EMPIRICAL SYSTEMATICS FOR SELECTION OF THRESHOLD REACTION EXCITATION FUNCTIONS.

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Abstract

This report is devoted to empirical excitation functions systematics of threshold reactions (n,p), (n,α), (n,2n) and (n,3n). The shapes and maximum cross sections of excitation functions were analysed as functions of neutron excess (N-Z) and mass number A. Some systematical trends are shown for the fission and (n,2n) cross sections of fissile isotopes.

Introduction

At the present time in the world there are several national and international evaluated data libraries of general purpose and some specialised libraries. The data of these libraries are evaluated mainly on the basis of theoretical calculations and essentially discrepant very often. In this connection the problem appears to select more reliable evaluated data.

To solve the problem different systematics are developed on the basis of available experimental data and using in some cases nuclear reaction theory models as well. There are many systematics of neutron cross sections in the incident neutron energy of 14-15 MeV. These systematics play important role in nuclear data evaluation, however their predictions does not solve the problem of data discrepancies in the energy range above 15 MeV, particular for reactions with high energy thresholds. Usually the value (N-Z)/A is used as a parameter in those systematics.

However, some works were made to analyse shapes of excitation functions and cross sections at its maxim. The important results have been obtained by H.Vonach et al in the work /1/ for (n,2n) reaction. The similarity of (n,2n) excitation function shapes for heavy nuclei (A>100) was shown and universal excitation function and systematics of the peak cross sections were proposed. In the works /2,3/ Yu.Trofimov proposed relations for evaluation of (n,p) reaction cross sections at the maximum of the excitation functions and for determination of the neutron energy corresponding to the maxim.

Independently in the works /4-7/ the systematics were developed on the basis of comparison of excitation functions by shapes and cross sections in particular points of excitation functions (in maximum for threshold reactions and in maximum and minima for fission reactions).

The following values were considered as parameters of nuclear reaction excitation functions: reaction threshold, difference of thresholds of the main and competing reactions (for example, (n,p) and (n,np)), cross section at the maximum of excitation function and position of the maximum on neutron energy scale.

The systematics mentioned above are empirical generalisation and to some extent are hypothesis needed in further investigation from point of view of limits their applicability and dependence on the leading parameters.

In the present paper some systematics and systematical trends for parameters, which characterise the threshold reaction excitation functions, are described. These empirical systematics were published earlier and used by authors in evaluation of nuclear data and for selection of neutron data for Russian library BROND-3 and for international library of fusion interest.

Systematics of (n,p) and (n,α) reaction excitation functions.

Analysis shows that the neutron excess (N-Z) and mass number A are main parameters, which determine the characteristics of the (n,p) and (n,α) reaction excitation functions. Because it is reasonable to arrange isotopes as table in dependence on (N-Z) and Z and compare excitation functions for isotopes with the same (N-Z) and Z. Below as an example the part of such table is given for A = 17-30.

Z N-Z	18	19	20	21	22	23	24	25	26	27	28	29	30
0	^{36}Ar		^{40}Ca										
1		^{39}K											
2	^{38}Ar		^{42}Ca		^{46}Ti		^{50}Cr		^{54}Fe		^{58}Ni		
3		^{41}K	^{43}Ca	^{45}Sc	^{47}Ti								
4	^{40}Ar		^{44}Ca		^{48}Ti	^{50}V	^{52}Cr		^{56}Fe		^{60}Ni		^{64}Zn
5					^{49}Ti	^{51}V	^{53}Cr	^{55}Mn	^{57}Fe	^{59}Co	^{61}Ni	^{63}Cu	
6			^{46}Ca		^{50}Ti		^{54}Cr		^{58}Fe		^{62}Ni		^{66}Zn
7												^{65}Cu	^{67}Zn
8			^{48}Ca								^{64}Ni		^{68}Zn
9													
10													^{70}Zn

As a result of comparison of available experimental data the following systematical trends were observed in dependence on (N-Z) and A:

1. The maximum of (n,p) reaction cross sections for the isotopes of a given element in semilogarithmic scale decreases linearly within experimental uncertainties (Fig.1). For the different elements these linear dependencies are practically parallel and equidistant (this was pointed by D.Gardner in 1962 for 14.5 MeV neutrons /8/).

