

Theoretical determination of (d, n) and (d, 2n) excitation functions of some structural fusion materials irradiated by deuterons

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Abstract Nuclear fusion is one of the world's primary energy sources. Studies on the structural fusion materials are very important in terms of the development of fusion technology. Chromium, nickel, zinc, scandium, titanium, and yttrium are important structural fusion materials. In this paper, for use in nuclear science and technology applications, the excitation functions of the $^{50}\text{Cr}(d, n)^{51}\text{Mn}$, $^{58}\text{Ni}(d, n)^{59}\text{Cu}$, $^{64}\text{Zn}(d, n)^{65}\text{Ga}$, $^{66}\text{Zn}(d, n)^{67}\text{Ga}$, $^{45}\text{Sc}(d, 2n)^{45}\text{Ti}$, $^{47}\text{Ti}(d, 2n)^{47}\text{V}$, $^{48}\text{Ti}(d, 2n)^{48}\text{V}$, and $^{89}\text{Y}(d, 2n)^{89}\text{Zr}$ nuclear reactions were investigated. The calculations that are based on the pre-equilibrium and equilibrium reaction processes were performed using ALICE–ASH computer code. A comparison with geometry-dependent hybrid model has been made using the initial exciton numbers $n_0 = 4\text{--}6$ and level density parameters $\alpha = A/5; A/8; A/11$. Also, the present model-based calculations were compared with the cross sections obtained using the formulae suggested from our previous studies. Furthermore, the cross section results have been compared with TENDL data based on TALYS computer code and the measured data in the literature.

Keywords Cross section · Fusion materials · Geometry-dependent hybrid model

1 Introduction

The cross section data are indispensable in a lot of applications in the history of nuclear physics. Especially, data on cross sections of nuclear reactions induced by deuterons are required to describe the nucleus–particle interaction. This interaction represents a good test for both nuclear models and evaluation of nuclear reaction data [1, 2]. The deuteron particle has a weak binding energy of 2.224 MeV. So, it is responsible for the high complexity of the interaction process, which involves a variety of nuclear reactions produced by the proton and neutron following the deuteron breakup [1]. The available cross sections for the nuclear reactions induced by the deuterons in literature show large discrepancies. Actually, because the experimental studies for these reactions are quite poor, more measurements and theoretical studies must be carried out. Hence, the nuclear models for particle-induced reactions are very useful since they can be provided for estimating the cross sections quickly [3]. Particularly, both experimental and theoretical cross section data around 14 MeV are of considerable importance for verifying the accuracy of nuclear models [4, 5]. On the other hand, the nuclear fusion will not contribute to acid rain and global warming because it will not produce SO_2 or CO_2 . So, it offers the best hope as an energy source for the future generations. The success of the energy production from fusion requires the development of structural materials for fusion reactors. In this framework, the selection of structural fusion materials is very important for nuclear fusion reactors. Chromium, nickel, zinc, scandium, titanium, and yttrium are important elements of structural fusion materials. In this paper, the deuteron reaction cross sections of these structural materials were calculated using different input

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parameters and nuclear models in the ALICE–ASH computer code [9]. And also, the (d, n) and (d, 2n) cross section systematics were used at cross section calculations for the investigated deuteron reactions. In the calculations, the effect on cross sections of the variation of initial exciton number and level density parameters has been investigated by the geometry-dependent hybrid (GDH) model [10] in the ALICE code. Also, the initial exciton configuration is an important input parameter in the GDH model [11]. We used three particles–one hole and four particles–two holes for initial exciton configuration in the pre-equilibrium reaction process. Furthermore, the cross sections for the considered nuclear reactions were estimated using different level density parameters via Fermi gas model. Therefore, the exciton numbers ($n_0 = 3p-1$ h to $4p-2$ h) and the nuclear level parameters ($\alpha = A/5; A/8; A/11$) were varied obtaining a good agreement between the experimental and model calculations.

