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Specifications for an International CODE INTERCOMPARISON FOR FISSION CROSS-SECTION CALCULATIONS

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I INTRODUCTION

The last international comparisons of nuclear models and codes organised by the NEA Data Bank concerned the calculation of the pre-equilibrium effects and the results were published in 1985 and 1989 [1]. It was emphasized in the specifications of the exercise that it is more correct to speak about a model intercomparison rather than a code intercomparison. The same remark applies to the present exercise which is devoted to fission cross section calculations. The models for the fission cross section calculations differ from each other in many aspects. The problem is still more complex if one considers that double, or triple, humped fission barriers should be used for accurate calculations of the fission cross section. Different models are also used for the evaluation of the level densities of the deformed nucleus just before undergoing fission. Consequently the specification of the parameters to be used in the exercise is quite complex; only a basic set of parameters could be defined and the participants in the exercise should adapt their own needs to this basic set.

The aim of the present exercise is to show how accurate could be the calculation of the fission cross section of exotic nuclei for which no experimental data exist. This accuracy could be checked by the calculation of the fission cross sections of the well known nuclei whose fission cross sections are supposed to be known with less than 5% uncertainty. But one should bear in mind that in most of the evaluations the results obtained are more a parametrisation aimed at reproducing the experimental data than the use of model parameters based on strong theoretical evidence, although one should admit that the evaluators start their evaluation with "realistic parameters"; but, at the end, when the calculated data fit the experimental data, the parameters of the model could be far from the "realistic" starting values, and then are no more realistic compared to the current theory.

A systematics for neutron reactions of the actinide nuclei, with emphasis on fission cross section calculations, was performed by E. Lynn and published in 1974 [2]. In the conclusion of his work, E. Lynn admitted that uncertainties of about 25 % could be expected for the calculation of the exotic nuclei fission cross sections, and that by using a consistent basis for level densities and fission barrier densities that he obtained by fitting the well known fission cross sections. It is quite unlikely that the present exercise could result in better evaluation of the accuracy; at least, it will show off the models and codes leading to consistent results, and those which should be disregarded in view of too important discrepancies.

The specification of the parameters will be restricted to the following:

1. Masses, Q values and related parameters;
2. Level scheme data;
3. Neutron transmission coefficients and corresponding optical model parameters;
4. Level density specifications for compound and residual nuclei;
5. Fission barrier specifications and fission barrier density;
6. Gamma ray competition parameters.

The fission cross section should be calculated in the energy range 50 keV to 3 MeV covering the fast reactor spectrum, for at least the following energy points: 50 keV, 500 keV, 1 MeV and 3 MeV. The selected nuclei are ^{239}Pu and ^{241}Am for which accurate fission cross sections exist in the experimental data base. The ^{240}Pu compound nucleus is an even-even nucleus and the ^{242}Am compound nucleus is an odd-odd nucleus. The target nuclei are odd-nuclei. Different treatments could be needed for low energy level density and fission barrier density and should be specified by the participants. The main quantity to be calculated is the fission cross section. Total, shape elastic, direct inelastic and compound nucleus formation cross sections are the direct result of the optical model calculations performed to provide the neutron transmission coefficients. In general, the codes available for fission cross section calculation calculate in the same run the cross sections in the competing channels, i.e. the (n,γ) and the (n,n') in the energy range concerned by the present exercise. These results should also be provided by the participants.

The width fluctuation corrections should be included in the calculations, and if possible details on the method of calculation should be provided by the participant.

II SPECIFICATION OF THE PARAMETERS

II.1 Mass, Q values, neutron binding energies etc..

The following values are found in "American Institute of Physics Handbook", third edition, 1982, reissue[1]:

Isotope	Mass (amu)	B_n(MeV)
^{238}Pu	238.04958	
^{239}Pu	239.05218	5.657
^{240}Pu	240.05384	6.534
^{240}Am	240.055	
^{241}Am	241.05685	6.660
^{242}Am	242.05957	5.535

II.2 Discrete level schemes

They are taken from the most recent Nuclear Data Sheets [12]. The energy levels, spin and parity are given in Table I and Table II for ^{239}Pu and ^{241}Am respectively. If participants need the ^{240}Pu or ^{242}Am levels for auxiliary calculations they may take them from the Nuclear Data Sheets.

