INVESTIGATION OF EXCITATION FUNCTIONS USING NEW EVALUATED EMPIRICAL AND SEMI-EMPIRICAL SYSTEMATIC FOR 14-15 MEV (n,*t*) REACTION CROSS SECTIONS

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ABSTRACT

The hybrid reactor is a combination of the fusion and fission processes. In the fusion-fission hybrid reactor, tritium self-sufficiency must be maintained for a commercial power plant. For self-sustaining (D-T) fusion driver tritium breeding ratio should be greater than 1.05. Working out the systematics of (n,t) reaction cross sections is of great importance for the definition of the excitation function character for the given reaction taking place on various nuclei at energies up to 20 MeV. In this study, we have investigated the asymmetry term effect for the (*n,t*) reaction cross sections at 14-15 neutron incident energy. It has been discussed the odd-even effect and the pairing effect considering binding energy systematic of the nuclear shell model for the new experimental data and new cross section formulas (*n,t*) reactions developed by Tel et al. We have determined a different parameter groups by the classification of nuclei into even-even, even-odd and odd-even for (*n,t*) reactions cross sections. The obtained empirical formulas by fitting two parameter for (*n,t*) reactions were given. All calculated results have been compared with the experimental data. By using the new cross sections formulas (*n,t*) reactions the obtained results have been discussed and compared with the available experimental data.

Keywords: Tritium, (*n,t*) cross-section, empirical and semi empirical formulas, hybrid reactor, fusion reactor,

1. INTRODUCTION

The hybrid reactor is a combination of the fusion and fission processes. The fusion plasma is surrounded with a blanket made of the fertile materials (U^{238} or Th^{232}) to convert them into fissile materials (Pu^{239} or U^{233}) by transmutation through the capture of the high yield fusion neutrons (Şahin et al., 1986, 2002a, 2002b, 2003, 2005; Übeyli and Tel, 2003). The fertile materials may also undergo a substantial amount of nuclear fission, especially, under the irradiation of the high energetic 14.1 MeV- (D,T) neutrons. Tritium self-sufficiency must be maintained for a commercial power plant. For self-sustaining (D-T) fusion driver tritium breeding ratio should be greater than 1.05. So, working out the systematics of (n,t) reaction cross sections is of great importance for the definition of the excitation function character for the given reaction taking place on various nuclei at energies up to 20 MeV.

The neutron incident energy around 14-15 MeV is enough to excite the nucleus for the reactions such as (*n, p*), (*n, d*), (*n, 2n*), (*n, t*) and (n,α). The systematic experimental studies for the cross sections of (*n, charged particle*) such as $\sigma(n, p)$ and $\sigma(n, \alpha)$ at 14 – 15 MeV have been studied over the years for a large number of nuclei (Levkovskii, 1974; Pearlstein, 1965; Adam and L. Jeki, 1969; Ait-Tahar, 1987; Korovin Yu and Konobeyev Yu, 1995; Belgaid and Asghar, 1998; Habbani and Osman, 2001). Moreover, applications of statistical and thermodynamical methods to the calculation of nuclear process for heavy nuclei go back to the fundamental work of Weisskopf and Ewing (Weisskopf , 1937; Weisskopf and Ewing, 1940). On the other hand, a number of empirical and semi-empirical formulas with different parameters for cross sections calculations of the reactions (n, p), (n, t), (n, α) and $(n, 2n)$ at the different neutron energies has also been proposed by several authors (Kumabe and Fukuda, 1987; Molla and Qaim, 1977; Manokhin et al., 2001) and Tel et al. (Tel et al, 2003) suggested using these new experimental data to reproduce a new empirical formula of the cross sections of the (n,p) reactions. This formula depends on the asymmetry parameter, $s = (N - Z)/A$, and has the pairing effect on the binding energy systematics of nuclear shell model. Tel *et al.* also obtained a new appropriate coefficient by using this formula for $(n,2n)$, (n,α), (n, d) and (n, t) reactions (Tel et al, 2003; 2007a; 2007b; Aydın, et al., 2007).

The neutron scattering cross sections and the emission differential data have a critical importance on fusion reactor (and in the fusion-fission hybrid reactor) neutronics. These data can be extensively used for the investigation of the structural materials of the fusion reactors, radiation damage of metals and alloys, tritium breeding ratio, neutron multiplication and nuclear heating in the components, neutron spectrum, and reaction rate in the blanket and neutron dosimetry. There are several new technological applications on the fields of fast neutrons such as accelerator-driven incineration / transmutation of the long-lived radioactive nuclear wastes into short-lived or stable isotopes (Rubbia, et al., 1995; Rubbia et al., 1996; Betak et al., 1999). Especially, in accelerator driven subcritical systems for fission energy production and /or nuclear waste transmutation as well as in intermediate- energy accelerator driven neutron source, ions and neutrons with energies beyond 20 MeV, the upper limit of existing data files that were produced for d-T fusion applications, will interact with materials. As well, there can be found several biomedical applications i.e., production of radioisotopes and cancer therapy.