. The maximum of (n,p) reaction cross sections in semilogarithmic scale increases also practically linearly within experimental uncertainties as a function of Z for the isotopes with the same (N-Z). These both dependencies for different elements seem to be almost parallel and equidistant (Fig.1).

The spread of cross sections around averaged linear dependencies is determined by the value $\Delta Q=(Q_{nnp}-Q_{np})$. At bigger $\Delta Q=(Q_{nnp}-Q_{np})$ the cross sections lie higher, but at less $\Delta Q=(Q_{nnp}-Q_{np})$ bellow. There are some indications that with the increase of A the influence of $\Delta Q=(Q_{nnp}-Q_{np})$ on this spread relative to averaged dependence decreases.

With increasing of the (N-Z) values the slopes of linear dependencies decreases. However, there are no enough experimental data to prove this argument.

2. For the isotopes with the same (N-Z) value the shapes of excitation functions are similar. In any case this takes place for reactions in mean mass numbers and for isotopes with

close values of $\Delta Q=(Q_{nnp}-Q_{np}.)$. Influence of $\Delta Q=(Q_{nnp}-Q_{np}.)$ on the shape did not investigated because of little amount of experimental data.

In Fig.2 the normalised experimental (n,p) reaction excitation functions for isotopes ^{48}Ti, ^{52}Cr, ^{56}Fe, ^{64}Zn, having the same values (N-Z) = 4. The functions are normalised to ^{48}Ti(n,p) reaction excitation function. The spread of curves are within experimental uncertainties.

All the mentioned systematical trends are supported by theoretical calculations based on the present day understanding of nuclear reaction mechanism.

As an example of application of these systematics let us compare excitation functions for ^{56}Fe and ^{58}Ni. Large spread of experimental data did not permit to describe reliably the ^{58}Ni(n, α) reaction excitation function (Fig.3). However the ^{56}Fe(n, α) reaction excitation function (Fig.4) is determined reliably enough. As far as the $\Delta Q=(Q_{nnp}-Q_{np}.)$ for both reactions are practically equal one can propose that positions of maximum of both excitation functions relative to threshold are the same. Shifting the ^{56}Fe(n, α) reaction threshold to that for ^{58}Ni and having in mind the systematics dependence of cross section at maximum of excitation function one can obtain the ^{58}Ni(n, α) reaction excitation function given in Fig.3. This curve is supported by recent experimental data.

3. For (n, α) reaction excitation functions the similar dependencies are observed. However the slope of linear dependencies in semilogarithmic scale are noticeably less than for (n,p) reactions.

Those systematics for (n,p) and (n, α) reactions are observed for the mass numbers from 10 to 100 and for (N-Z) = 0 -15.

As far as a position of the maximum of the (n,p) reaction excitation functions above $E_{th}+Q_C$ (where Q_C is Coulomb barrier) is proportionally to the value of $(Q_{nnp}-Q_{np})$, where Q_{nnp}-and Q_{np} are reaction energies of (n,np) and (n,p) reactions, respectively, it is useful to compare these values for different isotopes in the process of selection and evaluation of the (n,p) reaction excitation functions.

The systematics of (n,2n), (n,3n) and (n,np) - reactions.

The value of cross section in the maximum of (n,2n) reaction excitation function depends essentially on interrelation of (n,2n) and (n,np) reaction energies ($Q_{n,2n}$ and $Q_{n,np}$, respectively). Let us consider two cases: $Q_{n,2n} \leq Q_{n,np}$ and $Q_{n,2n} > Q_{n,np}$.