Additional levels for ^{239}Pu (not defined in the Nuclear Data Sheets) have been included in Table I in order to obtain a better temperature representation and a better estimation of the competition between the fission and inelastic cross sections; they are marked with an asterisk. The spin and parity of some ^{241}Am levels are not well known, particularly above 1 MeV; Participants should use the levels below 0.5 MeV only and assign the spin and parity for those levels for which these are missing; the continuum should start at 0.4 MeV with the parameters given in Table III and Fig. 2.

II.3 Neutron transmission coefficients

The neutron transmission coefficients are given in Appendix I for ^{239}Pu and Appendix II for ^{241}Am (they will also be supplied on diskette to the participants). They are the results of coupled channel calculations [3]. The direct inelastic components, which may be used as input in some codes could be ignored since they do not affect the calculation of the fission, compound inelastic and capture cross sections. The transmission coefficients supplied **must** be used by participants.

The following deformed optical model parameters for ^{241}Am are taken from Fort [13] and were used in ECIS [14] by Lagrange to calculate the transmission coefficients:

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[1] Although the basic parameters can also be found in the more recent Nuclear Data Tables 19(1988)281, the present values have been kept because the corresponding B_n values were used for the determination of the level density parameters of Table III. This has no importance for the exercise.

$$\begin{array}{lll} V_R & = 47.0 - 0.3\,E & \\ W_D & = 2.7 + 0.4\,E & E < 10\ \mathrm{MeV} \\ & = 6.7 & E > 10\ \mathrm{MeV} \\ V_{so} & = 7.5 & \\ \beta_2 & = 0.22, \quad \beta_4 = 0.036 & \end{array}$$

For ^{239}Pu Lagrange performed a microscopic model calculation and no optical model parameters are available.

TABLE I -^{239}Pu

Energy	Spin	Parity
0.0000	0.5	+
0.0078	1.5	+
0.0573	2.5	+
0.0757	3.5	+
0.1638	4.5	+
0.1940*	5.5	+
0.2855	2.5	+
0.3170*	6.5	+
0.3301	3.5	+
0.3600*	7.5	+
0.3874*	4.5	+
0.3916	3.5	-
0.4350*	4.5	-
0.4620*	5.5	+
0.4698	0.5	-
0.4880*	5.5	-
0.4921	1.5	-
0.5055	2.5	-
0.5118	3.5	+
0.5380*	4.5	+
0.5550	3.5	-
0.5830	4.5	-

TABLE II -^{241}Am

Energy	Spin	Parity	Energy	Spin	Parity
0.0000	2.5	-	0.6702	1.5	+
0.0418	3.5	-	0.6820	2.5	-
0.0936	4.5	-	0.7320		
0.1580	5.5	-	0.8220		
0.2059	2.5	+	0.8840		
0.2340	6.5	-	0.9520	2.5	-
0.2350	3.5	+	0.9820		
0.2390			1.0200		
0.2720	4.5	+	1.0640		
0.2730			1.1060		
0.3200	5.5	+	1.1320		
0.3800	6.5	+	1.1360		
0.4590			1.1630		
0.4718	1.5	-	1.2270		
0.4950			1.5500		
0.5045	2.5				
0.5430					
0.5490	3.5				
0.6231	0.5	+			
0.6369	1.5				
0.6521	0.5				
0.6532	1.5	+			

II.4 Level density parameters for compound and residual nuclei.

