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Evaluation of $n + {}^{16}Fe$ reaction cross section at 14*MeV* incident energy

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Abstract

Cross section calculations have been carried out by some earlier scientists independent of energy surface imaginary potential. These have been characterized by a lot of disparity between authors and literature values. In this work, special attention was devoted to the increase in the accuracy of the calculation of nuclear data needed for structural materials. To do this, optical model (OM) scat 2 was applied using the deformed optical para magnetization. The results showed that the total cross section is numerically the sum of the shape elastic and compound nucleus formation cross section. Results obtained are in good agreement with literature values within ± 5%.

Keywords
Cross section, transmission coefficient, compound nucleus, and multiple particles.

1.0 Introduction

For the sake of preciseness, we retain the term "model" for those phenomenological theories of nuclear collisions that prescribe probabilities of compound nucleus formation. The expression "strong absorption model" is identified with those theories in which the chance of collision without compound nucleus formation is very small; the expression "moderate absorption model" labels those theories in which the chance is appreciable [1].

Generally, the evaluation of cross section leans as far as possible on experimental data [2]. But these may be insufficient, incoherent, sparse, etc. Hence, a lot of computer codes have been developed and are in use for studying nuclear reactions at various energies. These codes are generally used to predict and generate cross sections where experimental facilities are either not available [1] or are grossly inadequate or where the results of experiments need to be validated. A characteristic feature of neutron-induced reactions is the existence of a well-defined cross section. The total cross section is ill defined in the reactions induced by charge particles, since it contains the Rutherford scattering cross section which becomes extremely large for very small scattering angles. It then largely becomes an atomic phenomenon.

In previous work, the calculation of neutron cross sections took many paradoxes for grated. This has resulted in varying results in their calculations with large discrepancies. For

this, there has been persistent need for updates of results to resolve the discrepancies particularly between experimental and calculated values. This work has examined the cross sections within the range $25 < A < 65$ around 14*MeV* using the optical model code SCAT-2. This was necessitated by the conflicting results of previous workers. This work is limited to Iron (Fe) whose selection is informed by its proximity and its importance in the industrialization of this developing nation. It is also important in the spectral measurements related to the fusion reactor technology, fast neutron dosimetry and in radiation damage studies. The program SCAT-2 was one of the codes selected in the International Nuclear Model Inter Comparison (PRB3) of 1980 [2].

Above the resonance region, the general procedure to perform an evaluation should be directed towards an output that would generate

(i) transmission coefficients
(ii) strength functions
(iii) angular distributions $f(\theta, E)$
(iv) Cross sections (total compound and shape elastic) and
(v) Polarization $P(\theta, E)$

The SCAT-2 program includes 19 subroutines and uses the unit of length in *fm*, cross section in *mb(1mb =1 fm^2)* and energy in MeV. The allowed particles are neutron (n), proton (p), deuteron (d), triton (t), helium-3 (τ) and alpha (α). The main parts of the program are sketched in the following table:

Table 1.1

INPUT	*Physical system: (m, z) + (m, z) --> μ, k, z* Optical model potential: form factors (geometry) depths Solve the radial *Schrodinger* equation
PROCESSING	(1) Define the internal and external regions --> matching radius (2) External region --> Coulomb functions (3) Internal region --> step-by-step integration (4) Matching --> Partial scattering amplitudes η_{ij}
OUTPUT	Transmission coefficient T_{ij}, *T, (--> CNodes)* Strength functions Angular distributions $f(\theta, E)$, $a_1(E)$ Cross sections -Total -Compound (--> *CNodes)* -Shape elastic Polarization $f(\theta, E)$