2 Theoretical calculation methods

Recently, a lot of theoretical calculation and experimental data analysis on the pre-equilibrium reaction mechanism have been reported because of the strong competition between the pre-equilibrium and equilibrium emissions of light particles [8, 11–13]. Energetic light particles in the pre-equilibrium emissions have generally been emitted at the initial stage of interactions of target nucleus with incident particle. Actually, the features of excitation functions at low, medium, and high incident energies may reveal the characteristics of the nuclear reaction mechanism. The equilibrium decay process dominates at the portion with low energy of the excitation function, but the pre-equilibrium decay becomes important with increasing incident energies, and a slowly decreasing tail at the excitation function becomes apparent [12]. Hence, the excitation functions for nucleon emissions in a nuclear reaction may be measurable at incident energies where pure evaporative processes are greatly favored. In addition, the time scale at which the pre-equilibrium emissions occur is very short, $\approx 10^{-21}$ s, while the equilibrium nuclear processes take a longer time, 10^{-16} – 10^{-18} s. Several models for explaining the pre-equilibrium and equilibrium reaction mechanisms have been proposed, including the Weisskopf–Ewing model, Hauser–Feshbach model, hybrid model, exciton model, and geometry-dependent hybrid model. The ALICE-ASH code has widely been used for the analysis of experimental values. This may be because of the fact that theoretical calculations with ALICE code are usually found to give reasonably good agreement with the measured values [12]. The ALICE–ASH code is a modified and advanced version of

the ALICE code. This code can calculate the cross sections, angular distribution, and energy of particles in nuclear reactions produced by nuclei and nucleons with projectile energies up to 300 MeV [9]. The equilibrium particle emission can be calculated using the Weisskopf–Ewing (WE) model [14]. The basic nuclear input parameters in the WE model are the nuclear level density parameter, nuclear binding energy, inverse nuclear reaction cross section, and pairing energy. The probability of evaporation in the WE model is calculated as follows,

$$W_x(\varepsilon_x) \propto (2S_x + 1)\mu_x \varepsilon_x \sigma_x^{\text{inv}}(\varepsilon_x) \frac{\rho(Z', A', U)}{\rho(Z, A, E)}, \quad (1)$$

where the term “ x ” denotes the type of particle. The terms “ S_x ”, “ μ_x ”, and “ ε_x ” are the spin, reduced mass, and emitted particle energy, respectively. The term σ_x^{inv} is inverse reaction cross section. The term “ E ” represents excitation energy for the emitting nucleus. $\rho(Z, A, E)$ and $\rho(Z', A', U)$ represents the nuclear level density for the x —particle emitted from the nucleus and the residual nucleus with “ U ” excitation energy, respectively [9].

The hybrid model [15] and GDH model [10] can be used to calculate the particle spectrum. The pre-equilibrium particle spectrum in GDH model is written as follows,

$$\frac{d\sigma}{d\varepsilon_x} = \pi\lambda^2 \sum_{l=0}^{\infty} (2l+1)T_l \sum_{n=n_0}^{\infty} X_n \frac{\omega(p-1, h, U)}{\omega(p, h, E)} \frac{\lambda_x^e}{\lambda_x^e + \lambda_x^+} gD_n, \quad (2)$$

where the “ λ ” and “ T_l ” represent the reduced de-Broglie wavelength of projectile particle and the transmission coefficient for l -th partial wave, respectively. X_n symbolizes the number of x —nucleons for the n —exciton state. “ ε_x ” and “ n_0 ” are the channel energy of nucleon and the initial exciton number, respectively. $\omega(p, h, E)$ represents the exciton state density at “ E ” excitation energy with “ p ” particles and “ h ” holes. “ D_n ” is a depletion factor determined by the work of Ref. [16], which takes into consideration the depletion of the n -exciton state due to nucleon emission. The final excitation energy is written as follows,

$$U = E - Q_x - \varepsilon_x. \quad (3)$$

Here the term “ Q_x ” is the separation energy of nucleon. In addition, the emission rate of nucleon is written as follows,

$$\lambda_x^e = \frac{(2S_x + 1)\mu_x \varepsilon_x \sigma_x^{\text{inv}}(\varepsilon_x)}{\pi^2 \hbar^3 g_x}. \quad (4)$$

The term “ g_x ” denotes single particle density. The density is equal to $\frac{Z}{14}$ for protons and $\frac{N}{14}$ for neutrons. The intranuclear transition rate is written as follows,

$$\lambda_x^+ = V\sigma_0(\varepsilon_x)\rho_l, \quad (5)$$

where “ ρ_l ” denotes the average nuclear matter density at the distance from $l\lambda$ to $(1+l)\lambda$. The term “ V ” represents the velocity of a nucleon in nucleus and also the term “ σ_0 ” is the nucleon–nucleon scattering cross section corrected for the Pauli principle [9].