Because of above mentioned cases, it is needed to form new data about the cross sections of nuclear reactions for the energy around 20 MeV (ENSDF, 1998; Maclane, 1997). Therefore, more many experiments have been carried out to obtain and detect neutrons for different energy ranges. For an instance, the method of energy measurement by means of velocity determination is a widely used technique and known as time of flight (TOF) (Walt, 1960). Additionally, obtained data from various techniques are necessary to develop more nuclear theoretical calculation models in order to explain nuclear reaction mechanisms and the properties of the excited states for different energy ranges. Furthermore, the experimental cross section data of neutron around 14–15 MeV energy and particle emission spectra have a profound importance for understanding the binding energy systematics, the basic nucleon-nucleus interaction, nuclear structure and refined nuclear models.

In the present study, firstly only empirical formulas of the (*n,t*) cross sections were obtained at the energy range of 14 – 15 MeV for different parameter groups by using fitting procedure. Secondly, by using Tel et al. formula (Tel et al., 2003) two different parameter groups by the classification of nuclei into odd-*A*, even-*A* for (*n, t*) reaction cross sections have been determined. In this way, it has been discussed odd-even effect and basic nucleon-nucleus interaction considering the new experimental data and the new cross section formulas developed by Tel et al.. (Tel et al, 2003) for (*n,t*) reactions. The current obtained results have been also investigated and compared with the other the theoretical and experimental results proposed in early studies.

2. EMPIRICAL SYSTEMATIC for 14-15 MeV NEUTRON REACTION CROSS SECTIONS

Recently nuclear data files have been prepared to study the neutron transport, nuclear heating and gas production, and radiation damage for materials irradiated by fast neutrons (ENSDF, 1998; Maclane, 1997). These data files include the information about total cross sections, elastic and inelastic cross sections for threshold reactions, energy and angular distributions for secondary neutrons, protons and α-particles. However, nuclear models are frequently needed to provide the estimations of neutron-induced reaction cross sections, especially when experimental data are scarce or very difficult to perform. If the calculations on nuclear models are carried out using global parameters that have not been sufficiently validated by the experimental data, the obtained numerical results can be quite unreliable. The calculations employed to various model codes have shown that the results may vary depending on the codes and input parameters when no experimental data are available. Furthermore, a large number of experimental data have been published on the (*n, charged particle*) and (*n,2n*) reaction cross sections induced by 14-15 MeV neutrons (ENSDF, 1998; Maclane, 1997). According to previous reports (Levkovskii, 1974; Pearlstein, 1965; Adam and Jeki, 1969; Ait-Tahar, 1987; Korovin and Konobeyev, 1995; Belgaid and Asghar, 1998; Habbani and Osman, 2001) the cross sections for many nuclei significantly vary with the mass number A, neutron number N and proton number Z of the target nucleus. In addition, the attributable effects to the asymmetry parameter, $s= (N-Z)/A$, as well as to the isotopic, isotonic and odd-even properties of nuclei have been observed in the data.

The empirical cross sections of reactions induced by fast neutrons can be approximately expressed as follows,

$$\sigma(n,x) = C\sigma_{ne}\exp[as] \tag{1}$$

where σ_{ne} is the neutron non-elastic cross section, and the coefficients C and a are the fitting parameters determined from least-squares method for different reactions. The non-elastic cross sections have been measured intensely for many nuclides in the MeV range, enabling us to find out their variation with atomic mass. The neutron non-elastic cross section is given by πR^2, where R is the nuclear radius and

$$\sigma_{ne} = \pi r_0^2 (A^{1/3} + 1)^2 \tag{2}$$

where, $r_0 = 1.2 \times 10^{-13}$ cm.

Equation (1) represents the product of two factors, each of which might be assigned to a stage of nuclear reaction within the framework of the statistical model of nuclear reactions. The exponential term represents the escape of the reaction products from a compound nucleus. It has a strong *(N-Z)/A* dependence implied by Eq.(1). This case has already been shown by (Betak, et al., 2005) for neutron-induced reaction cross sections. There are also several formulas describing the isotopic dependence of cross sections for different reactions at neutron energy of 14.5 MeV. The measured cross sections exhibit a large gradient for the lighter masses ($Z \leq 30$) with increasing asymmetry parameter and then become almost constant for medium and heavy mass nuclei (starting from $A \leq 100$).

The best fitting can be obtained with the new free parameters in order to provide the minimum value of the following expression,

$$\chi^2 = \frac{1}{N}\sum_i^N \left(\frac{\sigma_{exp}^i - \sigma_{cal}^i}{\Delta\sigma_{exp}^i} \right)^2 \qquad (3)$$

where $\sigma_{\exp}^i$ and σ_{cal}^i are the experimental and the calculated cross sections, respectively, and $\Delta\sigma_{\exp}^i$ is the error associated with $\sigma_{\exp}^i$. Details on the results of the best fitting parameters and the values of χ^2 can be found for (*n,p*), (*n,* α), (*n, 2n*), (*n, d*) and (*n ,t*) reactions in (Tel et al., 2003; 2007a; 2007b; Aydın, et al., 2007).