1. $Q_{n,2n} \leq Q_{n,np}$. In this case (n,2n) dominates and the maximum (top) cross sections of the (n,2n)-reaction excitation functions are determined by the following equation /5/: $\sigma_{top} = 65.4\ A^{2/3}$ mb, where A is atomic mass number. Experimental data support this relation for A = 50-210. However theoretical calculations permit to suppose that this relation is suitable for mass numbers in the range of 10-50.

2. The (n,2n)-reaction excitation functions in the neutron energy region from the threshold to the maximum of excitation functions are similar and can be described by the $\sigma = \sigma_{max}\ (\Delta E/\Delta E_m)^{1.35} \exp[1.4(1-\Delta E/\Delta E_m])$, where σ_{max} - cross section at the maximum, $\Delta E=E-E_{th}$, E_{th} - threshold energy, $\Delta E_{max} = E_{max} - E$, E - neutron energy, E_{max} - neutron energy at the maximum of excitation function and corresponds to (n,3n) reaction threshold.

This relation gives a reasonable result but the normalised function (Table 1) is better adjusted to experimental data (especially near threshold) and recommended for the use instead of the relation.

Table 1. Normalised excitation function of (n,2n)-reaction

$\Delta E/\Delta E_{max}$	σ/σ_{max}	$\Delta E/\Delta E_{max}$	σ/σ_{max}	$\Delta E/\Delta E_{max}$	σ/σ_{max}
0.05	0.03	0.35	0.60	0.65	0.91
0.10	0.09	0.40	0.68	0.70	0.93
0.15	0.18	0.45	0.75	0.75	0.95
0.20	0.30	0.50	0.81	0.80	0.97
0.25	0.42	0.55	0.85	0.85	0.98
0.30	0.53	0.60	0.88	0.90	0.99

The influence of difference ($Q_{n,3n}$ - $Q_{n,2n}$) on excitation function shape was not investigated, however there are grounds to suppose that such influence can be noticeable as far as this difference is within 5-12 MeV and normalised function for isotopes with different ($Q_{n,3n}$ - $Q_{n,2n}$) can be no exact similar and differ from averaged normalised function.

3. $Q_{n,2n} > Q_{n,np} + Q_C$. In this case the (n,2n) cross section in the maximum of the excitation function is below the values, calculated from the equation mentioned above, and the difference is determined by contribution of the (n,np) reaction cross section at the same neutron energy. At this condition the maximum of both reaction excitation functions are near 20 MeV and the sum of the (n,2n) reaction cross section and the (n,np) reaction cross section is approximately equal to $\sigma_{top} \approx \sigma_{n,2n} + \sigma_{n,np}$.

If $Q_{n,2n} > Q_{n,np}$, then σ_{max} is determined from experimental data or from other considerations however the shape of excitation function is described by the same normalised function.

In the Fig. 5 one can see the (n,2n), (n,p), (n,np) and (n,xp) reaction excitation functions of ^{58}Ni evaluated on the base of experimental data.

The values of (n,2n) and (n,np) reaction cross sections at the maximum of its excitation functions can be evaluated as 80 and 870 mb, respectively. In the sum it gives 950 mb that is close to 978 mb, predicted by equation for σ_{top}.

The ^{58}Ni (n,np) reaction excitation function, plotted in Fig.5, in the energy range above Coulomb barrier can be approximated by the normalised function, which almost similar that for (n,2n) reaction.

The sum of (n,np) and (n,p) reaction excitation functions (Fig.5) gives the (n,xp) reaction excitation function. As one can see there is a reasonable agreement with the experimental (n,xp) reaction cross sections measured by S.Grimes et al. and S.Saraf et al. The (n,p) reaction excitation function was evaluated on the base of reliable experimental data.

The shapes of the (n,3n) reaction excitation functions are similar in the neutron energy region from the threshold up to the neutron energy at the maximum of the excitation function (at 10-11 MeV above the threshold) and can be approximated by the equation:

$$\sigma = \sigma_{max} (\Delta E/\Delta E_m)^{3.3} \cdot \exp[3.3(1-\Delta E/\Delta E_m]),$$

where ΔE and ΔE_m are counted from the (n,3n) reaction threshold, σ_{max} is determined by the equation: $\sigma_{max} \approx 10$ A mb, where A is atomic mass number.

