CROSS SECTION EVALUATION OF THE (n, alpha) REACTION WITH FAST NEUTRONS ON $^{64}$Zn AND $^{147}$Sm NUCLEI USING THE HAUSER-FESHBACH APPROACH*

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Abstract. In the (n, α) reactions induced by neutrons with energy about some MeV the experimental data are very poor due to the difficulty of the measurement of the cross section. In this energy region of the incident neutrons the cross section is of order of tens mb or lower for emission of charged particles. It is supposed for both nuclei that the nuclear reaction is going by formation of an intermediate compound nucleus and this is suggested by the differential cross section experimental data. For the theoretical evaluation it was used the Hauser-Feshbach approach.

In this approach it is important to obtain the penetrabilities for neutron in the entrance channel and for charged particles (protons, alphas) in the exit channels. We have obtained the penetrabilities starting from quantum mechanical considerations and after that using them for obtaining the cross section. For this purpose we realized computer programs where it was implemented the regular and irregular functions in the integral form without any approximation. The theoretical and experimental evaluations of the $^{64}$Zn and $^{147}$Sm are important from theoretical point of view, nuclear reactor materials studies and astrophysical researches. Experimental data were measured using a double grided ionization chambers at electrostatic generators of FLNP - JINR Dubna (Russia) and Institute of Heavy Ions Physics from Pekin University (China).

Key words: fast neutrons, penetrability, cross sections.

1. INTRODUCTION

In this work will be evaluated the cross section in the $^{64}$Zn(n,α)$^{61}$Ni and $^{147}$Sm(n,α)$^{143}$Nd reaction with fast neutrons. For incident neutrons with energy of some MeV the experimental data are poor and therefore are of interest new theoretical and experimental investigations. For both nuclei we have chosen to start

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the evaluation using the Hauser-Feshbach approach [1]. In this formalism it is
supposed that the nuclear reaction is going by formation of a compound nucleus
CN) and the assumptions of the statistical model of nuclear reaction [2] are working.

After the interaction of the incident particle with the target nucleus the
formed CN has a time of life much longer than the time necessary to the incident
particle to traverse the target nucleus and therefore is considered that the CN
“forgets” how was formed and decays on one of possible channels. The CN and
residual nucleus is characterized by a large number of states. The nuclear potential
is considered to act in a finite range. Outside of this range the nuclear potential is zero.
The consequences of these assumptions are: there are not interference terms in the
cross section and the differential cross section is symmetrical to 90° in the SCM.

The 64Zn nucleus is medium one and the 147Sm is heavy. The experimental
differential cross section of 64Zn(n, α) reaction [3] and some new unpublished data
for 147Sm suggests that the dominant mechanism for these reaction is by formation
of a CN. It is obvious that for this incident neutron energy range of some MeV’s
other reaction mechanisms can give their contribution but this can be confirmed by
new experimental data on cross sections.

2. BASICS FORMULAS

For the evaluation of the cross section for (n, α) reactions in the frame of the
Hauser-Feshbach (HF) approach will be used the relation:

\[
\sigma_{\text{nn}} = \tau_\text{nn}^2 \sum_c T_c T_{\text{fluct}} F_{\text{fluct}}^{-1},
\]

where the terms are: \(\tau_\text{nn}\) = neutron reduced wave length, \(T\) = penetrability coefficient
for different particles (PC), \(T_{\text{fluct}}\) = widths correction fluctuation factor (WCF),
\(F_{\text{fluct}}\) = channel.

The penetrability coefficient represents the probability of a particle to pass a
potential barrier. In this approach the determination of the penetrability is very
important for the particles in the incident channel and for all possible outgoing
channels. The summation in (1) is realized over the incident channel and all
possible open outgoing channels.

Expression (1) is called the improved HF formula because first time this
relation was determined without the WCF factor. In the CN mechanism, according
with the Bohr hypothesis the CN “forgets” how is formed and therefore the
correlation between incident and outgoing channels is zero. However the
experience shows that is not always true and WCF factor indicates this correlation.
If there is no correlation between the incident and one emergent channel the WFC
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The way of obtaining of the PC can be found in many books, courses and manuals for quantum and nuclear physics. One is the semi-classical approach where the PC has the form:

\[
T(l, E) = \exp \left\{ -\frac{8m}{\sqrt{\pi^2}} \int_{0}^{\infty} \left[ V(r) + \frac{zZe^2}{r} + \frac{\hbar^2(l + 1)}{2mr^2} - E \right]^{1/2} dr \right\},
\]

(2)

where: \(m = \) reduced mass, \(V^\circ = \) the real part of the nuclear potential, \(\frac{zZe^2}{r} = \) Coulomb potential, \(z = \) charge of the particles, \(Z = \) charge of the nucleus, \(e = \) elementary charge, \(r = \) radius, \(\frac{\hbar^2l(l + 1)}{2mr^2} = \) centrifugal barrier.