The TENDL based on TALYS model code is a nuclear data library, of which output contains in ENDF format nuclear data for use in both basic physics and applications. It has been updated annually since 2008. The TENDL database library includes data for stable and unstable target nuclei. The TENDL includes sub-libraries for bombarding photon, proton, neutron, deuteron, triton, ^3He , and ^4He particles from 10^{-5} eV up to 200 MeV [17].

The semi-empirical and empirical formulae based on the systematics of the measured excitation functions have been widely used to evaluate the cross sections at different energy ranges. These formulae work very well for a quick prediction of the cross sections. In general, the empirical and semi-empirical formulae of the nuclear reactions contain the exponential dependence of nuclear cross sections upon the proton and neutron numbers in the nucleus. In recent years, the cross section systematics for different nuclear reaction channels were suggested by various studies [4, 18–21]. In previous investigations, we presented new empirical formulae to describe the cross sections of (d, n) and (d, 2n) nuclear reactions produced by deuteron particles. The empirical nuclear cross section formula of (d, n) reactions induced by deuterons at energy of 8.6 MeV is given as follows [20],

$$\sigma(d, n) = 14.1 \left(A^{1/3} + 1 \right)^2 e^{-2.54s}. \quad (6)$$

On the other hand, for (d, 2n) nuclear reactions at incident energies between 11.57 and 18.91 MeV, it is assumed that the cross section systematic including non-elastic and Coulomb effects is given as follows,

$$\sigma(d, 2n) = 0.64Z^2 \left(A^{1/3} + 2^{1/3} \right) e^{-17.52s}, \quad (7)$$

where the term “ s ” is the asymmetry parameter [21].

3 Results and discussion

In this paper, the cross sections of the ^{50}Cr (d, n) ^{51}Mn , ^{58}Ni (d, n) ^{59}Cu , ^{64}Zn (d, n) ^{65}Ga , ^{66}Zn (d, n) ^{67}Ga , ^{45}Sc (d, 2n) ^{45}Ti , ^{47}Ti (d, 2n) ^{47}V , ^{48}Ti (d, 2n) ^{48}V , and ^{89}Y (d, 2n) ^{89}Zr nuclear reactions were calculated using different input parameters in the ALICE–ASH computer code and also the cross section formulae. Furthermore, the calculated cross sections for these nuclear reactions are compared with the available experimental data [22] and TALYS-based TENDL library data [17]. The excitation functions are

presented in Figs. 1, 2, 3, 4, 5, 6, 7 and 8 as a function of projectile particle energy. The WE model for equilibrium state and the GDH and hybrid models for pre-equilibrium state in these calculations were used. Changing the initial exciton number and nuclear level density parameter in pre-equilibrium GDH model calculations of the effects on the calculated cross sections was investigated. The Fermi gas model with $\alpha = A/8$ parameter is used to calculate the nuclear level density in the equilibrium model. The initial exciton number and level density parameter in the hybrid model calculations are taken as $n_0 = 4$ and $\alpha = A/8$, respectively. The initial exciton number in the GDH model calculations are taken as $n_0 = 4$ –6. In addition, the nuclear level parameters for initial exciton numbers ($n_0 = 3p - 1h$ to $4p - 2h$) in the GDH model are taken as $\alpha = A/5$; $A/8$; $A/11$. Thus, the effects of these input parameters on the cross sections are investigated.

