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CROSS SECTION EVALUATION OF THE TRANSACTINIDES HAVING ODD MASS NUMBERS IN THERMAL AND RESONANCE ENERGY RANGES

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Abstract

A generalized non-uniform "picket-fence" model (GNM) to compute the truncated level contributions to the neutron cross-sections in the thermal and resolved resonance-energy regions is proposed; the truncated levels are the unresolved resonances and the bound levels. This model is applied for 18 transactinium nuclides having odd mass numbers.

Cross Section Evaluation of the Transactinides Having Odd Mass Numbers in Thermal and Resonance Energy Ranges

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1. Introduction

The physics design of fission reactors requires the largest needs for accurate nuclear data, particularly neutron cross sections /1/.

In this work, a generalized nonuniform "picket-fence" model (GNM) to compute the truncated level contributions to the neutron cross sections in the thermal and resolved resonance energy regions is proposed.

The truncated levels are the unresolved resonances and the bound levels, that is the levels outside the resolved resonance region.

This model represents a development of the nonuniform picket-fence model for even-even actinides, elaborated by Vasiliu in 1984 /2/, which in its turn is based on a uniform model developed by Olsen, de Saussure, Perez at ORNL in 1973-79 /3/ and successfully applied for ^{238}U.

The generalized model (GNM) is applied in this paper for 18 transactinium nuclides having odd mass numbers.

The transactinium isotopes have been chosen due to their great importance both for thermal and fast reactor design, and for the fuel cycle problems / 4- 5/.

2. The Resonance Nuclear Data in the ENDF/B Library

The evaluated neutron nuclear data are stored on magnetic tapes in different formats for different libraries /6/.

Generally, the cross sections have a pointwise reprezentation in the thermal and fast neutron energy ranges, and a parametric one in the resonance region.

To provide evaluated cross section data from the library for various neutron multigroup and cell calculations in the resonance region, the single or multilevel Breit-Wigner, Adler-Adler, Reich-Moore, Lane-Lynn formalisms and statistical model, /7/, /8/, are used, taking into account the background corrections. These corrections are stored into the library to compensate the differences between the cross sections computed from the resonance parameters and the "evaluated" (recommended) cross sections.

In the resonance energy range, the cross sections are calculated both from resolved resonance (RR) parameters and from average parameters of the unresolved resonance (UR), without taking into account the resonance "tails" from a region to the cross section from another region.

The truncated resonance contributions have been considered negligible for long time. The resolved resonance tails have a small contribution to the lower reference energies of the unresolved region, but the unresolved resonance tails have a significant influence on the cross section in the RR region.

Some attempts to estimate these contributions /9/, /10/, /11/ have been considered unsuitable for practical purposes.

The main hypothesis of the uniform picket-fence model (UM) are given in /12-14/ and the specific features of the non-uniform picket-fence model for even-even actinides (NM) are mentioned in /2/.

3. The Generalized Nonuniform Model (GNM)

In this work, the nonuniform model for even-even actinides was generalized becoming suitable for any type of nucleus (with any value for the spin of target, taking into account the distribution of the resonances in accordance with the orbital angular momentum $\bar{\ell}$ and with the total angular momentum $\bar{J}$, as well as with the corresponding resonance parameters ("s" or "p" waves). Using the average parameters for unresolved resonances, evaluated from resolved resonance parameters /16/, the truncated level contributions to the total, elastic, radiative capture and fission cross sections have been calculated for the thermal and resolved resonance energy ranges.

The level density is given by Fermi's formula. For given "ℓ" and "j", the numbers of the truncated levels for outside region of the RR resonances, up to a limit energy E_L, are the followings:

$$N_{1,2} = \mathrm{INT}\left[\frac{e^{\frac{\sqrt{a_j U_o}-2}{U_o}\cdot 10^6(\mp E_L - E_o)}}{\frac{\sqrt{a_j U_o}-2}{U_o}\langle D(\ell,j)\rangle \cdot 10^{-6}} - 1\right] + 1 \qquad (1)$$

where: E_L-E_o and $-E_L-E_o$ are the right and left energy regions of the RR, where the truncated levels are considered; a_j is the level density parameter; $U_o = S_n - P$ with S_n the binding energy of the neutron in the compound nucleus and P is the pairing energy for the compound nucleus (= P(Z) + P(N)); E_o is the energy of the first resonance or energy of the bound level (negative resonance).

The truncated resonance energies are calculated by (2):

$$E_I = E_o + \frac{1}{\frac{\sqrt{a_j U_o} - 2}{U_o} \cdot 10^6} \ln\left[1 + \frac{\sqrt{a_j U_o} - 2}{U_o} \langle D(\ell,j)\rangle \cdot 10^6 (I-1)\right] \quad (2)$$

The equation (2) is valid for given "ℓ" and "j". The distance between two successive truncated levels, I and I+1, is obtained by a recurrence equation:

$$D_{I+1} = E_{I+1} - E_I = \frac{1}{\frac{\sqrt{a_j U_o} - 2}{U_o}} \ln \frac{1 + \frac{\sqrt{a_j U_o} - 2}{U_o} \langle D(\ell,j)\rangle \cdot I}{1 + \frac{\sqrt{a_j U_o} - 2}{U_o} \langle D(\ell,j)\rangle (I-1)} \quad (3)$$

The calculation of the contribution of the truncated resonance having an E_i energy to the total cross section at the reference energy E, is based on the Breit-Wigner single-level formalism (the level-level interference in the framework of the Breit-Wigner-multi-level formalism is negligible, the distance between E and E_i being quite large):

$$\sigma^{i\infty}_{tot} = \frac{4\pi}{k^2}[A^{\infty}_i \cos(2kR) - B^{\infty}_i \sin(2kR)] \quad (4)$$

where R is the effective scattering radius.

