparison with others commonly used methods. In Chapter III the adopted method for description of gamma and neutron competition channels is briefly discussed. Chapter IV presents the results and their interpretation in connection with the double humped fission barrier model.

II. Level density.

Level density formalism.

The principal idea of the semimicroscopical Combined Method is as follow: the energy range in which level density are being considered is divided in two intervals, the first one is from zero to some value of nucleus excitation energy U_d, the second is from U_d to final value U_f. In the first interval level density is calculate in the frame of combinatorial BCS model and in the second one are made in the frame of quantum- statistical superfluid model [1-4]. In both cases same parameters (Single particle spectrum and pairing strength constants) are used.

The use of such method guaranties the smooth joining of discrete and continuous parts of the level density. The method allows to achieve smooth joining without fitting the parameters, because both calculations are fulfilled in the same model.

The combined method described above allows us to account for the structure of the transition spectrum at low excitation energies, both the shell and superfluid effects and permits to describe the level density in a wide energy range.

Only this method was used for all level density calculations. Axial-symmetry shape was considered for compound and residual nuclei, and the axial-asymmetry and mass- asymmetry properties of the first and second saddle points of fission barrier respectively, were taken into account.

The following expression was used for level density calculation of axial symmetric nuclei

$$\rho_{ax}(U,I) = \frac{(2I+1)\ \omega(U)\ K_{vib}(U)}{\sqrt{8\pi}\ \sigma_{\parallel}} \exp\left[-\frac{I(I+1)}{2\ \sigma_{\perp}}\right] \qquad (1)$$

In this formulae the contribution of rotational states is taken into account. Here $\omega(U)$ is the intrinsic level density. It was calculate in the frame of quantum-

statistical superfluid model. K_{vib} values are calculate in the liquid drop vibrational model [8].

$$K_{vib}(T) = \exp\left\{1.7\left(\frac{3mA}{4\pi G_{LD}}\right)^{2/3} T^{4/3}\right\} = \exp\left[x\ T^{4/3}\right] \qquad (2)$$

G_{LD} is the surface tension coefficient, $T= -\frac{\partial U}{\partial(\ln\rho(U))}$ is the nuclear temperature.

Spin cutoff parameter $\sigma^2_{\perp}$ and $\sigma^2_{\parallel}$ are calculated in the following way,

$$\sigma^2_{\perp} = \frac{F_{\perp}\ T}{\hbar}$$
$$\sigma^2_{\parallel} = \bar{\Omega}^2 g\ T \qquad (3)$$

here g is the single particle level density near the Fermi energy, $\bar{\Omega}^2$ is the value of average single particle square projection on the symmetry axis of deformed nucleus.

The energy dependence of the moment of inertia $F_{\perp}$ is approximated in the following way

$$F_{\perp} = \begin{cases} (F_o - F_{rig})\left[1 - \frac{U}{U_{crit}}\right] & U<U_{crit} \\ F_{rig} & U>U_{crit} \end{cases} \qquad (4)$$

were F_o is the moment of inertia in the ground state, U_{crit} is the maximum value of the transition energy from superfluid to normal state for neutron and proton systems, F_{rig} is the rigid body moment of inertia of nucleus.

The nuclear shape at the internal barrier has been suggested to be axially asymmetric [9,10]. The level density at the first saddle point were calculated within quantum statistical superfluid model in the approximation of small violation of axial symmetry. This means intrinsic level densities were taken at the axial symmetry deformation but its violations was accounted in the total density

$$\rho_{ns}(U,I) = K_{vib}(U)(2I+1)\ w(U)\ \exp\left[-\ \frac{I(I+1)}{2\ \bar{\sigma}^2}\right] \qquad (5)$$

were $\bar{\sigma}$ is an average spin cutoff parameter for rotations about the other two axes, and may be taken approximately equal to $\sigma_{\parallel}$.

The level density at second saddle point was calculated take into account the mass symmetry violation. In this case, rotational state with odd parity come in to play in addition to the rotational states with even parity [11]. Thus, the level density of Eq.(1) should be increased by a factor of 2.