The code EXIFON is based on an analytical model for statistical multistep direct and multistep compound reaction (SMD/SMC) models. It predicts emission spectra, angular distributions and activation cross sections including equilibrium, pre-equilibrium, as well as (collective and non-collective) processes. Multiple particle (second chance) emissions are considered up to three decays of the compound system. The model is restricted to neutron, proton and alpha particle induced reactions with neutrons, protons, alphas and photons in outgoing channels. The range of validity includes. Target mass numbers $A > 20$ and bombarding energies below 100*MeV*. In this code, a unique description of (*a, xb*) where *a, b = n, p,* α and γ (neutron, proton, alpha and gamma ray)based on many body theory and random matrix physics as well as excitation functions (activation cross sections) in proposed within a pure statistical multistep reaction model where

$$(a, xb) = (SMD) + (SMC) + (MPE)$$

The first term denotes the statistical multistep direct (SMD) part while the second the second term symbolizes the statistical multistep compound (SMC) emission. The sum of these two terms that is (SMD + SMC) represents the first chance emission process. Otherwise the multiple particle emission (MPE) reactions which are considered in a pure SMC concept and includes the second-chance, third-chance emissions etc. Hence their cross sections are given by

$$\frac{d\sigma_{a,xb}}{dE_b}(E_a) = \frac{d\sigma_{a,b}^{SMD}}{dE_b}(E_a) + \frac{d\sigma_{a,b}^{SMC}}{dE_b}(E_a) + \frac{d\sigma_{a,xb}^{MPE}}{dE_b}(E_a)$$

A is known as projectile, *b* is known as ejectile and *x* is possible ejectile. Nuclear reactions are usually measured by the probability of interaction that will take place. The probability per unit area per unit time is known as the cross section. Therefore the cross section is the probability that a reaction will take place and it has a unit of area. It is measured in cm^2 but the unit commonly used is barn (b) where $1b = 10^{-24}$ *cm*.

2.0 Basic theory

Considering two interacting particles of coordinates r, and r_2 , there exists a potential $V(r_1, r_2)$ between them. The corresponding *Schrodinger* equation is

$$\left[\frac{-\eta^2}{2m_1}\nabla_1^2 - \frac{\eta^2}{2m_2}\nabla_2^2 + V(r_1, r_2) - E\right]\Psi(r_1, r_2) = 0 \qquad (2.1)$$

where *E* is the total energy of the system, m_1, and m_2 are the masses of the particles and η is the plank constant. This two body problem is reduced to a one body problem in the centre of mass system. The coordinate *R* of the centre of mass is defined by $(m_1 + m_2)R = m_1 + m_2$ and; the relative coordinate *r* of the two particles is $r = r_1 + r_2$. Ignoring the center of mass motion, the transformed equation becomes

$$\left[\frac{-\eta^2}{2\mu}\nabla^2 + V(r) - E\right]\Psi(r) = 0 \qquad (2.2)$$

For free propagation ($V = 0$), the solution of equation (2.2) is the incident plane wave

$$\Psi(r) = exp(ik.r) \qquad (2.3)$$

where *k* is the wave vector with $k^2 = \frac{2\mu E}{\eta^2}$. A spherical outgoing wave and the asymptotic form of the wave function is

$$\psi(r) = \exp(ik.r) + \frac{1}{r} f(\theta)\exp(ikr).$$

The radial wave equation becomes for a central potential

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\eta^2}\mu(r) + \frac{l(l+1)}{r^2}\right]U_1(r) = 0$$

where $\mu = M/(m+M)$ and U(r) is the given potential. These asymptotic and radial equations can be solved in the internal region of the nucleus for a given potential $U(r) = 0$.