Having $kR \ll 1$, $\cos(2kR) \sim 1$ and $\sin(2kR) \approx 2kR$ were approximated.

Denoting:

$$A_i^{\infty} = \frac{1}{4}\,\frac{\Gamma_n^i\Gamma^i}{(E_i-E)^2+(\Gamma^i/2)^2}$$

$$B_i^{\infty} = \frac{1}{2}\,\frac{\Gamma_n^i(E_i-E)}{(E_i-E)^2+(\Gamma^i/2)^2} \qquad (5)$$

and neglecting $(\Gamma^i/2)^2$ which is very small in relation to $(E_i-E)^2$, the contribution of the N^+ levels from ΔE interval above the RR region and of the N^- levels below this region, will be:

$$\sigma_{tot}^{\infty}(E,\Delta E) = \sum_{\ell}\sum_{j} g_j \sum_{i=N^-}^{N^+} \sigma_{tot}^{i\infty} \qquad (6)$$

The widths of the truncated resonances are considered those of the unresolved resonances.

If the average widths are dependent on energy, the width of the level having energy E_i, is obtained by interpolation.

For the elastic cross section, the contribution of the I-th level with energy E_i, will be given by a general recurrence equation:

$$\sigma_{el,I}^{\infty}(E) = \sigma_{el,I-1}^{\infty}(E) + \frac{\pi}{k_o^2}\,\frac{\langle\Gamma_n^o(\ell,j)\rangle^2}{(E_I-E)^2} - \frac{4\pi R}{k_o}\,\frac{\langle\Gamma_n^o(\ell,j)\rangle}{(E_I-E)} \qquad (7)$$

where $k_o = k/\sqrt{E}$, $k_o = 2{,}19677\cdot 10^9\,\frac{A}{A+1}$, A being the mass of the nucleus divided by the neutron mass.

For the capture and fission cross sections, the general equation which gives the contribution of the I-th level at a reference energy E is:

$$\sigma^{\infty}_{x,I}(E) = \sigma^{\infty}_{x,I-1}(E) + \frac{\pi}{k_o^2} \frac{<\Gamma^o_n(\ell,j)><\Gamma x(\ell,j)>}{\sqrt{E}(E_I-E)^2} \qquad (8)$$

where $<\Gamma x(l,j)>$ is the average radiative capture or fission width.

The contribution of the I-th truncated level to the total cross section at a reference energy E, is obtained by adding all these previous contributions:

$$\sigma^{\infty}_{tot,I}(E) = \sigma^{\infty}_{tot,\ I-1}(E) + \frac{\pi}{k_o^2} \frac{<\Gamma^o_n(\ell,j)><\Gamma(\ell,j)>}{\sqrt{E}(E_I-E)^2} -$$

$$- \frac{4\pi R}{k_o} \frac{<\Gamma^o_n(\ell,j)>}{(E_I-E)} \qquad (9)$$

It can be seen that, for the capture and fission cross sections, the corrections decrease rapidly with E_I, and have a small dependence on the number of truncated levels.

For the elastic cross sections, the correction is diminished by increasing the number of truncated levels.

The contribution of the resolved resonance to the thermal cross sections will be calculated by the Breit-Wigner Single-Level approximation, at the limits of the RR region - by the Breit-Wigner multi-level approximation.

The level density parameter will be computed using Lynn's and Gilbert-Cameron's formalisms.

A threshold energy of the generalized model was established, generally being the threshold energy of the inelastic process /16/.

4. Truncation Contributions to the Cross Sections of Transactinides Having Odd Mass Numbers

In this chapter, the obtained results using the generalized nonuniform model and comparatively, the uniform model, for 18 transactinides having odd mass numbers are presented.

For this purpose, the programs REZIN, CORA and PARAM have been written.

Due to the very small distances between the levels for these actinides, as compared with even-even actinides, the number of the truncated resonances is about 2x(15000 ÷ 20000) for a nucleus. In order to reduce the computing time, all truncated levels were considered as "s" waves only.

4.1. Dependence of the Truncation Correction on the Total Angular Momentum j

The results obtained by GNM for the fission of ^{231}Pa are presented in Fig. 1.

For all cross section types, the truncation correction component corresponding to j=1 is less than that for j=2, the total correction being a sum of these two components.

Excepting the elastic scattering, the correction has a 1/E type dependence up to about 13 eV where it has a minimum, then begins again to increase.

For the elastic scattering, the correction is constant up to ~ 0.0253 eV, then diminishes having even negative values.