Parameters of level density calculation.

The single particle spectra were obtained by means of the WSBETA code [12] with Chepurnov parameters [13] of nuclear potential.

The spectrum at equilibrium deformation for compound and residual nuclei were fitted to reproduce the low-lying quasiparticle states of these nuclei and the ground state of neighbor nuclei. At equilibrium deformation β_2=0.2 and β_4=0.06 were taken.

The single particle spectra at extreme points of fission barrier were calculated at deformations β_2=0.55, β_4=0.12 and β_2=1.16, β_4=0.06 [14], corresponding roughly to the fission barrier according to theoretical calculation of nuclear potential energy in the frame of Strutinsky method.

The pairing strength constants for neutron and proton system were taken respectively G_n=24.5/A MeV and G_p= 27.5/A MeV for all extreme points of fission path.

Level density for compound and residual nuclei.

Level density calculations for ^{239}Pu, ^{240}Pu, ^{240}Am, ^{241}Am at equilibrium deformations were performed taking into account the axially symmetric properties of these nuclei.

The level spacing data is fitted taking in to account the K_{vib} enhancement (see table 1). Is well known that the contribution of K_{vib} arise mainly from the residual interactions which are not considered in the BCS

hamiltonian. Obtained K_{vib} values are used to normalize the level density in the statistical calculation of nuclear reaction cross sections.As can be seen from Figs.1-4, even at low energies the Combined Method describes rather well the experimental $\rho(U)$ values.

TABLE 1 :Level density at equilibrium deformation

		^{239}Pu	^{240}Pu	^{241}Am	^{242}Am
D_s^{obs}		7.7	2.31	0.372	0.55
D_s^{cal}		7.64	2.32	0.37	0.55
D_p^{cal}		2.58	1.05	0.19	0.28
Γ_γ^s		34.00	39.40	65.00	43.80
Γ_γ^p		34.00	36.80	65.00	85.00
X_{vib}		1.10	1.00	0.10	2.20
Gilbert & Cameron	P(N)	0.00	0.43	0.43	0.00
	P(Z)	0.61	0.61	0.00	0.00
	Δ	0.61	1.04	0.43	0.00
	T	0.50	0.5	0.50	0.50
	E_c	5.40	4.15	3.55	3.12
	a	29.70	27.0	25.7	28.0
	σ^2	50.8	45.9	44.2	48.3

One is more commonly used method in level density calculations is the Gilbert & Cameron formulae ,which also were performed. The results are shown in Figs.1-4,where are compared with those of Combined Method. They do not differ

to much one from another because both are fitted to reproduce the level spacing at neutron binding energy and cumulative number of states at low energy, but in general their energy behavior is not the same. At higher energies Gilbert & Cameron formulae systematically gives higher values of ρ^{tot}. This is due to the fact that according to this formulae a is an energy independent parameter and therefore can not consider the variations of shell effects with the energy.

Level density and discrete transition state spectra at saddle point

The quasiparticle transition states spectra were calculated in BCS +blocking model at extreme points of deformations corresponding roughly to the fission barriers. The BCS equations were solved separately for protons and neutrons, using the pairing constant G_p=27.5/A MeV and G_n=24.5/A MeV.

On each of the quasiparticle states rotational bands were built with the moment of inertia corresponding to the deformation

$$E^{IK\pi} = E^{K\pi} + \frac{\hbar^2}{2\,F_\perp}\left[\, I(I+1) - K^2 \right] \qquad (6)$$

Discrete spectrum of transition states was used only up to 1 MeV . The effect of the mass-asymmetry violation on the external barrier was accounted by doubling the number of states, and the effect of the axial-symmetry violation on the internal barrier was simulated by (2I+1) times increase of the number of rotational states [11].

In Figs.5-8 the results of level density calculation at both saddle points are shown. In these figures, the results of level density calculation with a commonly used constant temperature formulae ,using parameters proposed by Lynn [15], are shown too. Although the energy dependence of both calculations are roughly similar, there are some differences. As shown in figures, the constant temperature formulae revels some irregularities, which do not have any

physical explanation. Nevertheless, the calculation carried out by the Combined Method have a more confident physical basis.