If $U(r) \leq 0$, the imaginary part of the complex potential has the effect of absorbing flux from the incident beam. To calculate the total absorption cross section, we first of all evaluate the total inward flux over a large sphere of radius *R* and then divide by the number of incident particles per square centimeter per second [3]. Thus,

$$\sigma_A = \frac{\pi}{k^2}\sum(2L+1)(1-|S_L|^2) \tag{2.4}$$

while the elastic cross section is given by

$$\sigma_E = \sum_L^{\infty} 4\pi\Delta^2(2L+1)(1-R_e\eta_L) \tag{2.5}$$

The value $R_L\eta_L$ can also be represented by $S_{L,} = exp(2i\sigma_L)$ known as the scattering matrix element or transmission coefficient. The total cross section is the sum of the elastic and absorption cross section σ_E and σ_A. Therefore

$$\sigma_T = \sigma_A + \sigma_E = \frac{\pi}{k^2}\sum_L(2L+1)(1-|S_L|^2) + \frac{\pi}{k^2}\sum_L(2L+1)(1-|S_L|^2) \tag{2.6}$$

$$\sigma_L = \frac{\pi}{k^2}\sum_L(2L+1)(1-R_eS_L) \tag{2.7}$$

Transmission coefficient $T_l = 0$ for $S = 0$ and is equal to

$$\frac{1}{(2S+1)(2S+1)}\sum_{j=|l-s|}^{l+S}(2j+1)T_{ij}\text{ , for S < 0} \tag{2.8}$$

The optical model is useful only in discussing energy behavior in reactions such as scattering. Many of the interesting features of the microscopic structure of nuclei are accounted for indirectly only in this average way. Nevertheless, the optical model is successful in accounting for elastic and inelastic scattering and leads us to an understanding of the interactions of nuclei.

3.0 Calculations

The optical potential was taken in its conventional form consisting of its real potential with the Woods-Saxon form factor, a surface imaginary part with derivative of the Woods-Saxon form factor and a real spin-orbit Thomas terms. The solution has the form [4]

$$U(r) = V_c(r) - V_r f(r) - i[4Wg(r) + Wr f(r)] + C_{so}[LS]V_{so}h(r) \tag{3.1}$$

where the five terms represent the Coulomb Potential, the real volume potential, an imaginary surface potential and a spin orbit potential respectively; *f (r), g(r)* and *h(r)* are the form factors. For practical purposes the Coulomb Potential, *Vjr)* of the target nucleus is assumed to be the potential due to a uniformly charged sphere of radius *R*, [5].

$$V_c = \frac{ZZ'e^2}{r} \quad if\ r > R_c$$

$$V_c = \frac{ZZ'e^2}{2R_c}\left[3 - \frac{r^2}{R_0^2}\right] \quad if\ r < R_c \tag{3.2}$$

where Z and *Z'* are the charges of the incident particle and the target nucleus. On the other hand, the real potential has a Woods-Saxon form factor.

$$f(r) = \left[1 - \exp\left(\frac{r - R_1}{a_{11}}\right)\right]^{-1} \quad with\ R_1 = r_1A^{1/3} \tag{3.3}$$

and the imaginary potential factor can be either surface or volume peaked. A surface

peaked form factor can have either a derivative Woods-Saxon shape [6].

$$g(r) = \exp\left(\frac{r-R_2}{a_2}\right)\left[1-\exp\left(\frac{r-R_2}{a_2}\right)\right]^{-1} \quad with\ R_2 = r_2 A^{1/3} \tag{3.4}$$

Or a Gaussian shape

$$g(r) = Exp\left[-\left(\frac{r-R_2}{a_2}\right)^{-2}\right] \quad with\ R_2 = r_2 A^{1/3} \tag{3.5}$$

This is sometimes used for low energy neutrons. A volume from factor has a Wood-Saxon shape

$$f(r) = \left[1+\exp\left(\frac{r-R_3}{a_3}\right)\right]^{-1} \quad with\ R_3 = r_3 A^{1/3} \tag{3.6}$$

The spin orbit form factor has a Thomas shape

$$f(r) = \frac{1}{r}\frac{d}{dr}\ f(r) = \frac{1}{ra^4}\exp\left(\frac{r-R_4}{a_4}\right)\left[1+\exp\left(\frac{r-R_4}{a_4}\right)\right]^{-2} \quad with\ \ R_4 = r_4 A^{1/3} \tag{3.7}$$