3. RESULTS AND DISCUSSION

Empirical and semi – empirical formulae are applied for the creation of systematic studies. Empirical expressions contain the exponential dependence of cross – sections upon the number of neutrons and protons in nuclei. The empirical formulae use the evaporation model and ignore an important role of the pre – equilibrium mechanism of particle emission for medium and heavy nuclei. But the semi – empirical systematic are based on the use of analytical expressions for calculation of particle emission within the frame of pre – equilibrium exciton and evaporation models.

The odd-even and the nucleon binding energy systematics have been compared with the (*n,t*) measured cross sections with the empirical fits as shown in Figs. 1-2. The (*n,t*) reaction cross sections include coulomb effect as seen in Figs. 1 – 2. In these reactions, it can be also seen that the reaction cross sections decrease by the increasing of the asymmetry parameter (Figs. 1–2). According to Levskovskii's formula (Levkovskii, 1974), the proton and alpha emission probabilities increase with increasing relative proton number. The same relation can be also expected for *d, t* and α emission. Besides, pre-equilibrium process are important mechanisms in nuclear reactions induced by light projectiles with incident energies above 10 MeV (Griffin, 1966; Betak, 1975; Blann and Vonach, 1983). The pre-equilibrium reaction effects strongly depend on the asymmetry parameter. Particularly, in the region I($A = 40 \sim 62$), the (*n,p*) reaction is possible with compound process whereas this reaction is possible with pre-equilibrium process in region III (A=90 ~ 160). Moreover, in the intermediate region II (A= 63 ~ 89) this reaction is also governed by both processes in the regions I and III (Kumabe and Fukuda, 1987). In Figs. 3-5, reaction cross sections were classified according to odd-even properties by depending up on asymmetry parameter. As it can be obviously seen from Figs. 3–5, the reaction cross sections separate with each other (with relative to odd-even properties) according to the raising of asymmetry parameter. This separation can be observed mostly for (*n,t*) reactions. This case shows a strong pairing effect by depending up on the target nuclei mass number-A.

Detailed investigations for (*n,p*), (n,α) and (*n,2n*) reaction cross sections have been performed in previous studies (Tel et al, 2003; 2007a; 2007b;2007c). In the present study, we have only investigated the (*n,t*) reaction cross sections at the energy of 14–15 MeV in two different groups by using Tel et al. formula as it can be seen in Figs. 3–5. Since there is not enough experimental data for the (*n,t*) reactions, it has been determined two different parameter groups by the classification of nuclei into the odd-A and the even-A. As it can be clearly seen from Fig. 1-2 the (*n,t*) reaction cross sections separate with each other due to increasing of the asymmetry parameter. Therefore, by using only empirical formula we could not perform a good fitting for this case . However, for the (*n,t*) cross sections values, a good fitting was achieved by considering the even-even correction (Figs. 3-5).

We have used the number of 25 experimental (*n,t*) reaction cross sections data taken from Refs. (ENSDF, 1998; Maclane, 1997; Belgaid, et.al, 2003) for fitting procedure. We have used the nuclei which their mass numbers change from A = 46 to 209, the atomic numbers change from Z = 22 to 83 and also the neutron numbers change from N = 24 to 126. In Figs. 1-5, the experimental (*n,t*) cross sections of these nuclides have been fitted to depending on the asymmetry parameter. In Figs. 3-5, we have introduced the two formulas by fitting two parameters for each formula presented by the considering of pairing effect of the nuclear shell model. We could not be able to use the even-even, the even-odd and the odd-even systematic because of the lack of sufficient experimental data.

The coefficients C and a were determined by the least-squares fitting method and the empirical formulas obtained by fitting the two parameter for the (*n,t*) reactions are given in the Table I and also in Figs. 1-5, respectively. Besides, The comparison of calculations empirical and semi-empirical formulas with experimental for (*n,t*) reactions 14-15 MeV incident neutrons are given in the Table II and also in Figs. 6-7, respectively.

When the more experimental data for the neutron scattering and emission differential cross sections have been obtained by using the new technology, it can be explained more reliable results and developed more nuclear reaction mechanisms and nuclear models. As a result, the precise knowledge of the systematic for different neutron induced reactions is of great importance in the account of the understanding the binding energy systematics of the nuclear shell model. Also, the present kind of studies lead to improve and clarify the binding energy systematic of the nuclear shell model and the estimation of unknown data for the development of nuclear reaction theories.

SUMMARY AND CONCLUSIONS

In this paper, we have discussed the odd-even effect and the pairing effect considering binding energy systematic of the nuclear shell model for the new experimental data. We have determined a different parameter groups by the classification of nuclei into the even-even, the even-odd and the odd-even for (*n,t*) reactions cross sections. The obtained empirical formulas by fitting two parameter for the (*n,t*) reactions were given and the following conclusions can be summarized as follows:

1. The (*n,t*) reaction cross sections for 14-15 MeV decrease by the increasing of the asymmetry parameter.

2. The tritium emission probabilities increase with increasing relative proton number.

3. The pre-equilibrium reaction effects strongly depend on asymmetry parameter for the (*n,t*) cross sections.

4. A good fitting of the (*n,t*) cross section values was achieved by considering the pairing correction.

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Figure Captions

Fig. 1. Systematic of (*n,t*) reaction cross sections (in μb) induced by 14-15 MeV neutrons. Experimental data were taken from Ref. (ENSDF, 1998; Maclane, 1997; Belgaid, et al., 2003).