III. Gamma ray competition parameters and others quantities used in calculation.

For the calculation of γ-ray competition, recently developed energy-dependent Breit-Wigner (EDWB) giant dipole resonance (GDR) with adoption of a stronger nuclear deformation dependence [16] are used to predict the electric dipole gamma-ray strength function $f_{E1}(\varepsilon_\gamma)$. The EDWB GDR shape has given much better results in reproducing the physical observed magnitudes.

Normalizations at neutron binding energy are performed by using the s-wave and p-wave radiative widths $(\Gamma_\gamma^s, \Gamma_\gamma^p)$ and spacings (D_{obs}^s) given in table 1.

Neutron transmission coefficient $T_\ell(E_n)$ are taken of results of coupled channels optical calculations made by Lagrange [17].

IV. Results.

In the frame of Strutinsky method [18] the fission barrier take a double humped form for the most of actinides, including in this group the studied isotopes in present paper. Fission cross section of ^{239}Pu and ^{241}Am have been analyzed from 150 keV up to 3 MeV. The calculation have been made on the basis of the double humped fission barrier model with the assumption that the nuclear shape is axially asymmetric at internal barrier, while it is axially symmetric and mass asymmetric at external one [19].

Fission barrier parameters are fitting to give the best correspondence with the experimental data of fission cross section. Emphasis has been placed on reproducing the cross section values in the plateau region, thus near threshold structures arising from the coupling of class I and

class II states have been neglected in the present calculation.

Fission barrier parameters obtained in present paper are compared with the values of the other authors in table 2. For both nuclei is obtained height barriers values greater than the values of Lynn [15] that is so due to the significant difference of level densities at barrier deformations. Nevertheless like values was obtained in Ref.20, where authors used semimicroscopical approach in level density. The differences more significantly in barrier B can be explained with the different treatments of vibrational enhancement.

The final results of fission cross section calculations are shown in Fig.9,10. Good agreement with the experimental values is achieved. These results prove that the Combined Method is able to make an adequate description of level density in dependence of nuclear deformation for these nuclei.

The use of all available experimental data of fission cross section, allow us to obtain a systematic for fission barrier heights in the frame of explained above theoretical assumptions. The consideration of structural features of nuclei in a more realistic way becomes the obtained semi-microscopical systematic of the barrier more confident than others based in Fermi gas level density form.

TABLE 2: Fission barrier parameter deduced from the statistical analysis.

		^{240}Pu	^{242}Am
Ref.[19]	B_A	5.99	6.61
	$\hbar\omega_A$	1.00	0.60
	B_B	5.22	5.56
	$\hbar\omega_B$	0.70	0.42
Ref.[20]	B_A	5.57	6.50
	$\hbar\omega_A$	1.00	0.65
	B_B	5.07	5.70
	$\hbar\omega_B$	0.60	0.45
Present paper	B_A	5.90	6.60
	$\hbar\omega_A$	0.79	0.65
	B_B	5.55	6.23
	$\hbar\omega_B$	0.60	0.45

V. Conclusions.

Aplying the semimicroscopical Combined Method for level density formalism with an appropriate collective enhancement factor and discrete transition spectra deduced from single particle calculations in deformed nuclei at the transitions states of the double humped barrier, was reproduced the energy-dependence behavior of the fission cross section for ^{239}Pu and ^{241}Am. Good fits were obtained by assuming the first barrier axially-asymmetric and the second one mass asymmetric. Information of the barrier heights was obtained from the analysis.

Acknowledgment.

The authors are grateful to Dr. V.A.Rubchenya of Radium Institute for helpful comments and suggestion.