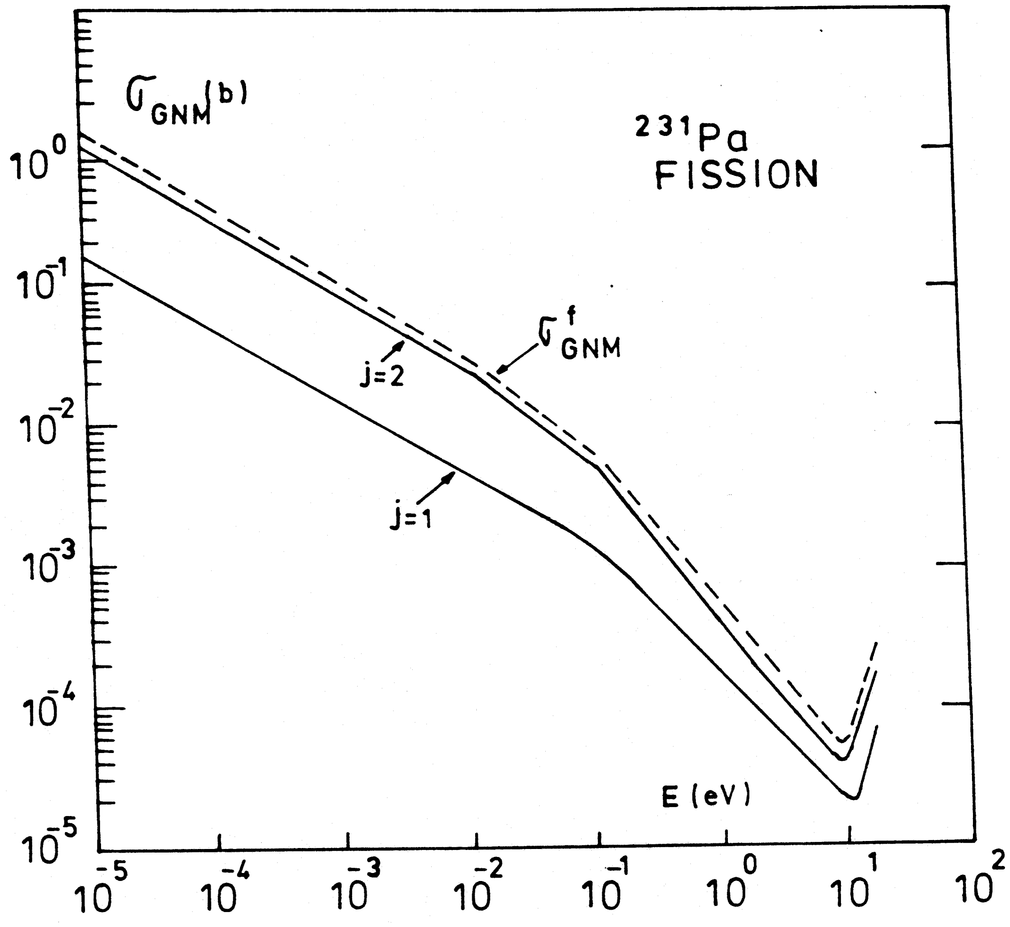

Fig.1.The dependence on J of the truncation correction for the fission of ^{231}Pa.