Fig. 2. The experimental points were fitted with $\sigma(n,t)_{empirical} = 7.09(A^{1/3}+1)^2 \exp\left[-8.91\, s\right]$ and correlation coefficient was determined as $R^2 = 0.20$. Experimental data were taken from Ref. (ENSDF, 1998; Maclane, 1997; Belgaid, et al., 2003).

Fig. 3. Systematic of (*n,t*) reaction cross sections (in μb) for even-*Z*, even-*N* ; odd-*Z*, even-*N* nuclides induced by 14-15 MeV neutrons. Experimental data were taken from Ref. (ENSDF, 1998; Maclane, 1997; Belgaid, et al., 2003).

Fig. 4. Systematic of (*n,t*) reaction cross sections (in μb) for even-*Z*, even-*N* nuclides induced by 14-15 MeV neutrons. The experimental points were fitted with $\sigma_{n,t} = 6.94(A^{1/3}+1)^2 \exp\left[-13.41\, s\right]$ and correlation coefficient was determined as $R^2 = 0.80$. Experimental data were taken from Ref. (ENSDF, 1998; Maclane, 1997; Belgaid, et al., 2003).

Fig. 5. Systematic of (*n,t*) reaction cross sections (in μb) for odd-*Z*, even-*N* nuclides induced by 14-15 MeV neutrons. The experimental points were fitted with $\sigma_{n,t} = 121.21(A^{1/3}+1)^2 \exp\left[-20.54\, s\right]$ and correlation coefficient was determined as $R^2 = 0.73$. Experimental data were taken from Ref. (ENSDF, 1998; Maclane, 1997; Belgaid, et al, 2003).

Fig.6. Ratios of the (*n,t*) experimental cross – sections to the cross – sections calculated with only empirical formula.

Fig.7. Ratios of the (*n,t*) experimental cross – sections to the cross – sections calculated with semi- empirical formula

Table Captions:

Table I. The coefficients C and a, and the empirical and semi-empirical formulas for (*n*,*t*) reactions.

TableII The comparison of calculations empirical and semi-empirical formulas with experimental for (*n*,*t*) reactions 14-15 MeV incident neutrons. Experimental data were taken from Ref. (ENSDF, 998; Maclane, 1997; Belgaid, et.al, 2003).

Table I.

C	a	$\sigma(n,x) = C\sigma_{ne} \exp\left[as\right]$	χ^2
7.09	-8.91	$\sigma(n,t)_{empirical} = 7.09(A^{1/3}+1)^2 \exp\left[-8.91\ s\right]$	15.94
6.94	-13.41	$\sigma(n,t)_{semi-empirical} = \begin{cases} 6.94(A^{1/3}+1)^2 \exp\left[-13.41\ s\right] & \text{Even Z- Even N} \\ 121.21(A^{1/3}+1)^2 \exp\left[-20.54\ s\right] & \text{Odd Z - Even N} \end{cases}$	5.05
121.21	-20.54		

Table II

Target	Reaction Products	Half life-Residual Nucleus and decay mode	Threshold Energy (MeV)	Q-value (MeV)	Excitation Energy (MeV)	σ_{exp} (in μb)	$\Delta\sigma_{exp}$ (in μb)	Empirical formula (in μb)	Semi-empirical formula (in μb)
^{46}Ti	^{44}Sc+^{3}H	3.93 h (EC)	13.475	-13.185	1.415	123	25	101.159	81.375
^{50}Cr	^{48}V+^{3}H	16 d (EC)	12.918	-12.662	1.938	77	20	108.993	89.060
^{55}Mn	^{53}Cr+^{3}H	STABLE	9.475	-9.304	5,296	990	198	72.797	431.984
^{54}Fe	^{52}Mn+^{3}H	5.59 d (EC)	12.657	-12.425	2.175	121	30	116.531	96.497
^{56}Fe	^{54}Mn+^{3}H	312 d (EC)	12.143	-11.928	2.672	46	12	87.428	62.018
^{59}Co	^{57}Fe+^{3}H	STABLE	9.079	-8.926	5.674	640	128	79.818	508.850
^{58}Ni	^{56}Co+^{3}H	78.8 d (EC)	11.259	-11.066	3.534	90	20	123.803	103.704
^{60}Ni	^{58}Co+^{3}H	70.8 d (EC)	11.698	-11.504	3.096	54	18	94.615	68.570
^{64}Zn	^{62}Cu+^{3}H	9.73 m (EC)	10.243	-10.084	4.516	78	16	101.626	75.045
^{70}Ge	^{68}Ga+^{3}H	68.1 m (EC)	10.504	-10.355	4.245	42	12	86.688	57.665
^{86}Sr	^{84}Rb+^{3}H	32.9 d (EC)	11.788	-11.652	2.948	30	8	73.778	42.772
^{88}Sr	^{86}Rb+^{3}H	18.8 d (EC)	12.195	-12.053	2.547	63	22	62.461	33.082
^{90}Zr	^{88}Y+^{3}H	106.6 d (EC)	11.473	-11.346	3.254	26.5	7	79.191	46.990
^{93}Nb	^{91}Zr+^{3}H	STABLE	6.263	-6.196	8.404	37	74.4	75.631	326.441
^{92}Mo	^{90}Nb+^{3}H	14.6 h (EC)	11.148	-11.027	3.573	70	21	99.399	65.752
^{103}Rh	^{101}Ru+^{3}H	STABLE	7.019	-6.950	7.651	730	146	74.522	293.303
^{102}Pd	^{100}Rh+^{3}H	20.8 h (EC)	9.310	-9.219	5.381	64	22	95.283	59.964
^{106}Cd	^{104}Ag+^{3}H	69.2 m (EC)	8.984	-8.899	5.701	86.5	15	100.582	64.361
^{114}Cd	^{112}Ag+^{3}H	3.14 h (b-)	10.366	-10.275	4.325	36	8	59.420	28.566
^{112}Sn	^{110}In+^{3}H	69.1 m (EC)	9.146	-9.064	5.536	77.5	13	92.500	55.876
^{141}Pr	^{139}Ce+^{3}H	137.2 d (EC)	5.989	-5.946	8.654	134	30	63.831	163.547
^{170}Er	^{168}Ho+^{3}H		6.967	-6.926	7.674	12.7	3.2	51.041	20.303
^{205}Tl	^{203}Hg+^{3}H	46.6 d (b-)	5.456	-5.429	9.171	33	6.6	52.034	77.507
^{204}Pb	^{202}Tl+^{3}H	12.2 d (EC)	6.034	-6.005	8.595	30	6	58.617	23.731
^{209}Bi	^{207}Pb+^{3}H	STABLE	2.698	-2.685	11.915	300	60	54.527	85.103