The Fermi-gas level density model is widely used at high excitation energy:

$$\rho(E,J,\pi) = \rho(E) \cdot \frac{2J+1}{2\sigma^2} \cdot e^{[-(J+0.5)^2/2\sigma^2]} \tag{I}$$

$$\rho(E) = \frac{1}{12\sqrt{2}} \cdot \frac{1}{\sigma} \cdot \frac{1}{a^{1/4}} \cdot \frac{1}{(E-\Delta)^{5/4}} \cdot e^{2\sqrt{a(E-\Delta)}} \tag{II}$$

At excitation energy equal to the neutron binding energy B_n, the average spacing D_{obs} of the levels excited by s-wave neutrons is known from the neutron resonance analysis. Using, for example, the following relations for the spin cut-off factor σ and for the nucleus temperature:

$$\sigma^2 = 0.0888 aTA^{2/3} \qquad \text{(III)}$$

$$T = (U/a)^{1/2} \quad \text{with} \quad U=E-\Delta \qquad \text{(IV)}$$

or other more sophisticated relations (which should be specified by the participants), the participants should evaluate the parameters a and σ from the values of D_{obs}, pairing energy Δ and neutron binding energy given in Table III. The pairing energies are taken from the values published by Gilbert and Cameron [4]. But other tables of P(N) and P(Z) are available in the literature [5,6].

At low excitation energy the Gilbert and Cameron constant temperature formula is used:

$$\rho(E) = \frac{1}{T_0} \cdot e^{\frac{(E-E_0)}{T_0}} \qquad \text{(V)}$$

The values of T_0 and E_0 which match the Fermi-gas formula and the constant temperature formula at the energy E_c are given in Table III. In the calculations the continuum should start at E_{cont}. E_c and E_{cont} are given in Table III.

TABLE-III
Compound nucleus parameters

Compound Nucleus	^{239}Pu	^{240}Pu	^{241}Am	^{242}Am
D_{obs}(eV)	7.70	2.31	0.372	0.55
Γ_γ(s)(meV)	34.	39.4	65.0	43.8
Γ_γ(p)(meV)	34.	36.8	65.0	85.
P(N)(MeV)		0.43	0.43	
P(Z)(MeV)	0.61	0.61		
Δ(MeV)	0.61	1.04	0.43	
B_n(MeV)	5.657	6.534	6.660	5.535
E_c(MeV)	4.191	4.152	3.825	2.882
T_0 (MeV)	0.4213	0.4054	0.4325	0.3858
E_0(MeV)	-0.9112	-0.1659	-0.9125	-1.0855
E_{cont} (MeV)	0.6	1.2	0.4	0.4

More sophisticated parameters for the constant temperature formula could be obtained from pairing correlation theory [7] and observed low lying band-heads for odd-A, even-even and odd-odd nuclei [2]. Such parameters will not be specified in the present exercise; if used, they should be specified by the participants.

If back-shifted Fermi-gas model of Dilg et al. [8] is used, parameters equivalent to those given in Table III should be specified by the participants.

D_{obs} and Γ_γ are taken from an evaluation performed at Cadarache [11]. Fig. 1 and Fig. 2 show the consistency between the experimetal levels and the level density parameters of Table III (15).

II.5 Fission barrier parameters and level density at saddle point.

The fission transmission coefficient through a single fission barrier is given by the well-known Hill-Wheeler relation:

$$T_f = [1 + e^{-2\pi\frac{E-E_f}{\hbar\omega_f}}]^{-1} \qquad \text{(VI)}$$

E_f and $\hbar\omega$ being the height and the curvature associated to the barrier. The total fission transmission coefficient is usually obtained by the following sum :

$$T_f(E,J) = T_f^{discrete} + T_f^{continuum} \qquad \text{(VII)}$$

with:

$$T_f^{\mathrm{discrete}} = \sum_\nu T\nu_f(E,J,\pi) \qquad \text{(VIII)}$$

and:

$$T_f^{\mathrm{continuum}}(E) = \int_0^\infty \rho_f(E^*-\epsilon,J,\pi) \cdot [1 + e^{(-2\frac{E-E_f-\epsilon}{\hbar\omega_f})}]^{-1} d\epsilon \qquad \text{(IX)}$$

where $E^* = B_n + E\,(A/A+1)$ in the center of mass.