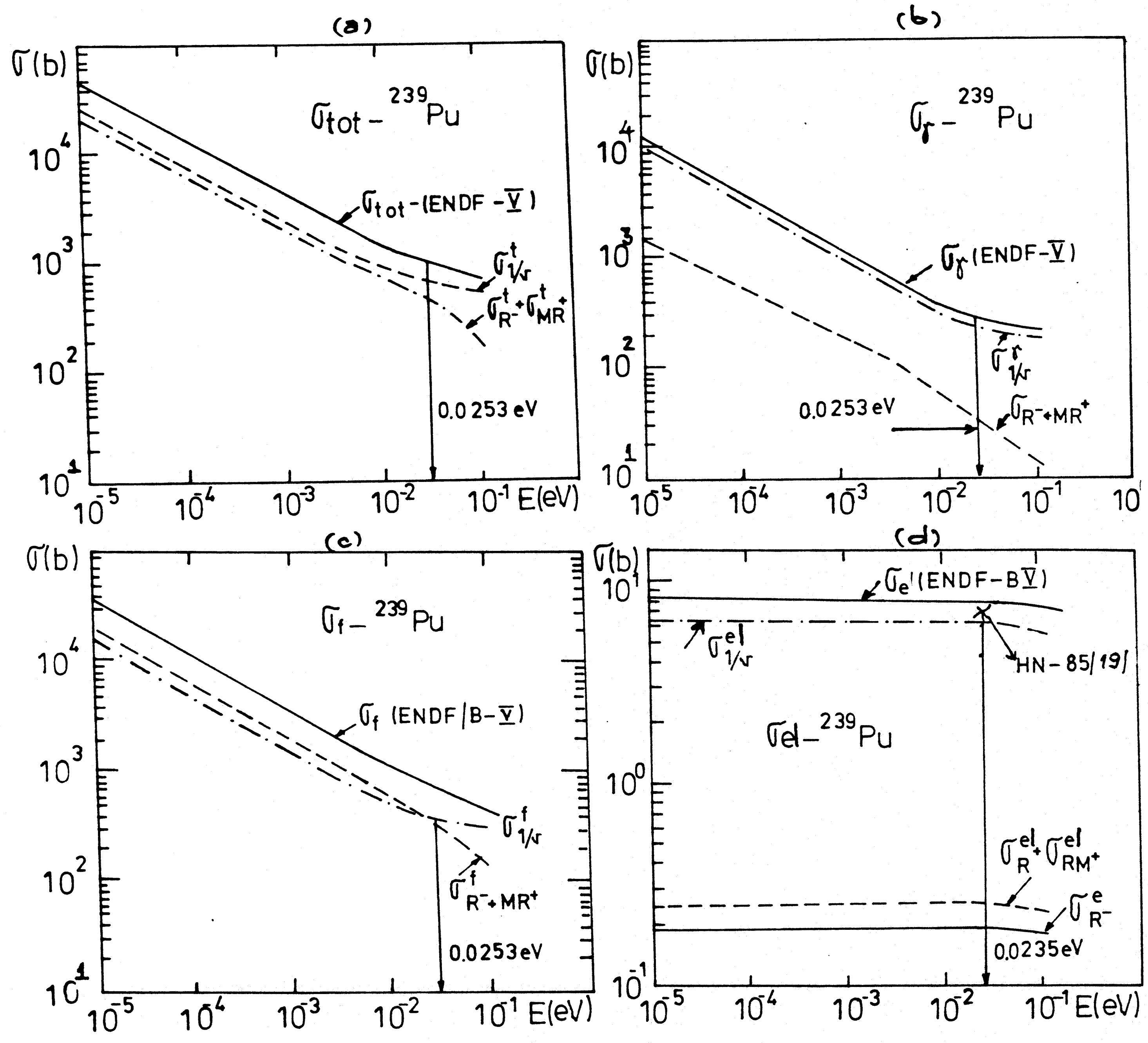

Fig.2.The contributions of the resolved resonances and the marginal resonances for total (a),radiative capture(b), fission (c), and elastic (d) cross sections.

4.2. Cross Section Analysis in Thermal Energy Range

4.2.1. The Resolved and the Contribution of the Marginal Resonances

The resolved resonance contributions to the cross section are of the 1/v type, and have been calculated by the CORA program. The contributions of the negative ($\sigma^{x}_{R}-$) and positive ($\sigma^{x}_{RM}+$) marginal resonances were computed by program REZIN.

In Fig. 2 these contributions to the total, radiative capture, fission and elastic scattering cross sections are shown for ^{239}Pu at thermal energies, between 10^{-5} eV and 0.1 eV. The evaluated cross sections from the ENDF/B library /18/ are also represented.

It should be noticed that there is a good agreement between calculated cross sections as a sum: $\sigma^{x}_{1/v} + \sigma^{x}_{R}- + \sigma^{x}_{RM}+$ and the evaluated cross sections from the ENDF/B-V library.

For thermal neutron elastic scattering on ^{239}Pu, the differences are ~ 10%.

At 0,025 eV, the calculated cross section is in good agreement with the experimental value in the reference /19/ within the limits of the experimental errors.

It is also to be mentioned that the potential elastic cross section is included in the resolved resonance contribution ($\sigma^{e}_{1/v}$).

It is only for elastic scattering, that the contribution of the positive resonances is significant, but the elastic cross section has small values comparatively with the total cross section.

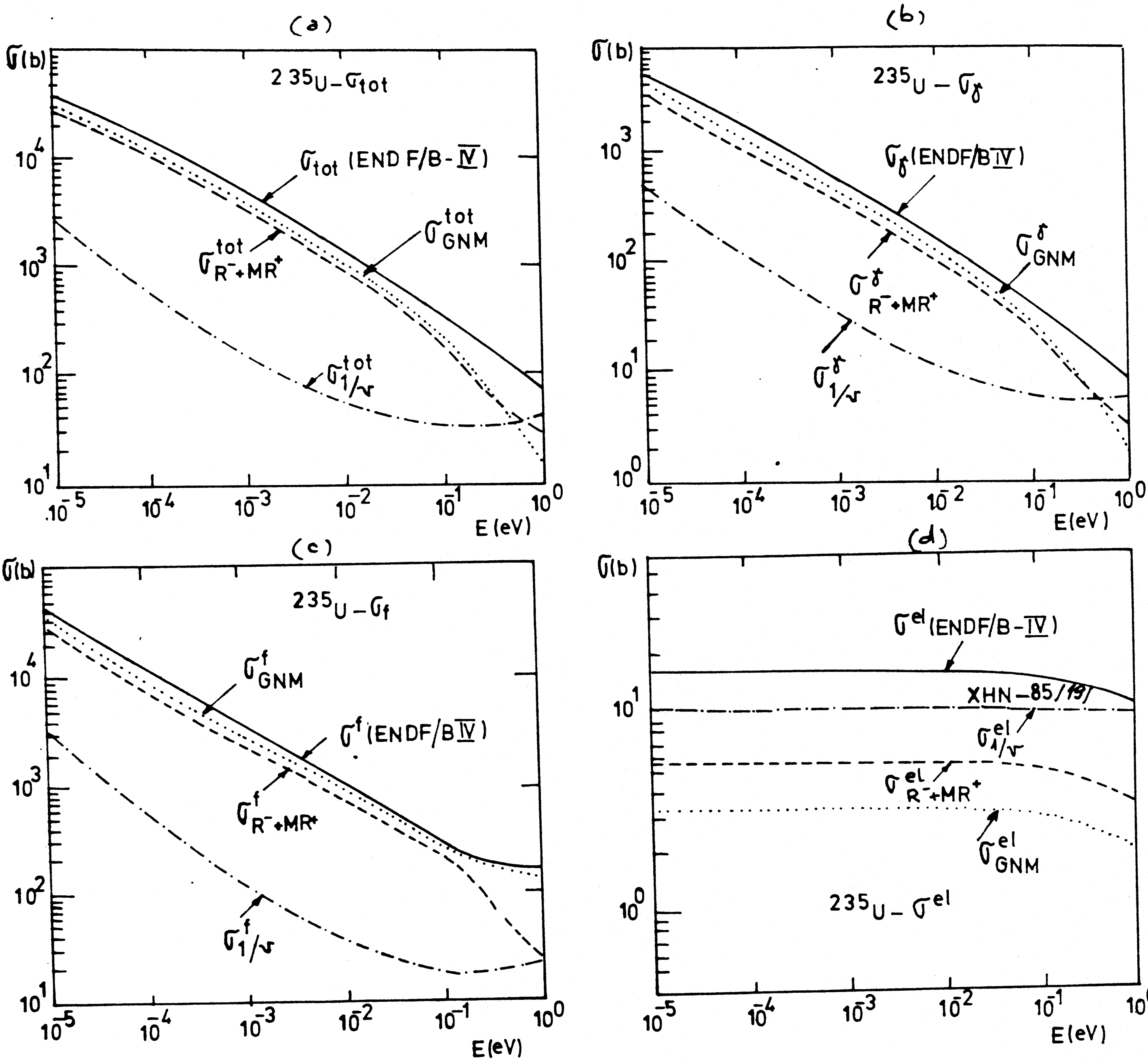

Fig.3. The truncation corrections for the cross sections of ^{235}U : (a) total; (b) radiative capture; (c) fission; (d) elastic.