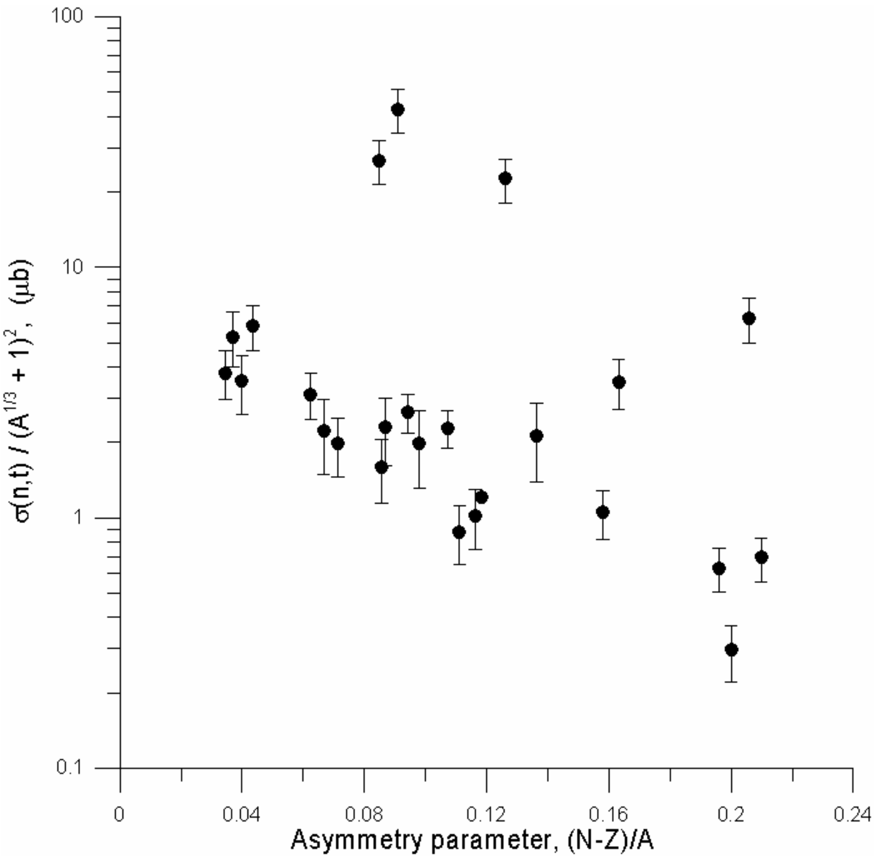
100
10
1
0.1
σ(n,t) / (A^1/3 + 1)^2, (μb)
0
0.04
0.08
0.12
0.16
0.2
0.24
Asymmetry parameter, (N-Z)/A