The first term corresponds to the sum over all the ν discrete barrier considered, and the second term corresponds to a continuum of fission barrier of density ρ_f.

At least the following questions have to be answered when performing fission cross section calculation:

1. Is the single fission barrier suitable for fission cross section calculations, or should one use a double humped fission barrier ?
2. What is the most accurate description of the level density at the saddle point for highly deformed nuclei?

Most of the codes use a double humped fission barrier. Two methods are generally used for the calculation of the corresponding transmission coefficients. In the first case, one considers the very crude assumption of uncoupled oscillators for the representation of the 2 barriers, which leads to a total fission transmission coefficient of [2,9]:

$$T_f(E,J,\pi) = \frac{T_a(E,J,\pi)\cdot T_b(E,J,\pi)}{T_a(E,J,\pi)+T_b(E,J,\pi)} \qquad \text{(X)}$$

T_a and T_b being calculated for each barrier set (inner barrier A and outer barrier B) by the equations (VII, VIII and IX). In the second method the Shrödinger equation is solved for the fission motion and the fission barrier transmission is obtained [9]. The deformation potential is represented by three smoothly joined parabolic sections and therefore is characterized by 6 parameters: E_a, E_b, E_{ii}, $\hbar\omega_a, \hbar\omega_b, \hbar\omega_{ii}$ (see reference [9]). This method is needed for intermediate class II structure calculations and for partial damping in the second well (particularly vibrational resonance Δ). In case of complete damping of class I levels into class II levels (at high excitation energy), one can assume that the inner and the outer barrier act independently and a total fission transmission coefficient similar to the equation (X) is obtained.

In the present exercise the participants are requested to use the first method or the equivalent second method in the assumption of complete damping in the second well, since no intermediate structure or vibrational resonance have to be taken into account in the energy range of interest for the nuclei chosen for the exercise. The second question is the formulation of the fission barrier density. The basic formulation is still the constant temperature formula at low energy above the fundamental barrier and the Fermi-gas formula at higher energy. But one must take into account the level density enhancements originating from rotational bands built on single particle levels [10]. The enhancement could be very large for the case of no axial asymmetry, but much smaller for axially symmetric nuclei. Since the two barriers A and B have different symmetry properties at the saddle point, the enhancement factors could be different for the A and B barrier densities. This kind of situation can be easily taken into account in the complete damping assumption where the A and B parameters can be specified separately.

The discrete transition states are usually specified by the head of the associated rotational bands, and automatically generated from the energy E_b of each band-head; or independent values of barrier heights can be provided.

The fission barrier parameters to be used in the present exercise are given in Table IV.

TABLE-IVa ^{242}Am

		Fission channels (Energy above the fundamental) Energy	J^π
Barrier A	$E_f = 6.215$ MeV	0.025	2-
	$\hbar\omega = 0.65$ MeV	0.239	2-
Barrier B	$E_f = 5.604$ MeV	0.000	3-
	$\hbar\omega = 0.45$ MeV	0.193	3-
		0.276	3-
		0.100	4-
		0.231	4-
		0.323	4-

TABLE-IVb ^{240}Pu

Barrier A	$E_f = 5.78$ MeV $\hbar\omega = 0.80$ MeV
Barrier B	$E_f = 5.46$ MeV $\hbar\omega = 0.60$ MeV

Fission Channels (Energy above the fundamental)

Energy (MeV)	J^π	K (Band)	Energy (MeV)	J^π	K (Band)
0.0000	0.0	0^+	0.6000	–1.0	0^-
0.0240	2.0		0.6240	–3.0	
0.0800	4.0		0.6800	–5.0	
0.1680	6.0		0.7680	–7.0	
0.2880	8.0		0.8880	–9.0	
0.4400	10.0				
0.4000	2.0	2^+	0.7000	–1.0	1^-
0.4240	3.0		0.7160	–2.0	
0.4560	4.0		0.7400	–3.0	
0.4960	5.0		0.7720	–4.0	
0.5440	6.0		0.8120	–5.0	
0.6000	7.0		0.8600	–6.0	
0.6640	8.0		0.9160	–7.0	
0.7360	9.0		0.9800	–8.0	
0.8160	10.0		1.0520	–9.0	
			1.1320	–10.0	