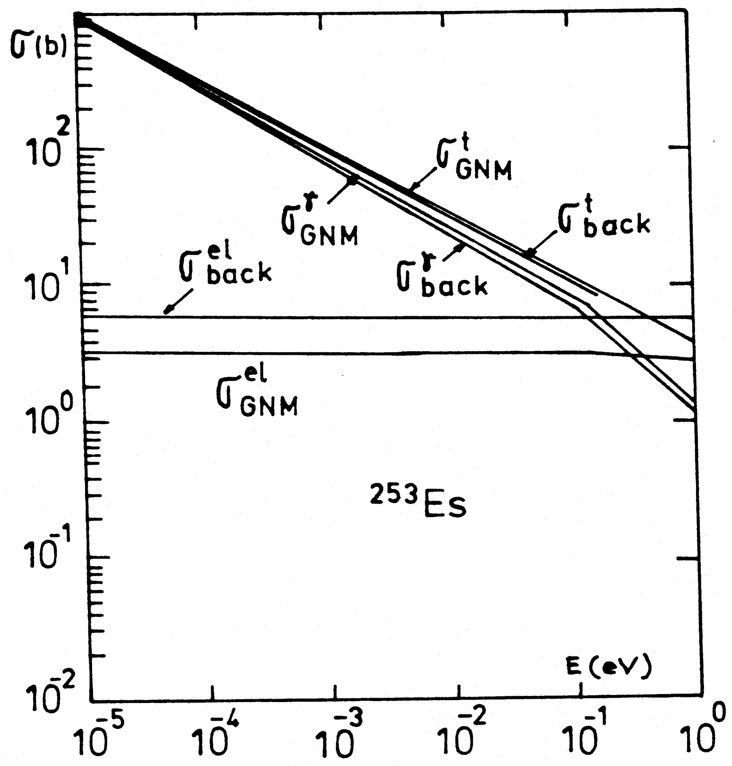

Fig.4.The truncation compensations for thermal cross sections of ^{253}Es computed by GNM and the background corrections.

4.2.2. **Truncation Corrections to Thermal Cross Sections**

In Fig. 3 the truncation corrections σ^x_{GNM} calculated by the generalized model for ^{235}U on thermal energy range, as well as the $\sigma^x_{1/v}$ contributions, the compensations due to the marginal resonances, $\sigma^x_{R^-} + \sigma^x_{RM^+}$, together with evaluated cross sections from the ENDF/B-IV library /17/ are shown.

A good agreement between the evaluated and calculated cross sections (sum of $\sigma^x_{1/v}$ and σ^x_{GNM}) for total, capture and fission cross sections is observed.

The difference for scattered thermal neutron on ^{235}U is ~ 10 per cent as compared with the ENDF/B-IV data. At 0,0253 eV, the calculated elastic cross section is in good agreement with the value given in /19/.

Generally, the truncation compensations and the negative resonance contributions are approximately the same.

The σ^x_{GNM} and background corrections σ^x_{back} for ^{253}Es are presented in Fig. 4.

A good agreement is observed, except for the elastic scattering (where the difference can be explained by the small values of the neutron widths computed on the basis of the strength function, S_o, having an average value of 1.2×10^{-4}, recommended for nuclei in this mass range).

It is to be mentioned that in the ENDF/B-V library, there is no other negative resonance for ^{253}Es.

A first conclusion is that in the thermal energy range the truncation compensations computed by the generalized model are approximately equal either with the marginal resonance contributions (mainly the negative resonances, because the positive ones have an unsignificant contribution in this range) or with the background corrections.

This was an expected result because the parameters of the negative resonances are chosen so as to fit the thermal cross section.

The compensation due to the negative resonances decreases rapidly in the neighbourhood of the RR region comparatively with the truncation compensation which includes the long distance effects.

This suggests that the evaluation of the negative resonance parameters must follow after the correction of the cross sections due to the truncated levels.

The uniform model does not provide good results in the thermal range, which is one of its limits suggested by the authors.

A detailed analysis of the cross sections at 0,0253 eV taking into account the truncation effects is given in /16/.

4.3. The Cross Sections in the Resolved Resonance Region (RR)

The total cross section for ^{233}U was estimated in the RR region by the Breit-Wigner single level (BWSL) and Adler-Adler (AA) formalisms, using programs RESEND /21/ and ADLER /22/, based on resolved resonance parameters from the ENDF/B library.

The results have been compared with Moore's /23/ experimental data. The truncation correction was computed by program REZIN.