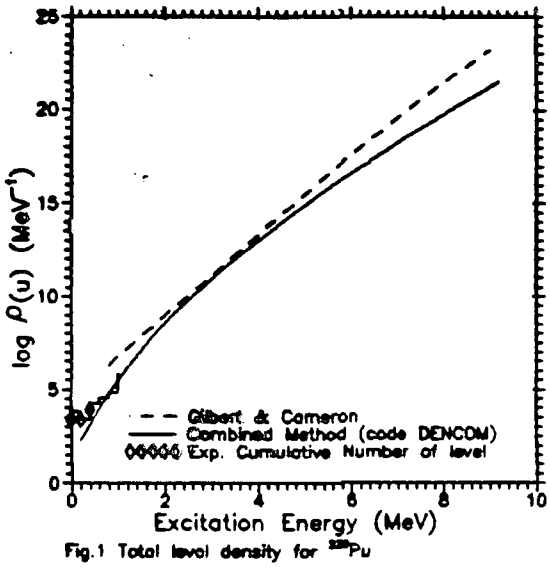

Fig.1 Total level density for ^{239}Pu

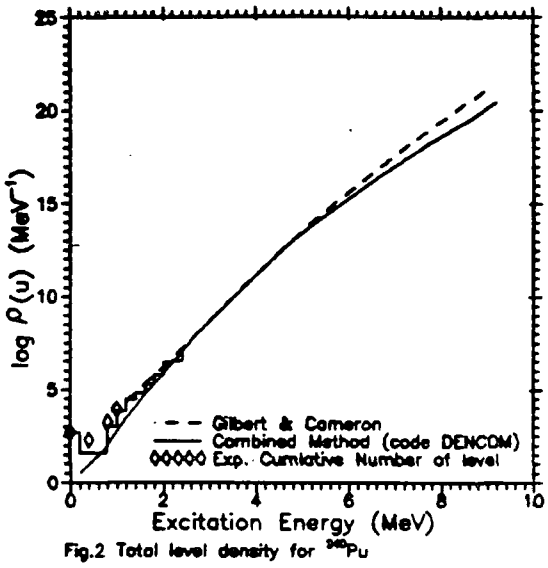

Fig.2 Total level density for ^{240}Pu

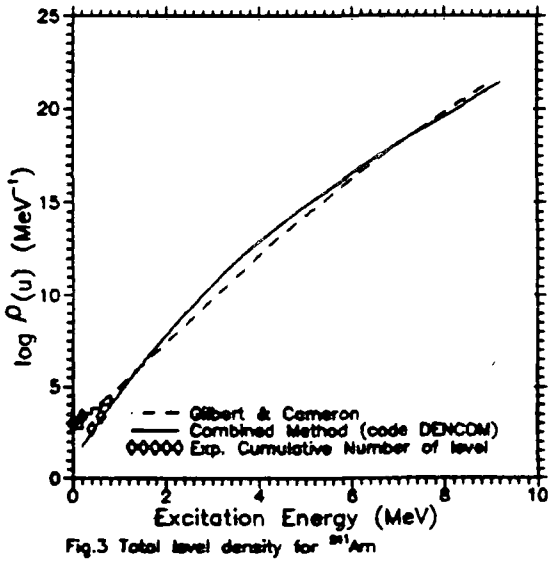

Fig.3 Total level density for ^{241}Am

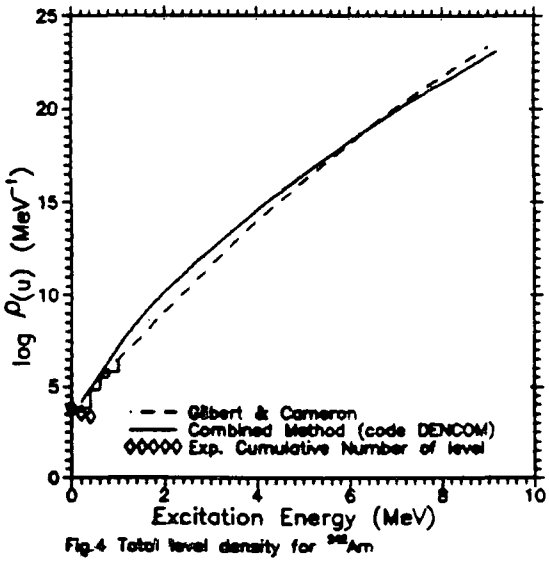

Fig.4 Total level density for ^{242}Am

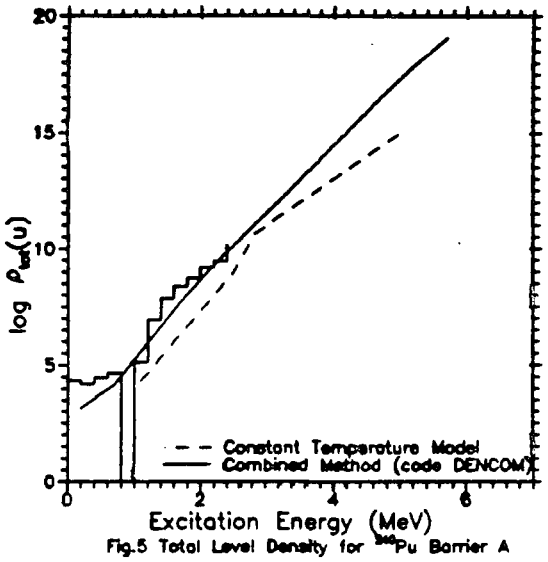

Fig.5 Total Level Density for ^{240}Pu Barrier A

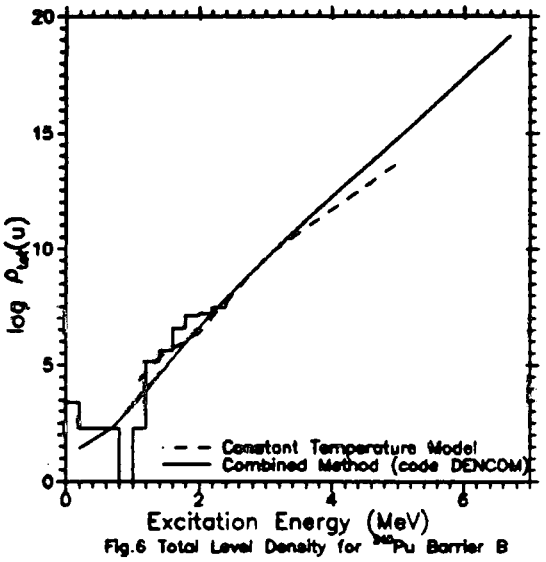

Fig.6 Total Level Density for ^{240}Pu Barrier B

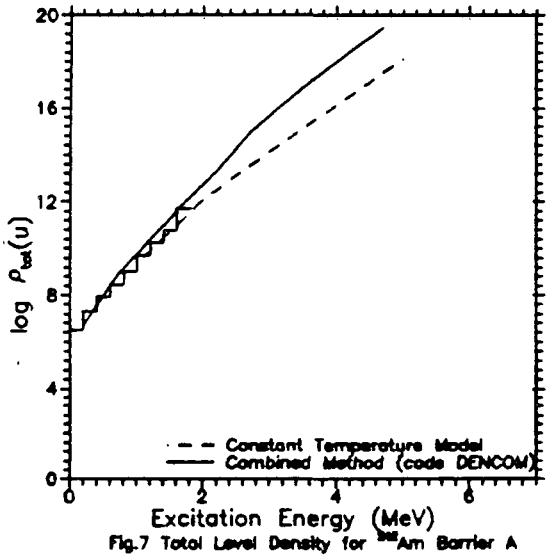

Fig.7 Total Level Density for ^{242}Am Barrier A

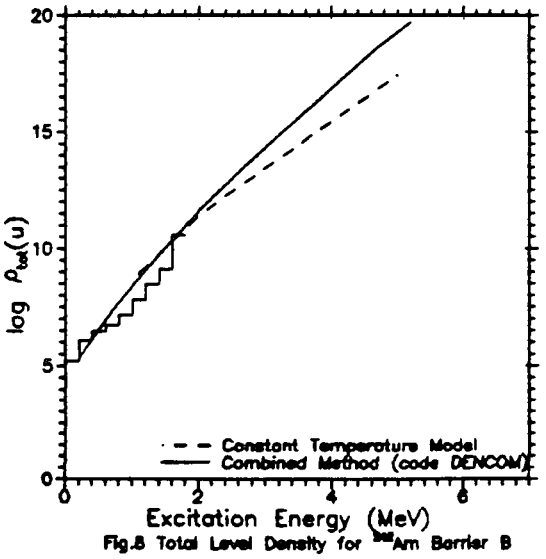