Fig. 1

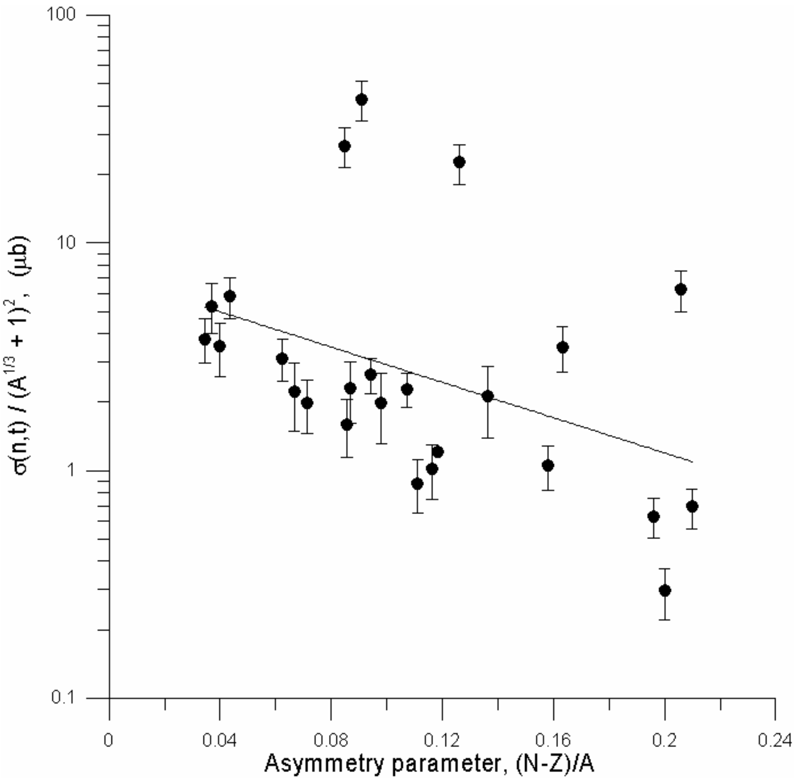
100
10
1
0.1
σ(n,t) / (A^1/3 + 1)^2, (μb)
0
0.04
0.08
0.12
0.16
0.2
0.24
Asymmetry parameter, (N-Z)/A

Fig.2

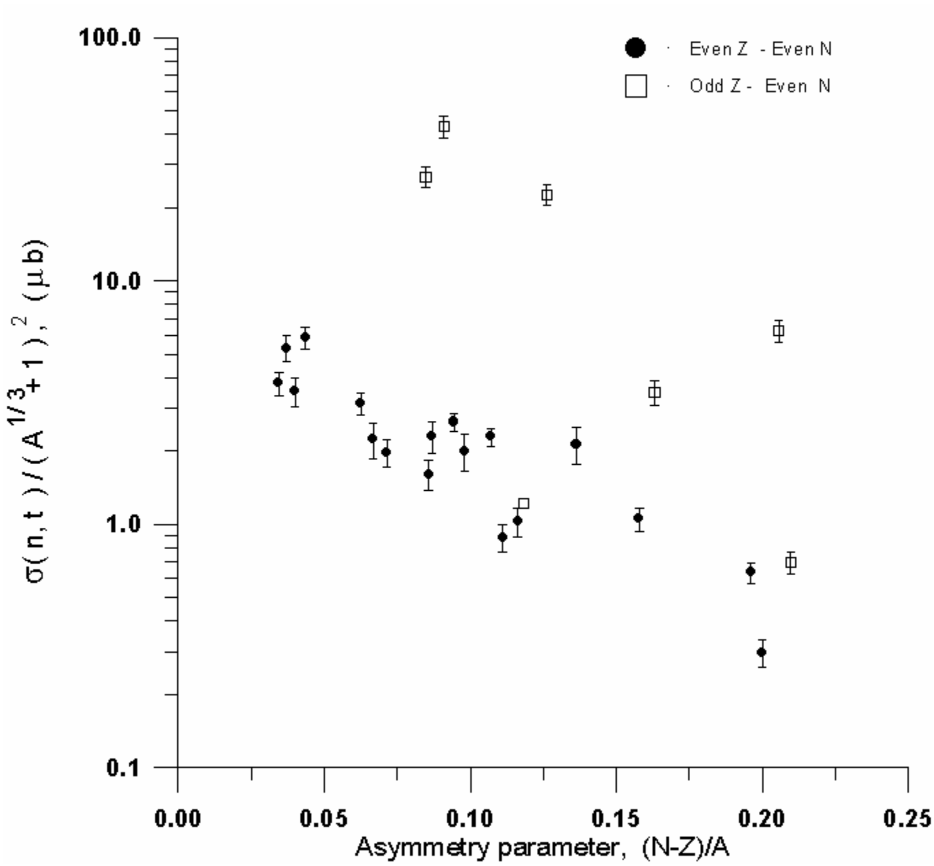
100.0
10.0
1.0
0.1
0.00
0.05
0.10
0.15
0.20
0.25
Asymmetry parameter, (N-Z)/A
σ(n,t)/(A^{1/3}+1)^2, (μb)
● Even Z - Even N
□ Odd Z - Even N