The spin orbit coupling constant, C_{so} is nearly equal to 2 $fm^{2.}$ The calculation was carried out using the deformed optical model parametization of [6] for medium mass nuclei at low energies expressed as

$$U = 52.095\text{-}0.735E\text{-}0.195E2\ \text{-}11.528(1\text{-}0.171E)\eta \tag{3.8}$$

$$W_s = 0.343\ \text{-}\ 0.337E + 0.304E2\ \text{-}1.234(1\text{-}1.366E)\eta \tag{3.9}$$

$$a_v = a_{so} = 0.645fm$$
$$r_v = r_s = 1.24\ fm$$
$$V_{so} = 7.4\ 1Me\ V$$

where E is the incident, η is the isotopic factor $(N - A)/A$

These calculations however show that the neutrons cross sections were calculated independent of energy surface imaginary potential, [4]. For the present postulations, it was necessary to include a little energy dependence to describe the cross section at higher energies by increasing the imaginary part of the potential. The optical parameters finally used were as follows:

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$$V_0 = 501\text{-}3EMe\ V,\ a_o = 052fm$$
$$W_s = 22 + 2EMe\ V,\ a_v = 0.40fm,\ r_0 = r_w = r_{so} = 1.23fm$$
$$V_{so} = 7.5MeV,\ a_{so} = a_o$$

For each incident energy, we used five (5) potential parameter sets of earlier scientists for ease of comparison. The parameter sets were those of Wilmore-Hodgson (I), Bechetti-Greeless (II), Fever-Rapaport (III), Bercilo-Cindro (IV) and Madland (V) respectively [7,8,9,10]. For each parameter set, the following calculations were performed:

(i) Transmission coefficients as a function of angular momenta.
(ii) The differential cross sections as function of scattering angles.
(iii) Calculations for cross sections (compound nucleus, shape elastic and total) as functions of

incident energies are shown in Tables 3.1, 3.2 and 3.3. Column 6 of these Tables represents the present calculations, which are in consonance with earlier results. All, calculations were limited to incident energies around 14*MeV*, i.e. 13.5 - 14.5*MeV*.

Table 3.1: Calculated compound nucleus cross-sections as calculated using the 5 parameters. *E* is energy in MeV and *P* is the parameter used.

PE	I	11	I I I	IV	V	PP
13.5	1.40	1.60	1.49	1.31	1.84	1.40
13.7	1.39	1.59	1.49	1.31	1.84	1.37
13.9	1.39	1.59	1.49	1.31	1.85	1.39
14.0	1.39	1.59	1.49	1.31	1.85	1.39
14.2	1.39	1.58	1.48	1.31	1.86	1.39
14.4	1.39	1.58	1.48	1.31	1.86	1.37
14.5	1.39	1.58	1.48	1.31	1.86	1.39

Table 3.2: Calculated shapes elastic cross-section using the parameter and the standard present parameter**.**

Parameter energy	1	I I	111	I V	V	PI,
13.9	1.26	1.29	1.33	1.22	1.34	1.26
13.9	1.25	1.28	1.31	1.20	1.33	1.25
13.9	1.23	1.26	1.30	1.18	1.33	1.23
14.0	1.22	1.26	1.29	1.17	1.32	1.23
14.2	1.20	1.24	1.27	1.15	1.32	1.20
14.4	1.18	1.23	1.26	1.14	1.31	1.18
14.5	I.A 8	1.23	1.25	1.13	1.31	1.18

Table 3.3: Calculated total cross section

Parameter energy	1	11	111	IV	V	PP
13.5	2.66	2.89	2.82	2.53	3.11	2.66
13.7	2.64	2.89	2.87	2.51	3.17	2.64
13.9	2.62	2.85	2.78	2.50	3.17	2.62
14.0	2.61	2.85	2.77	2.48	13.17	2.61
14.2	2.59	2.83	2.75	2.46	3.17	2.59
14.4	2.57	2.81	2.74	2.45	3.18	2.57
14.5	2.57	2.80	2.73	2.44	3.18	2.52

These results (Tables 3.1 – 3.3) were compared with earlier work using optical model code EXIFON we arrive at Table 3.4 below.