The ^{240}Pu fission channels are constructed from ^{240}Pu band heads at the first and second barrier for $K^+ = 0^+$, 2^+. 0^- and 1^- [15]. The fission channel continuum should be used from $E_{cont} = 1.2$ MeV with the following level density parameters (30 levels at $E_x = 1.132$ MeV) [15]:

$D_{obs} = 2.31$ eV
$\Delta = 1.04$ MeV
$a = 27.059$ MeV^{-1}
$E_c = 4.369$ MeV
$E_0 = -0.2993$ MeV
$T_0 = 0.4166$ MeV
$E_{cont} = 1.2$ MeV

similarly to the description of the ^{240}Pu level density (constant temperature formula and Fermi-gas formula).

For ^{242}Am fission channels, only 8 discrete fission channels are given [11]. Participants are requested to propose their own interpretation of the fission channel continuum to be used. One of these interpretations will be selected in the first results of the exercise and proposed to the participants in a second step of the exercise.

III CONCLUSION

The author of the present specifications realizes the difficulties of establishing a basic set of parameters which could be used for the various cross section calculation codes available for the evaluators. The present set is based on ^{239}Pu parameters supplied by Young [15], and ^{241}Am evaluation performed at Cadarache by using FISINGA [11] where some of the parameters have been taken directly from Reference [2], particularly the fission barrier densities. It is expected that the present parameters should produce fission cross sections not too far from the current evaluated data but will not exactly reproduce experiment or evaluations. The purpose of this exercise is to compare codes and models and not to compare with experiment.

If difficulties in understanding or using the specified parameters are encountered, or if errors are found, participants should contact P. Nagel at the NEA Data Bank.

IV ACKNOWLEDGEMENTS

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V REFERENCES

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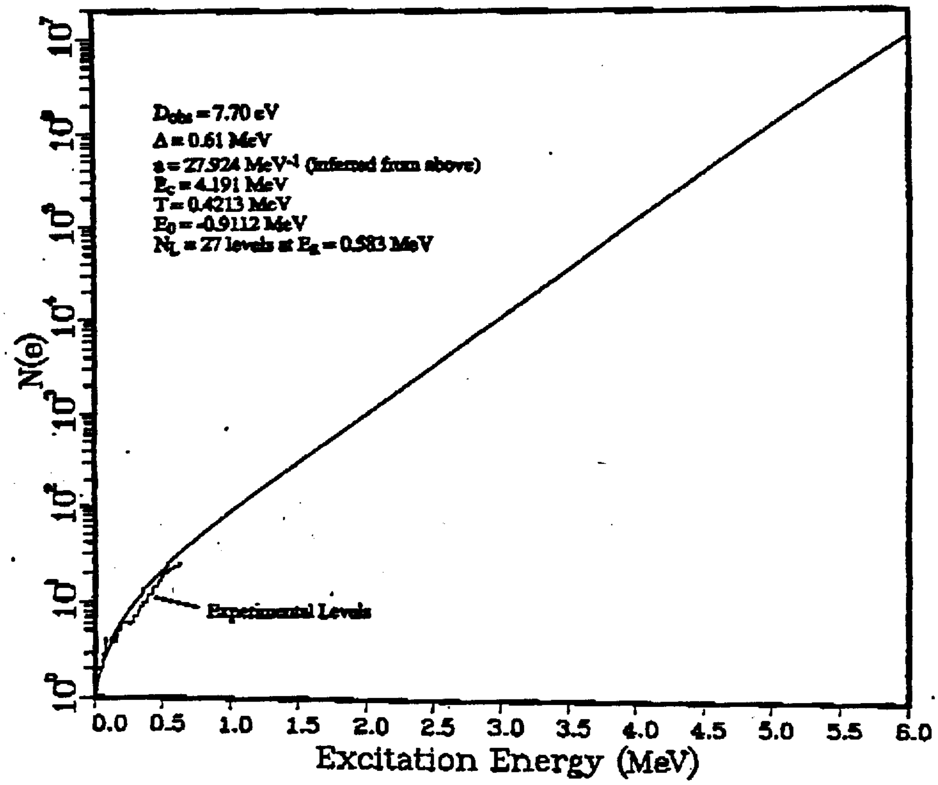
Fig. 1