3.1 (d, n) nuclear reactions

3.1.1 ^{50}Cr (d, n) ^{51}Mn nuclear reaction

The nuclear cross sections for the ^{50}Cr (d, n) ^{51}Mn reaction are presented in Fig. 1 up to the projectile energy of 15 MeV. According to the excitation functions obtained using different input parameters in the ALICE–ASH computer code, the maximum cross section is 252.9 mb at deuteron energy of 6 MeV. The available experimental cross sections reported by Klein et al. [23] at incident deuteron energies above 5.68 MeV are in good agreement with the calculated results using the initial exciton number $n_0 = 4$ in the pre-equilibrium hybrid and GDH models. Additionally, the cross section values obtained using the initial exciton number $n_0 = 4$ in the pre-equilibrium nuclear models are agreeing fairly well with the data of Cogneau et al. [24] at the energies below 10 MeV. The cross section values of the GDH calculations (for $n_0 = 6$ and $\alpha = A/8$) and TALYS-based TENDL library data match well with each other. The cross section results obtained using the systematic of Yiğit [20] is 279.4 mb at the deuteron energy of 8.6 MeV for the ^{50}Cr (d, n) ^{51}Mn nuclear reaction. From Fig. 1, it is shown that the cross section point obtained by the systematic [20] is higher than the experimental value of 191.6 mb reported by Cogneau et al. [24] at the deuteron energy of 8.6 MeV.

3.1.2 ^{58}Ni (d, n) ^{59}Cu nuclear reaction

The excitation functions for the ^{58}Ni (d, n) ^{59}Cu reaction are shown in Fig. 2 up to the deuteron energy of 15 MeV. The theoretical model calculations reach the maximum cross section value of 130.5 mb at 5.5 MeV energy. The cross section calculations are generally consistent with the

Fig. 1 Cross section values of the $^{50}\text{Cr}(d,n)^{51}\text{Mn}$ nuclear reaction with the data reported by Klein et al. [23], Cogneau et al. [24], and Yiğit [20]

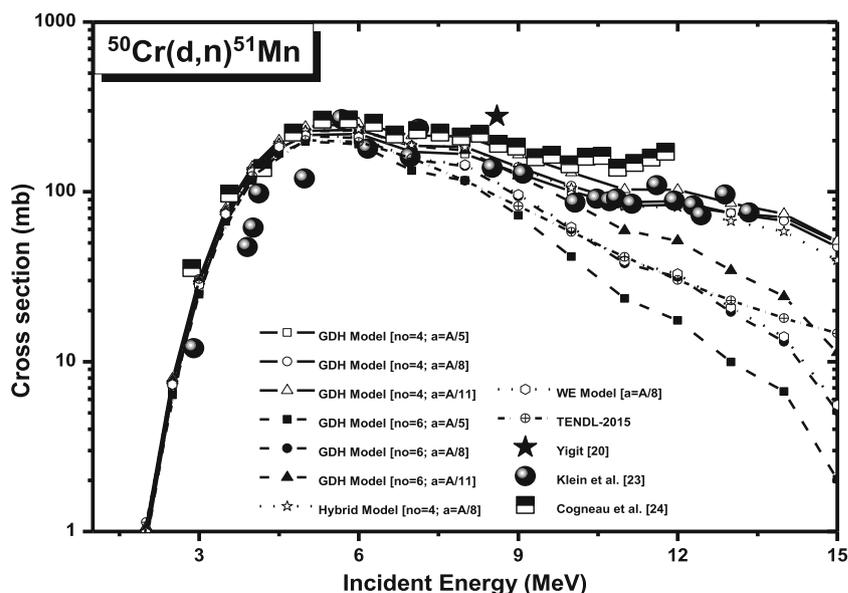
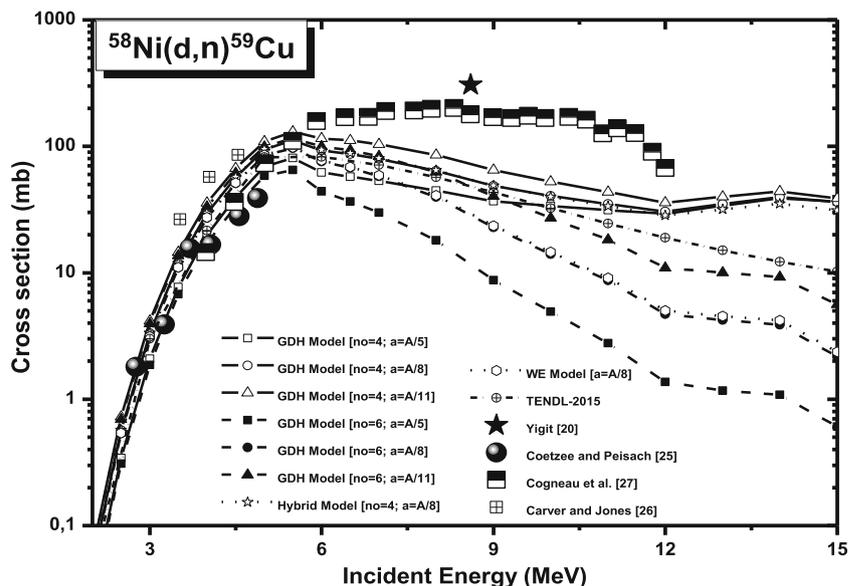