The semi-classical approach is appropriate if the particle energy is much lower than the height of the potential barrier. If the energy of the particle is closing to the top of the barrier height this approach is not so exact.

Another way for the PC evaluation is a quantum mechanical approach using the reflection factor. According with [4] the reflection factor is:

\[
U_i = \begin{vmatrix} D_i - R \frac{1}{W_i} \left( \frac{dW_i^-}{dr} \right) & W_i^- \\ D_i - R \frac{1}{W_i} \left( \frac{dW_i^+}{dr} \right) & W_i^+ \end{vmatrix}, \quad (3)
\]

and PC is:

\[
T(l, E) = 1 - |U_i(E)|^2. \quad (4)
\]

From (4) the PC cannot be greater than unity. The calculation of the PC using the reflection factor has a more general character. This can be understood after we know the functions and parameters involved in (3) and (4) these are:

\(W_i^- (r) = \) outgoing wave function, \(W_i^+ (r) = \) ingoing wave function, \(D_i = R \left[ \frac{1}{W_i} \left( \frac{dW_i^-}{dr} \right) \right]_{r=R} = \) logarithmic derivative, \(W_i = \) particle wave function in the nuclear potential, \(R = \) the channel radius, \(l = \) particle orbital momentum.
The \( W_l(r) \) wave function is a solution of the radial Schrödinger equation and we can write this function like a linear combination of the ingoing and outgoing functions pondered by reflection factor \([4]\)

\[
W_i(r) \sim W_i^{-}(r) - U_i W_i^{+}(r) \tag{5}
\]

The ingoing and outgoing functions are a combination of regular and irregular functions. In the case of neutral particles the regular and irregular functions are the Neumann and Bessel functions \((n_l, j_l)\) and in the case of charged particles the regular and irregular Coulomb functions \((F_l, G_l)\). For neutral and charged particles respectively we have:

\[
W_i^{+}(r) = kr \left[ n_l(kr) \pm i \cdot j_l(kr) \right],
\]

\[
W_0^{+}(r) = kr \left[ F_l(kr) \pm i \cdot G_l(kr) \right]. \tag{6}
\]

The regular and irregular functions and their derivatives are easy to calculate for neutral particles. For charged particles the situation is more complicated. Many authors, evaluating the PC, use some approximation for the Coulomb functions. In this work the regular and irregular Coulomb functions were evaluated without any approximation using their integral representation \([5]\).

\[
F_l - iG_l = \frac{e^{-\rho}}{(2l+1)!} c_l(\eta) \int_0^\infty e^{-t(1+\eta)} (1+t)^{l+\eta} dt,
\]

\[
c_l(\eta) = \frac{2^\eta e^{-\gamma} \Gamma(l+1+\eta)}{\Gamma(2l+2)}. \tag{7}
\]

For the evaluation of the PC we realized computer programs which compute all these functions, their derivatives, other functions and parameters. Also, in the investigated \((n,\alpha)\) reactions we took into account the other open channels like, proton, gamma and inelastic neutron channels. For the investigated nuclei, the contribution of gamma penetrability’s can be neglected (calculated after relations from \([6]\)).

We present now the neutron energy dependence of the PC for neutral and charged particle.

In Fig. 1 are represented the PC for neutrons. We have reproduced with our software some examples from \([4]\) for checking. The PC obtained by us respect the condition requested by relation (4) and are not greater than unity with the increasing of the energy.
Fig. 1 – The energy dependence of the PC for neutrons with orbital momentum $l = 0, 1, 2$.

Figure 2 represents the PC for charged particles. If for neutral particles the software procedure is simple and is working fast, for charged particles PC the procedure is more complicated and needs more time for running.

We have reproduced many examples from [4] but here we present the most significant two examples, one for neutrons and one for charged particles.