Systematics of fission and (n,2n) reaction cross section of fissile isotopes.

Analysis of available experimental data on fission cross sections for the isotopes in the region from thorium up to curium shows that for all isotopes the energy dependence of fission cross sections in the incident neutron energy of 1-20 MeV have similar structures: maximum in the energy intervals of 1-3 and 8-9 MeV and minima in the energy intervals of 5-6 and 11-13 MeV.

Because these maximum and minima are situated practically in the same neutron energy intervals for all isotopes it is possible to compare fission cross sections in these intervals in dependence on A and Z. It should be noted that in the 5-6 MeV interval there is (n,nf) reaction threshold, in the 11-13 MeV there are (n,2nf) reaction threshold, the maximum of (n,2n) reaction excitation function and (n,3n) reaction threshold. From theoretical model calculations one can see that at 11-13 MeV the inelastic scattering cross section is small (about 50 mb) and main contribution to nonelastic process cross section in this energy range gives the fission and (n,2n) reactions.

In Fig. 6 all available experimental data and calculated by STAPRE code /10/ are given. As it is seen the straight lines can approximate the fission cross sections of a given element. in some region.

In Fig. 7 the experimental and calculated (n,2n) reaction cross sections in the maximum of excitation function are presented. As one can see that there is linear dependence of this cross section as a function of atomic mass number A.

In Table 2 the sums of fission and (n,2n) reaction cross sections are given in the incident energy interval of 11-13 MeV. The sum changes weakly against Z and A and in the first approximation can be considered as constant in all range of isotopes from Th up to Am and equal to 2580+–50 mb. The theoretical calculations /10/ shows that for Cf and Bk the sum of fission and (n,2n) reaction cross sections lies within the same limits.

Table 2. The fission and (n,2n) reaction cross sections for 12 MeV.

Isotope	Fission cross section, mb	(n,2n) reaction cross section, mb	Sum of fission and (n,2n) reaction cross sections, mb
Th-232	350±30	2200±50	2550
U-235	1750±50	870±30	2550
U-238	1000±50	1500±100	2550
Np-237	2100±50	530±30	2630
Pu-239	2200±50	400±50	2600
Am-241	2350	250±20	2600

The normalised excitation function for (n,2n) reaction describes quite well the shape of the (n,2n) reaction cross sections from the threshold up to the maximum of the cross section for fissile isotopes ^{232}Th, ^{238}U, ^{237}Np.

Conclusion.

These systematical trends give good possibility of selection of more reliable and physically based excitation functions or at least to show confidence interval of values and exclude the excitation functions with considerable deviations in shapes and wrong absolute values.