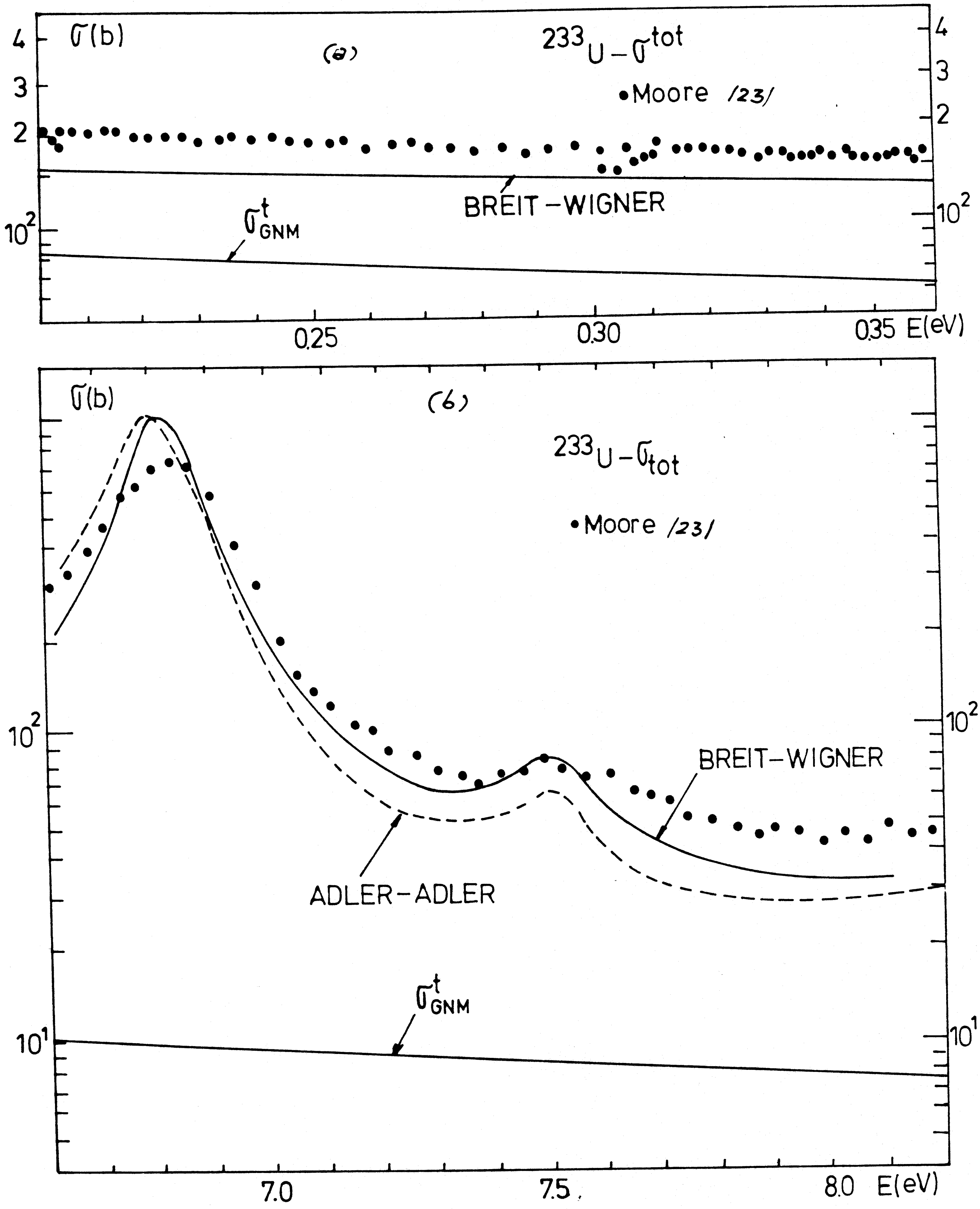

Fig.5. The total cross section of ^{233}U between 0.2 and 0.35 eV (a), and 6.6 and 8.2 eV (b).

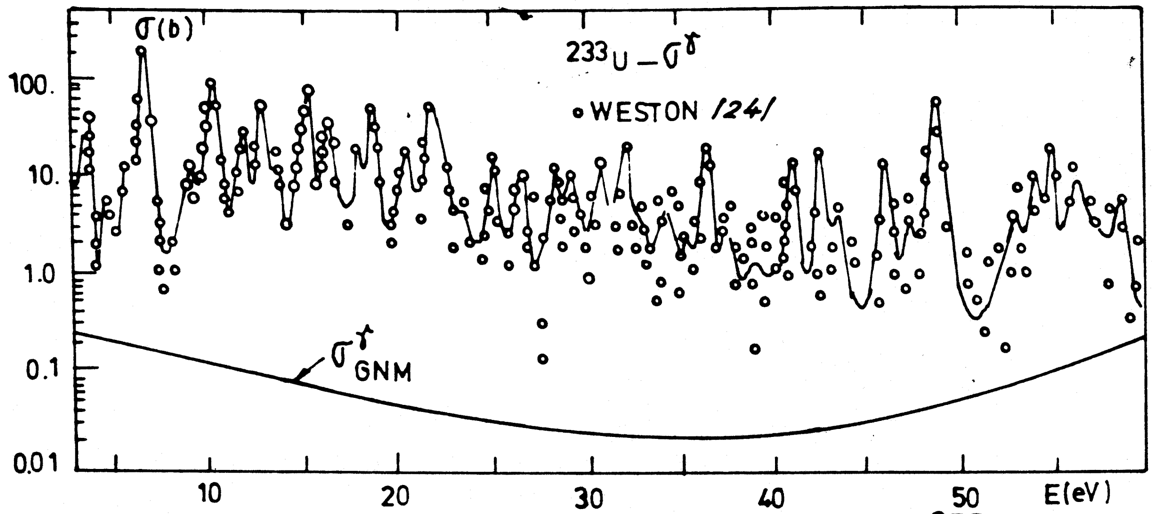

Fig.6.The radiative capture cross section of ^{233}U on energy range 3 - 60 eV.