^{239}Pu Levels



^{240}Pu Levels

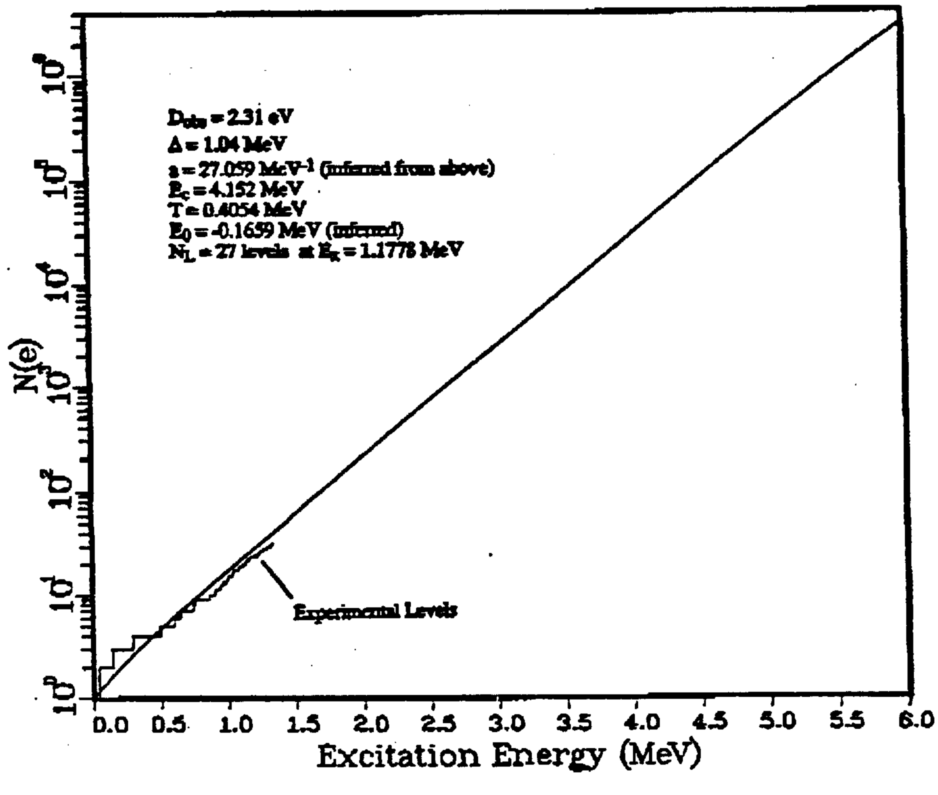
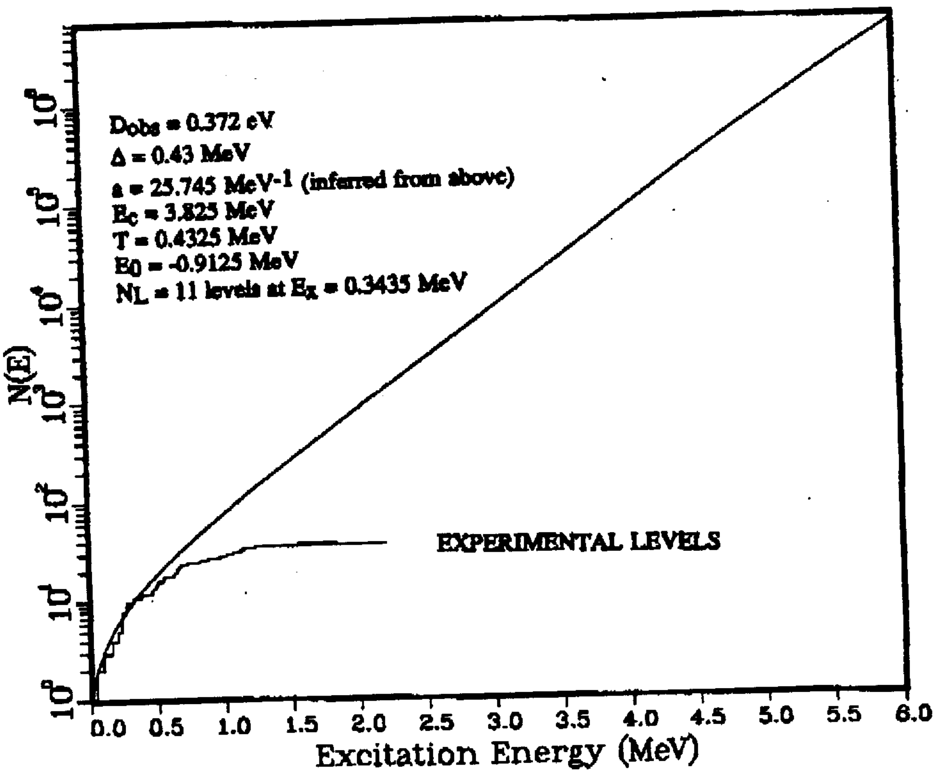