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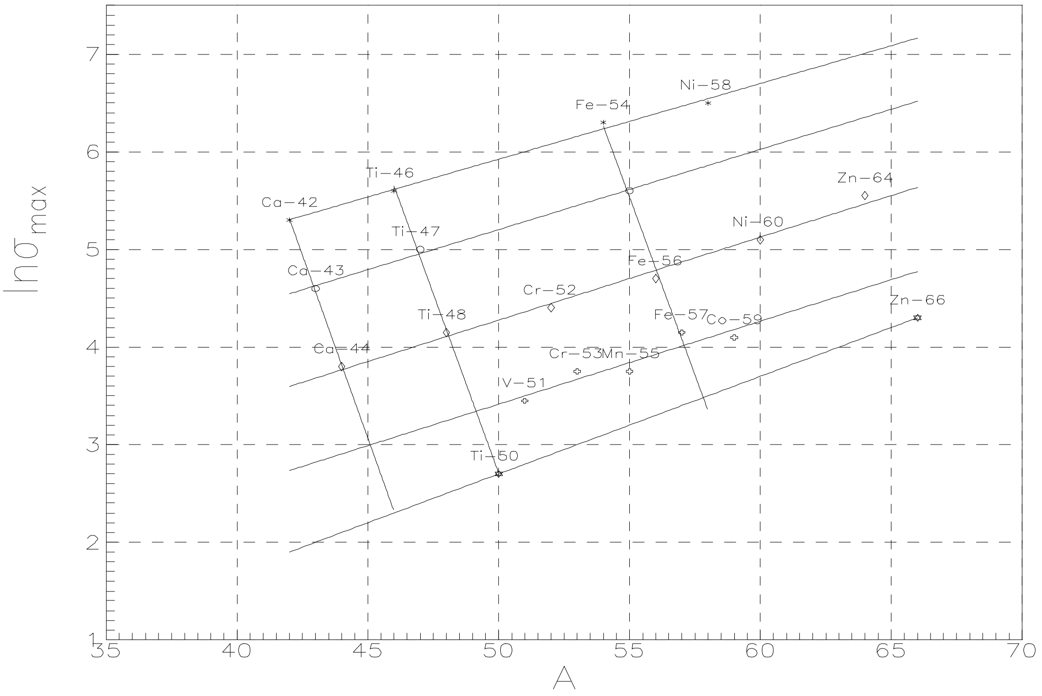

Fig.1. The (n,p) reaction cross sections at the maximum of the excitation functions against mass number A.

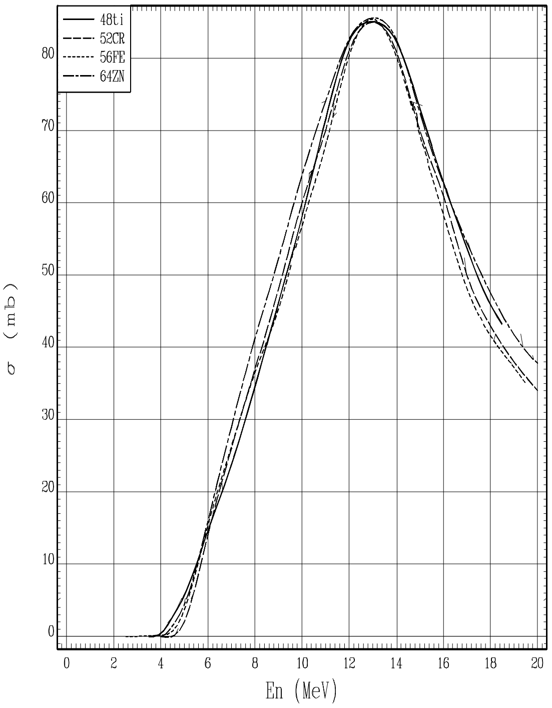

Fig.2. The normalised (n,p) reaction excitation functions for isotopes with (N-Z)=4.

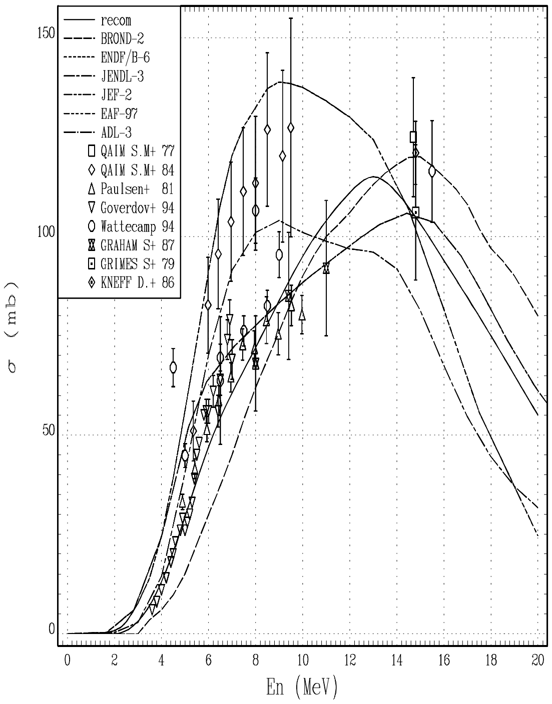

Fig.3. Cross section of ^{58}Ni(n,α)^{55}Fe reaction.