Fig.8 Total Level Density for ^{242}Am Barrier B

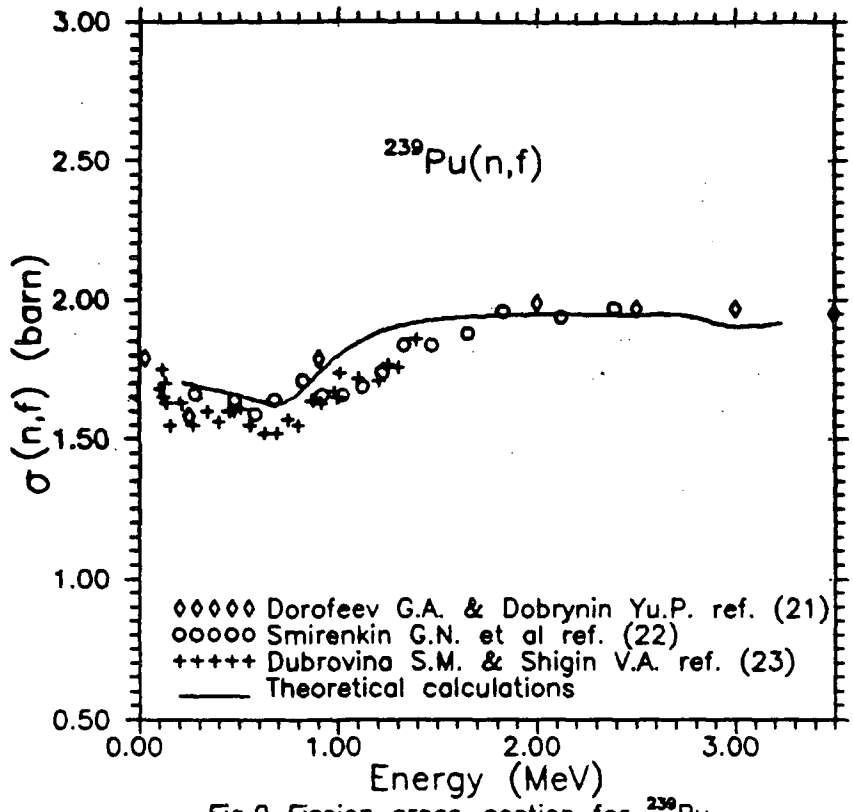

Fig.9 Fission cross-section for ^{239}Pu

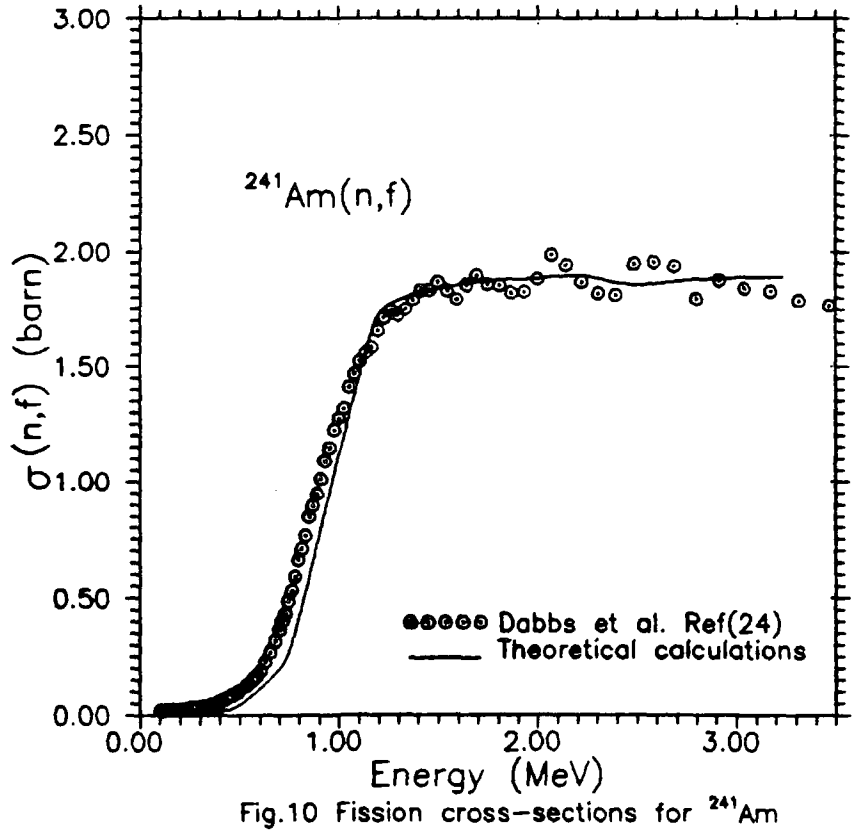

Fig.10 Fission cross-sections for ^{241}Am

References:

[1] P.Decowski, W.Grochulski, A.Marcinkowski, K.Siwek, Z.Wilhelmi, Nuc.Phys. A110 (1968) p.129.

[2] A.V.Ignatyuk, Yu.N.Shulin, Yad.Fiz8 (1968) p.1135.

[3] A.V.Rubchenya, Yad.Fiz 11 (1970) p.1028.

[4] T.Dessing, A.S.Yensen, Nuc.Phys. A223 (1974) p.569.

[5] S.A.Egorov, V.A.Rubchenya, Nuc.Phys. A494 (1989) p.75.

[6] S.A.Egorov, A.V.Rubchenya, Yad.Fiz 49 (1989) p.1580.

[7] S.A.Egorov, A.V.Rubchenya, F.V.Garcia, H.O.Rodriguez, INDC(CUB)-006, March, 1992.