Table 3.4: Comparison of results with calculations using OM code EXIFON

Optical model code SCAT-2	Optical model code exifon (2002)

Energy *MeV*	**Compound nucleus cross section**	**Shape elastic cross section**	**Total (T_1) Cross section**	**Statistical multistep compound nucleus**	**Multiple Particle emission**	**Total (T_2)**	$\left(\frac{T_1 - T_2}{T_1}\right)\%$
13.1	1.40	1.26	2.66	1.442	1.037	2.479	6.8
13.6	1.37	1.25	2.64	1.438	1.028	2.466	6.8
13.8	1.39	1.23	2.62	1.434	1.018	2.452	6.5

Table 3.4: Comparison of results with calculations using OM code EXIFON (contd.)

Optical model code SCAT-2				**Optical model code exifon (2002)**			
Energy *MeV*	**Compound nucleus cross section**	**Shape elastic cross section**	**Total (T_1) Cross section**	**Statistical multistep compound nucleus**	**Multiple Particle emission**	**Total (T_2)**	$\left(\frac{T_1 - T_2}{T_1}\right)\%$
14.0	1.39	1.22	2.61	1.429	1.009	2.438	6.5
14.2	1.39	1.20	2.59	1.425	1.000	2.425	6.3
14.4	1.37	1.18	2.57	1.421	0.991	2.412	6.2
14.6	1.39	1.18	2.57	1.417	0.928	2.399	5.1

Observations show that the values of the cross-sections in each case are approximately equal to the sum of the compound nucleus cross sections. The compound, shape elastic and total cross sections as functions of neutron energies for each isotope vary appreciably from one isotope to the other. Comparisons with previous experimental and calculated values (Table 3.4) are in good agreement within ±6% of calculations earlier done using EXIFON Code and other scientists. The differences may be due to the resulting differences between the laboratory energies of the projectiles (the laboratory system) and the center of mass energy system (CMS) used in measurements and calculations respectively.

It is also noticed that the compound nucleus, shape elastic and total cross sections using optical model code SCAT 2 approximately equal to the statistical multistep compound multi particle emission and the total cross section using the optical model code Exifon version 2 respectively.

These values are collated and used for comparison of results gotten from experimentation. Positive correlation helps in the determination of the right materials needed for dosimetry in the nuclear industry.

Generally, between incident energies 13*MeV* and 15*MeV*, the transmission coefficient oscillates sinusoidally at low angular momenta ($0 < L < 5$) and therefore decays exponentially to zero at approximately $L = 7$. This is because the wave function is exponential ($\Psi = exp(ikr)$), which comprises of the plane wave (real part) and the scattered wave (imaginary part)., It is also observed that at all incident energies and angular momenta the transmission coefficient is less than unity. Unlike in the case of transmission coefficients, calculations show that the differential cross sections, using the five parameter sets decay rapidly from each peak value to a minimum of zero at approximately 40° scattering angles which is less than the maximum scattering angle of a projectile (45°) at maximum height (i.e. $Sin40^0 < Sin45° = 1$) which is less than unity.

4.0 Conclusion

The main emphasis of this study was to devote special attention to the increase of the accuracy in the calculation and evaluation of nuclear data needed for dosimetry and structural materials around 14*MeV*. This is achieved by the inclusion of a little energy dependence to the earlier parametization of Cabezas [4]. The comparison of our data with

previous results using the statistical multi-step code EXIFON2 as presented in Table 4 shows a good agreement with most recent data.

Our data would be very helpful for new evaluations of cross sections for other materials and for reaction model calculations, as better data could constrain some of the nuclear parameters (level densities, for examples) entering into the calculations. By the

same token we see that the code SCAT 2 can be successful in reproducing experimental emission spectra for both different incident energies and different nuclei.

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