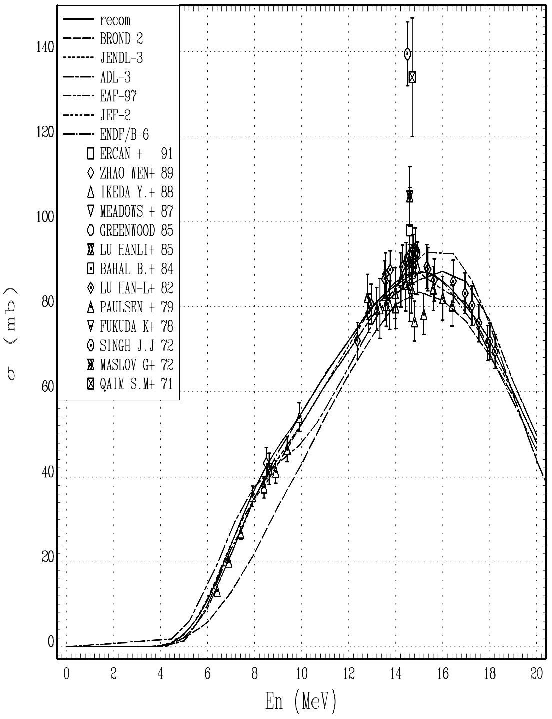

Fig.4. The experimental and evaluated data for ^{54}Fe(n,α)^{51}Cr.

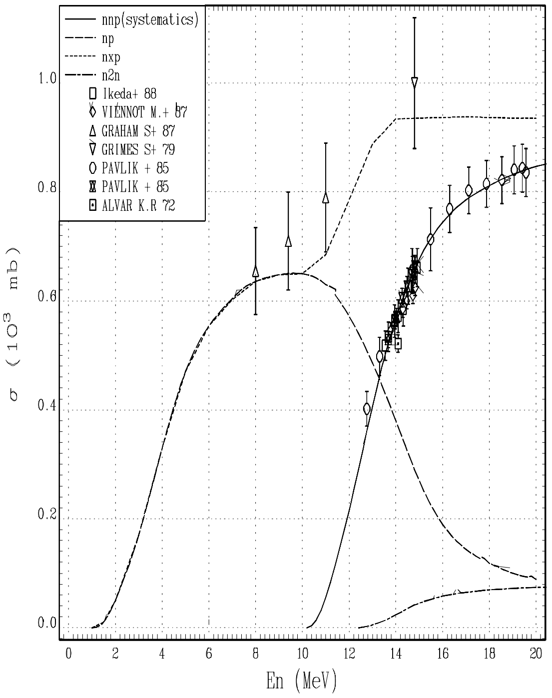

Fig.5. The (n,2n), (n,p), (n,np) and (n,xp) reactions on ^{58}Ni.