Fig. 2 – The energy dependence of the PC for $\alpha$ particles with orbital momentum $l = 0, 1, 2$. 
2.2. The WCF factor

The WCF factor represents the correlation between the ingoing and outgoing channels. For our evaluation we used the WFC factor proposed in [7], [8] (Moldauer expression).

\[
F_{ab}^{\text{fact}} = \left(1 + \frac{2\delta_{ab}}{v_a} \right) \prod_{c} \left(1 + \frac{2T_c x}{\nu_c \sum_{j} T_j} \right)^{\delta_{ac} + \delta_{bc} + \nu_a},
\]

(8)

\[v_a = 1.78 + \left( T_{a,212} - 0.78 \right) e^{-0.228 \sum E_c}.
\]

The \( v_a \) is an empirical parameter and was obtained by Monte Carlo simulation [9, 10]. The WCF factor as we already mentioned above is equal to unity for uncorrelated ingoing and outgoing channels usually for low energy and slowly decrease with increasing of the energy. We have presented all functions, parameters necessary to evaluate the \((n, \alpha)\) cross section using the HF approach. We will show only the results for \(^{64}\text{Zn}\) and \(^{147}\text{Sm}\) nuclei but the software realized by us it is possible to obtain the \((n, \alpha)\) cross section for any nuclei with appropriate modifications.

3. RESULTS. CROSS SECTIONS

In our evaluation the neutrons with orbital momentum with \( l = 0, 1 \) are considered for \(^{64}\text{Zn}\) and \(^{147}\text{Sm}\) only those with \( l = 0 \) suggested by experimental data [11]. After the book keeping of the momentums, spins and parities according with the laws of conservation, in the exit channels were considered particles with all possible orbital momentum and also were considered the possible states of the compound and residual nucleus.

Theoretical cross section is smaller than the experimental points but we consider this evaluation good enough. We choose for the beginning a square well nuclear potential without imaginary part for all neutron, alpha and proton channels (\( V_n, V_p, V_{\alpha} \) in Fig. 3). Our theoretical HF evaluation is practically the same with the calculation of the TALYS (http://www.talys.eu) software with the same potential. Choosing a square well potential in fact we made the calculation to run faster because with this potential the internal wave function \( W_i \) from (5) can be considered a plane wave simplifying in this way the calculation. If we take another nuclear potential (a Wood-Saxon potential) will be necessary to find numerically the \( W_i \) function by solving the radial Schrödinger equation and after to calculate the logarithmic derivative \( D_i \) and the reflection factor \( U_i \) from (3).
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Fig. 3 – The $^{64}$Zn(n, α) cross section. The HF evaluation (continuous line) is compared with experimental data [3].

Fig. 4 – The $^{147}$Sm(n, α) cross section. The HF evaluation (continuous line) is compared with experimental data [11].

The present evaluation is also quite good. We have taken the simplest potential and it was obtained the order of magnitude of the experimental data. It is necessary to try more potentials (different potentials for different channels) and to include the contribution of the neutrons with orbital momentum $l = 1$. 
4. DISCUSSIONS

The investigation of the (n, α) reaction on $^{64}$Zn and $^{147}$Sm nuclei is important from theoretical point of view and for applications. The study of (n, α) reaction with fast neutrons provides new information about the reaction mechanisms. This energy region is poor on experimental data and new cross section experimental data are important for astrophysical researches and nuclear material science. The nucleus $^{64}$Zn is a component element of nuclear facilities and walls and due to this reaction takes place an accumulation of Helium in the walls and constructions materials. In time the accumulation process modifies the properties of the construction materials, changing their mechanical resistance. We evaluated the (n, α) cross section for mentioned nuclei using the HF approach. For this purpose was realized a complex software able to compute all necessary functions based on quantum mechanical considerations. The software is flexible and can evaluate the (n, α) cross section for other nuclei, considering the neutron incident channel and all possible open exit channels. The software also can evaluate the influence of different radius channels. In the presented evaluation the radius for different channels has the usual form in which the radius of residual nucleus is summated with the radius of emitted particles. Our calculation realized with a square potential well, compared with the experimental data are in a good agreement. The obtained results suggest us to try more type of potential. It is obvious that new data on differential cross section would be very useful for determination of the predominant reaction mechanism because in this energy range not only the CN mechanism can contribute to the cross section.

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