Fig.3

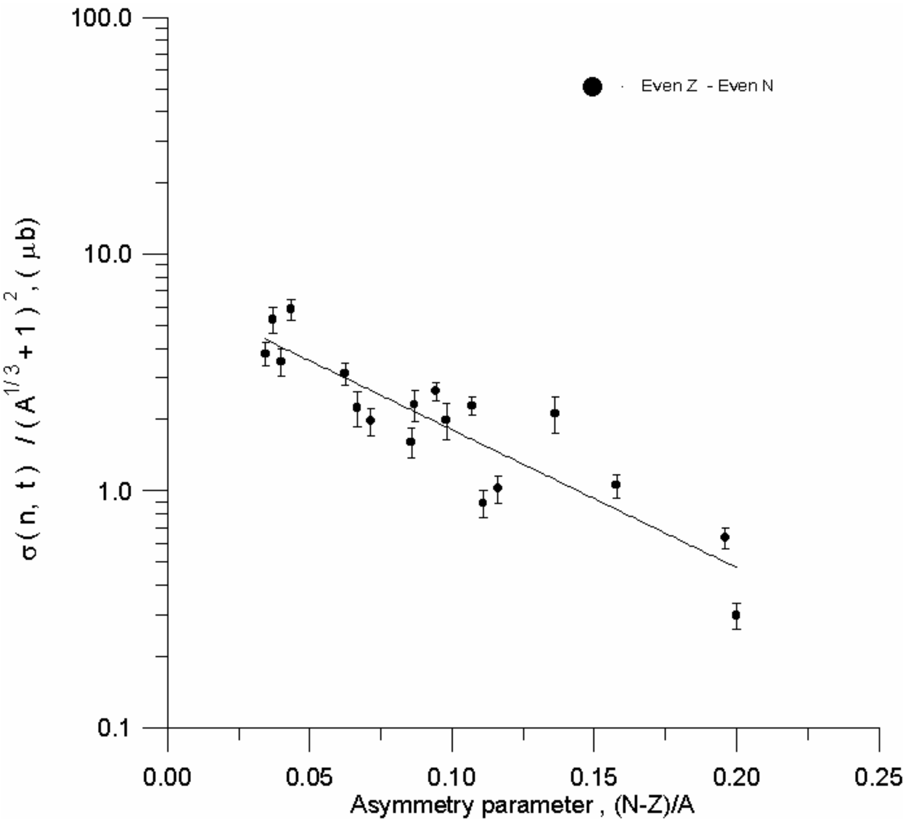
100.0
10.0
1.0
0.1
0.00
0.05
0.10
0.15
0.20
0.25
Asymmetry parameter , (N-Z)/A
σ(n, t) /(A^{1/3}+1)^2, (μb)
● Even Z - Even N

Fig.4

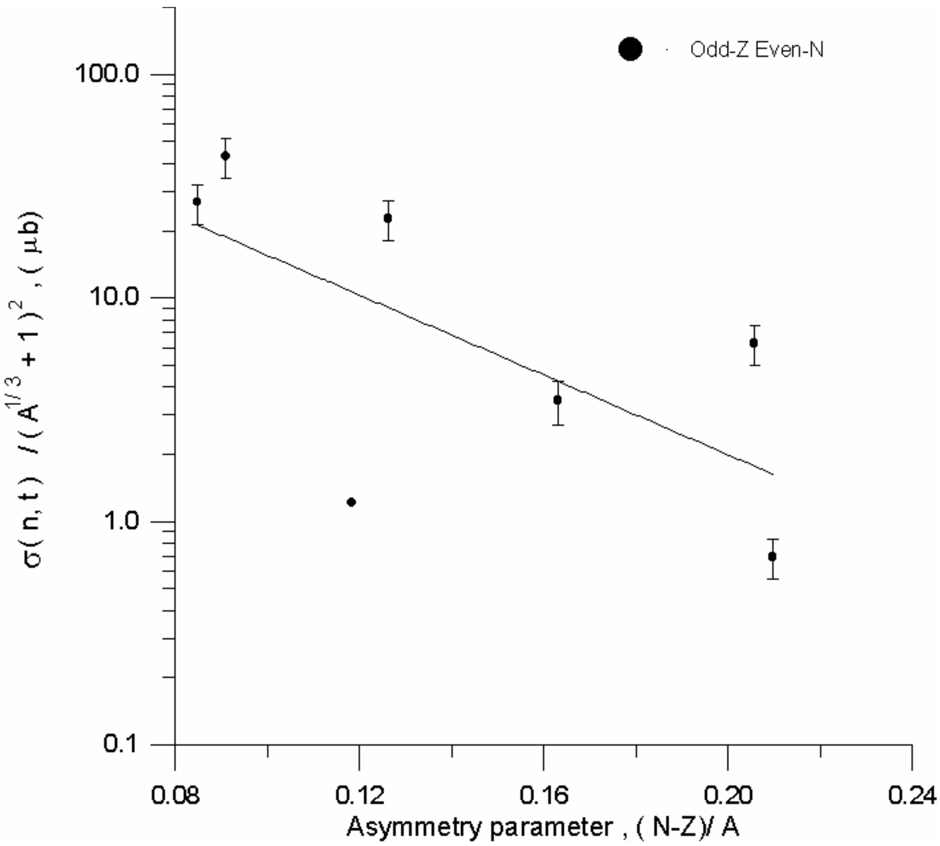
● Odd-Z Even-N
100.0
10.0
1.0
0.1
$\sigma(n,t)\ /(A^{1/3}+1)^2$, (μb)
0.08
0.12
0.16
0.20
0.24
Asymmetry parameter , (N-Z)/ A