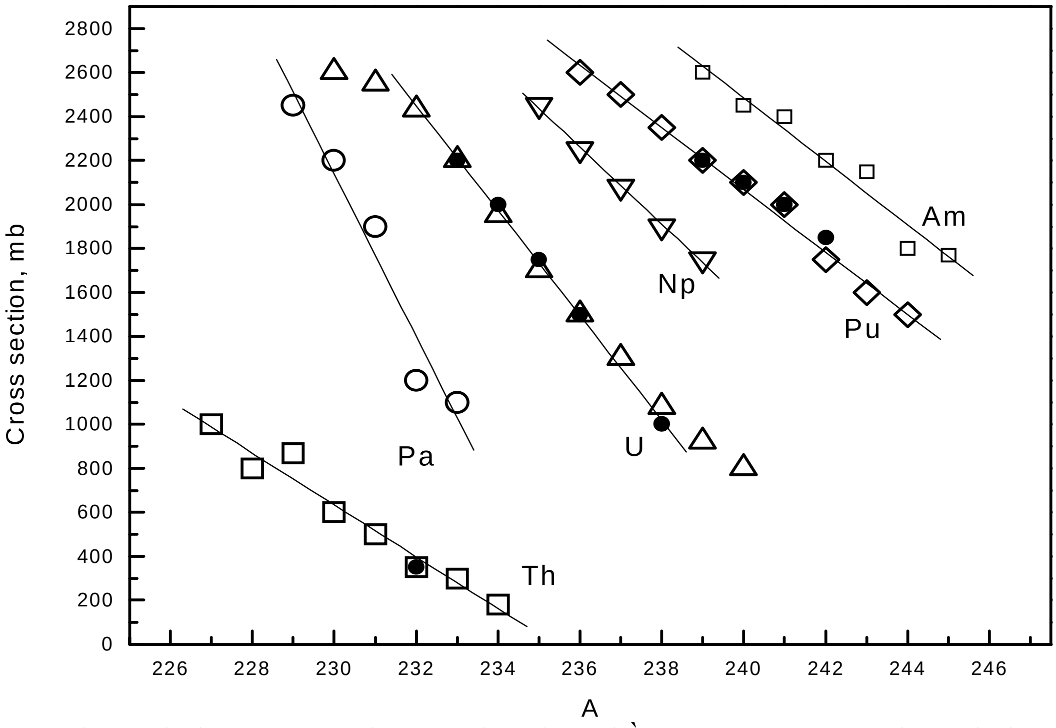

Fig.6. Fission cross section as a function of À at 12-13 MeV. Dark symbols - experiment, open symbols - calculation /10/.

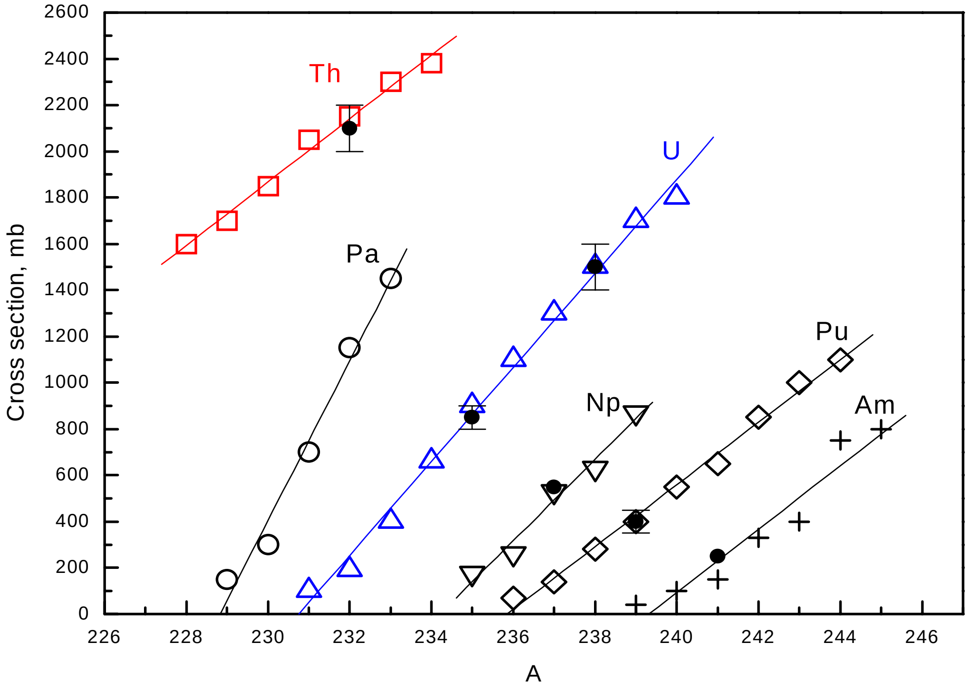

Fig.7. The (n,2n) reaction cross section at 12-13 MeV. Dark symbols - experiment, open symbols - calculation /10/.