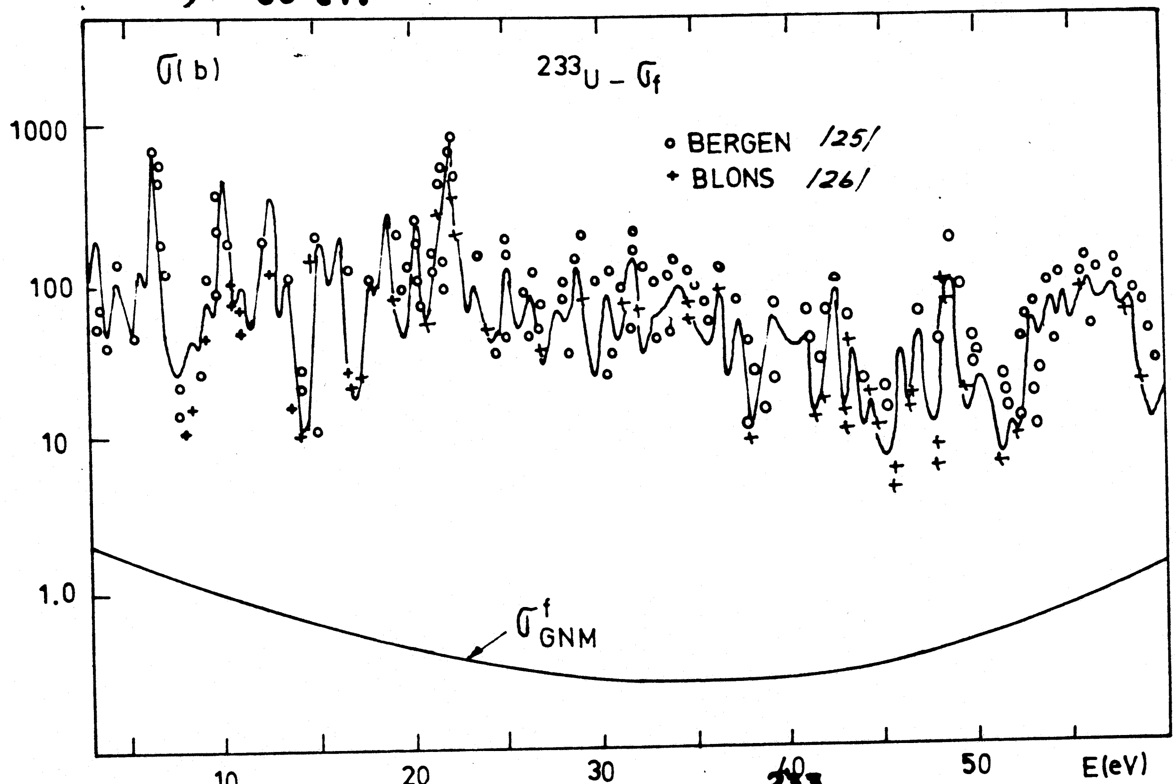

Fig.7. The fission cross section of ^{233}U between 3 and 60 eV and the truncation correction.

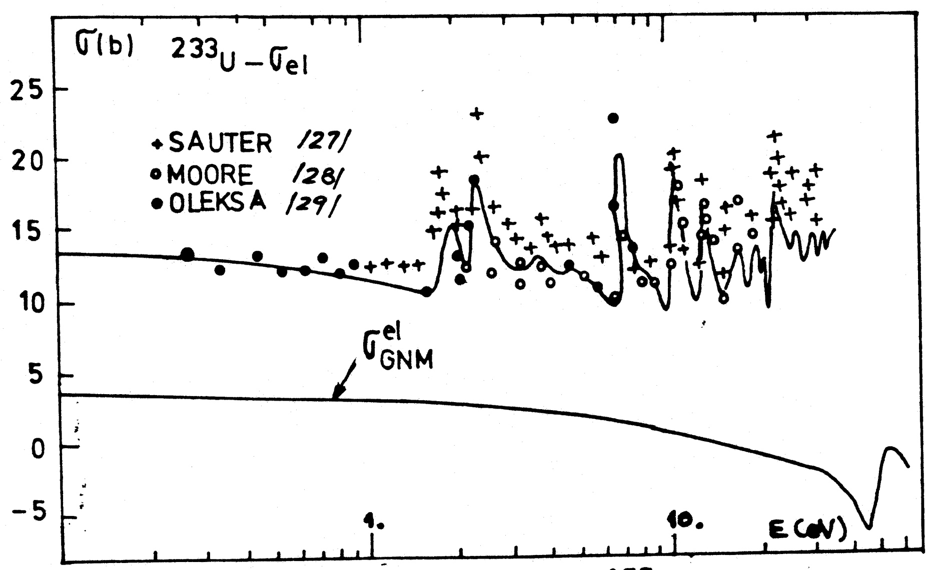

Fig.8.The elastic cross section of ^{233}U between 0.1 and 60 eV.

Up to ~ 10 eV (fig. 5), the σ^{x}_{GNM} is about 40 per cent of the cross section and added to the computed cross section (BWSL or AA), gives a good agreement with experimental data.

In the range 10-38 eV, σ^{x}_{GNM} decreases very much, giving an improvement of the cross section especially in the valleys between resonances.

Above 38 eV (up to ~ 60 eV), σ^{x}_{GNM} has negative values.