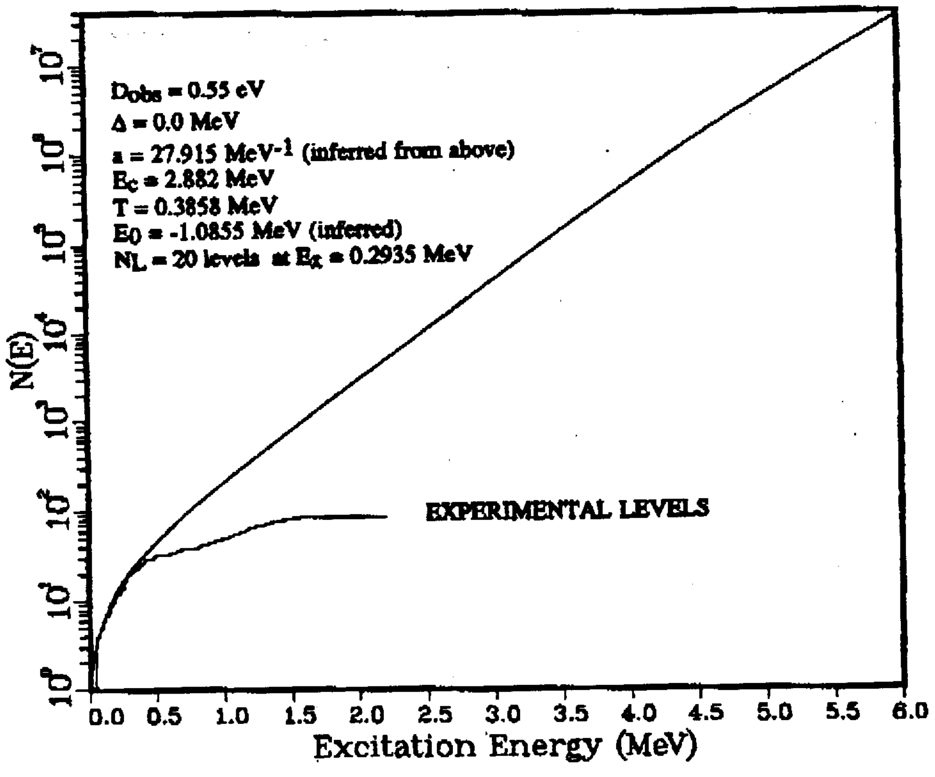


Fig. 2



^{241}Am Levels



^{242}Am Levels