Fig. 5

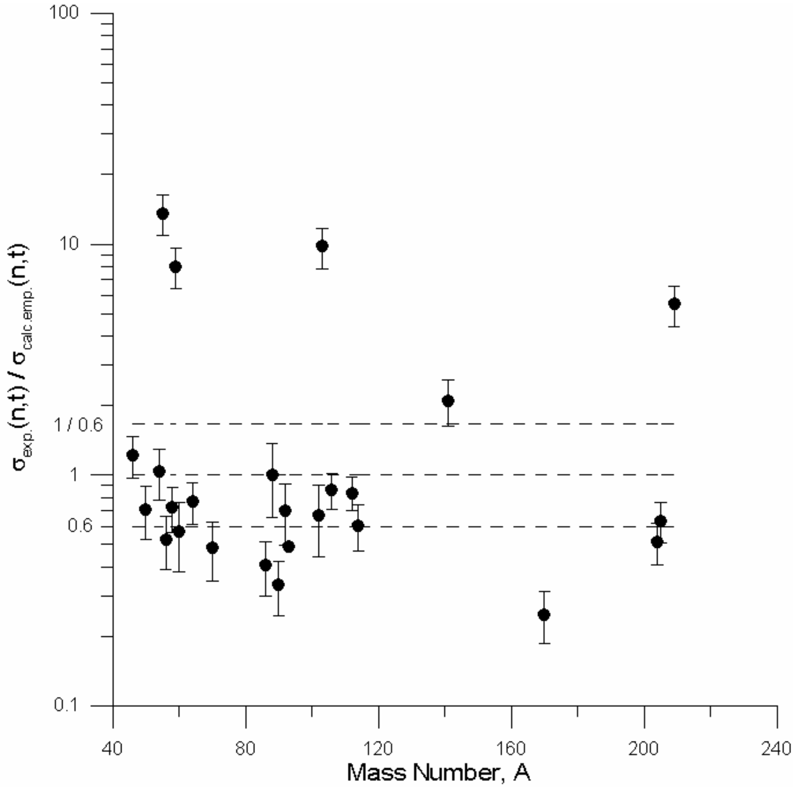
100
10
1 / 0.6
1
0.6
0.1
$\sigma_{exp.}(n,t) / \sigma_{calc.emp.}(n,t)$
40
80
120
160
200
240
Mass Number, A

Fig.6

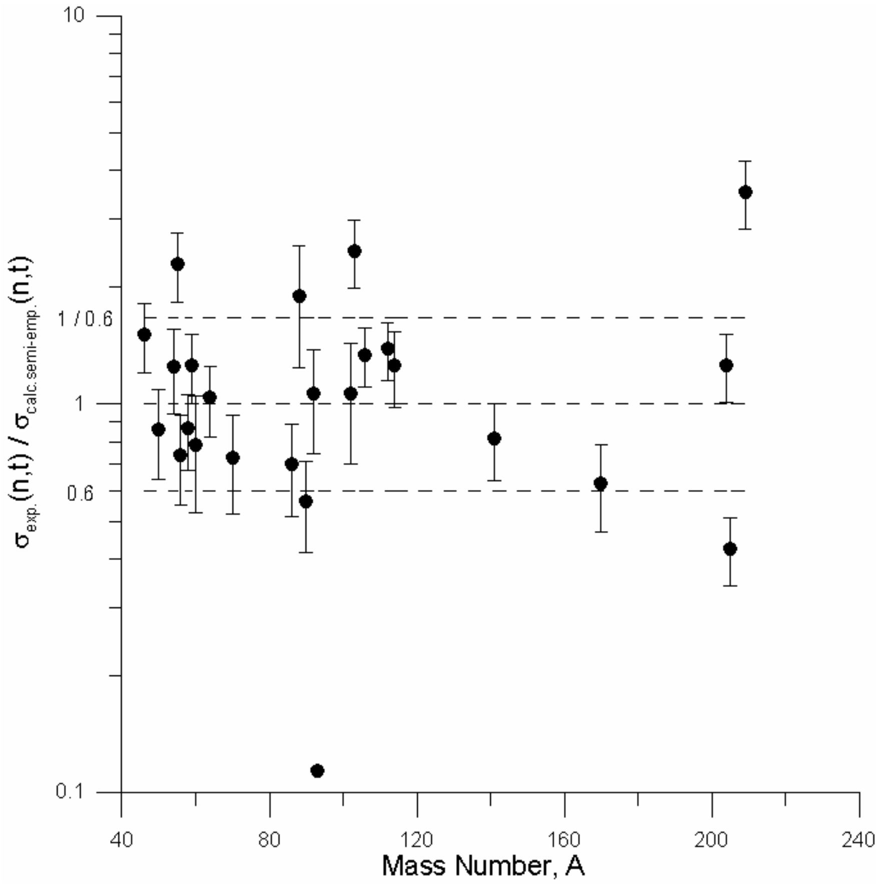
10
1 / 0.6
1
0.6
0.1
40
80
120
160
200
240
Mass Number, A
$\sigma_{exp.}(n,t) / \sigma_{calc.semi-emp.}(n,t)$

Fig. 7