[8] A.V.Ignatyuk in "Statistical properties of excited atomic nuclei INDC(CCP)-233/L (1985).

[9] V.V.Pashkevich, Nuc.Phys A133 ,(1969) p.400.

[10] S.E.Larsson, Proc.Int.Symp.on Phys and Chem.of Fission Rochester,1973 p.177(1974) IAEA.

[11] A.Borh, B.R.Mottelson, "Nuclear Structure, Vol I,p.142 (1969), VolII p.38 (1975).

[12] S.Cwiok, J.Dudek, W.Nazarewicz, J.Skalski, T.Werner. Comp.Phys.Comm. 46(1987) p.379.

[13] V.A.Chepurnov, Journal of Nucl. Phys. T6 N5 (1967).

[14] V.V.Pashkevich, Nuc.Phys A169 ,(1971) p.275.

[15] S.Bjornholm and J.E.Lynn, Rev.Mod.Phys. Vol.52 (1980)

[16] M.Avrigeanu, V.Avrigeanu, G.Cata, M.Ivascu, Rev. Roum. Phys 32 (1987) p.837.

[17] Ch.Lagrange, Intern. Nuclear Model and Code Comparison on Fission Cross-Section Calculations IAEA (1991).

[18] V.M.Strutinsky, Nuc.Phys. A95 (1967) p.420.

[19] Moller P., Nucl.Phys. A192 (1972) p.529.

[20] Ohsawa T., Shigemitsu Y., Ohta M., Kudo K. ,J.Nucl. Sci. Technol. Vol.21 (1984) p.887.

[21] G.A.Dorofeev and Yu.P.Dobrynin, Atomnaja Energija 2 (1983) p.10.

[22] G.N.Smirenkin, B.G.Nesterov, I.I. Bondarenko, Atomnaja Energija 13 (1984) p.366.

[23] S.M.Dubrovina and V.A.Shigin, Atomnaja Energija 6 (1984) p.453.

[24] J.W.T.Dabbs, C.H.Johnson, C.E.Bemis Jr, Nucl.Sci. and Eng.83 (1983) p.22.