In Fig. 6 the experimental capture cross sections obtained by Weston /24/ the truncation correction σ^{x}_{GNM}, as well as a linear fit to the experimental cross section are presented; σ^{x}_{GNM} decreases with the energy, having a minimum at about 35 eV.

The results obtained for the fission of ^{233}U, the Bergen's /25/ and Blons's /26/ experimental data, as well as a linear fit, are shown in Fig. 7. For elastic scattering, Sauter's /27/, Moore's /28/ and Oleska's /29/ experimental cross sections are shown in Fig. 8.

Above 30 eV, σ^{el}_{GNM} has negative values.

4.4. The Dependence of the Truncation Correction on Energy and Z Number

In Fig. 9 the estimation of the truncation contributions for radiative capture cross sections computed by the generalized nonuniform model are shown, for these 18 transactinides having odd mass numbers, as functions of energy and the Z number, on the 10^{-5} eV - 10^{2} eV region.

Excepting elastic scattering, the corrections have a

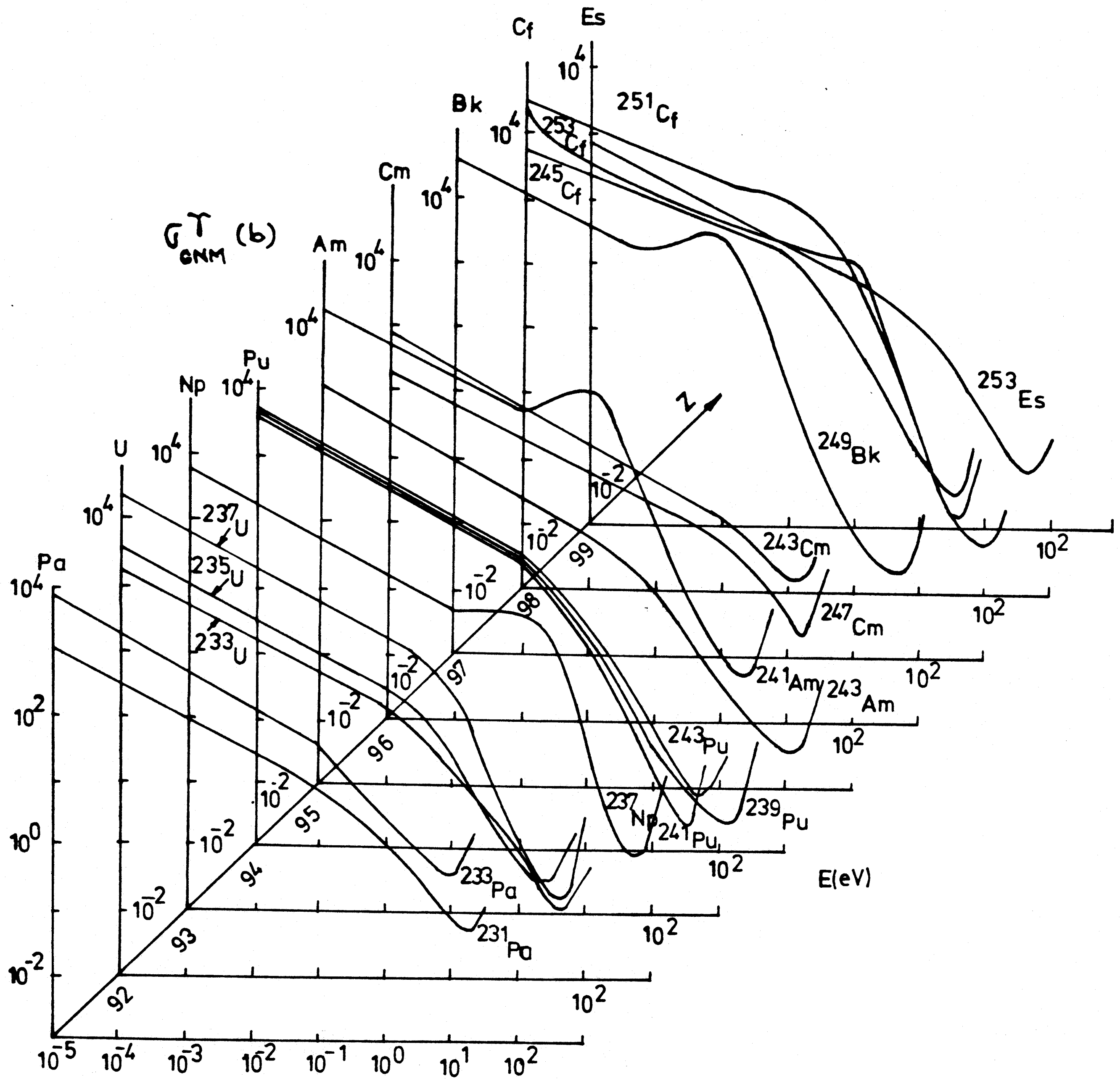

Fig.9.The truncation corrections of the radiative capture cross sections depending on energy and on atomic number Z for transactinides having odd mass numbers,

1/E type dependence in the thermal region, a minimum in the resolved resonance range and then begin again to increase. For elastic scattering, σ^{x}_{GNM} are constants on thermal range and then decrease.

5. Conclusions

The generalized model proposed in this paper can be used for any nucleus (for different values of the spin), on thermal and resolved resonance regions. The model computes the correction of the truncated levels (which can be "s" and "p" waves) to the total, elastic, radiative capture and fission cross sections.

The obtained results are generally satisfactory and these truncation corrections can be stored as "background" data in the ENDF/B files on thermal and resolved resonance regions and the generalized picket-fence nonuniform model gives a physical meaning to this "background".

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