Fig. 2 Cross section values of the $^{58}\text{Ni}(d,n)^{59}\text{Cu}$ nuclear reaction with the data reported by Coetzee and Peisach [25], Carver and Jones [26], Cogneau et al. [27], and Yiğit [20]



experimental values of Coetzee and Peisach [25] and Carver and Jones [26]. The experimental data reported by Cogneau et al. [27] at energies above 5.91 MeV give higher cross sections than the calculated excitation functions and TENDL evaluated data. On the other hand, four data points measured by Cogneau et al. [27] at energies below 5.91 MeV show a very good agreement with the model-based cross section values. It should be noted that the GDH model and hybrid model calculation results (for $n_0 = 4$ and $\alpha = A/8$) by the ALICE-ASH code for the investigated reaction give almost the same results. The cross section value obtained using the empirical formula of Yiğit [20] is higher than other predictions and the experimental result of Cogneau et al. [27] at deuteron energy of 8.6 MeV.

3.1.3 $^{64}\text{Zn}(d,n)^{65}\text{Ga}$ nuclear reaction

The cross section calculations and experimental data reported by Coetzee and Peisach [25] and Bissem et al. [28] for the $^{64}\text{Zn}(d,n)^{65}\text{Ga}$ nuclear reaction are shown in Fig. 3 up to the projectile energy of 26 MeV. The model-based cross section results are in good agreement with the data of Coetzee and Peisach [25]. Moreover, the nuclear excitation function reported by Bissem et al. [28] in the energy region of 11.7–25.8 MeV is in excellent agreement with the GDH model calculation results predicted by the initial exciton number $n_0 = 4$. The excitation functions have maximum cross section values about incident deuteron energies of 5–9 MeV. The cross section value

Fig. 3 Cross section values of the $^{64}\text{Zn}(d, n)^{65}\text{Ga}$ nuclear reaction with the data reported by Coetzee and Peisach [25], Bissem et al. [28], and Yiğit [20]

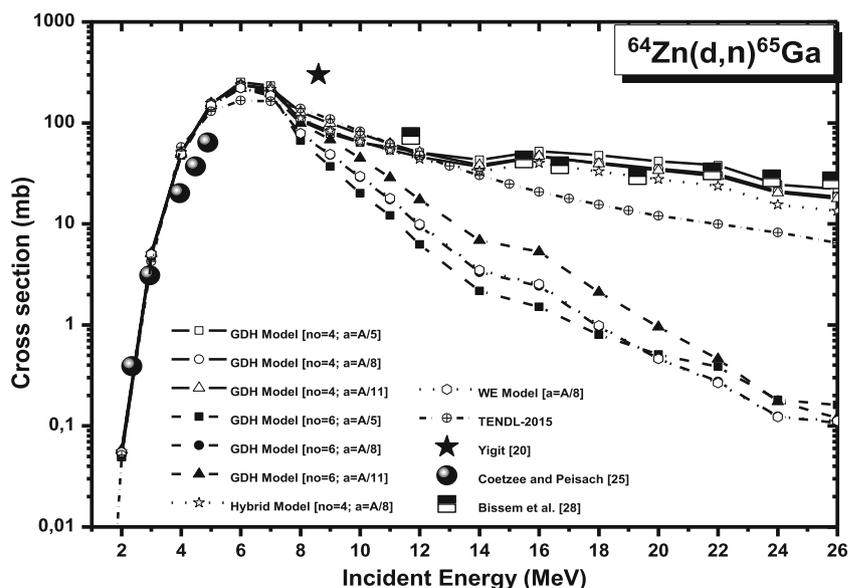
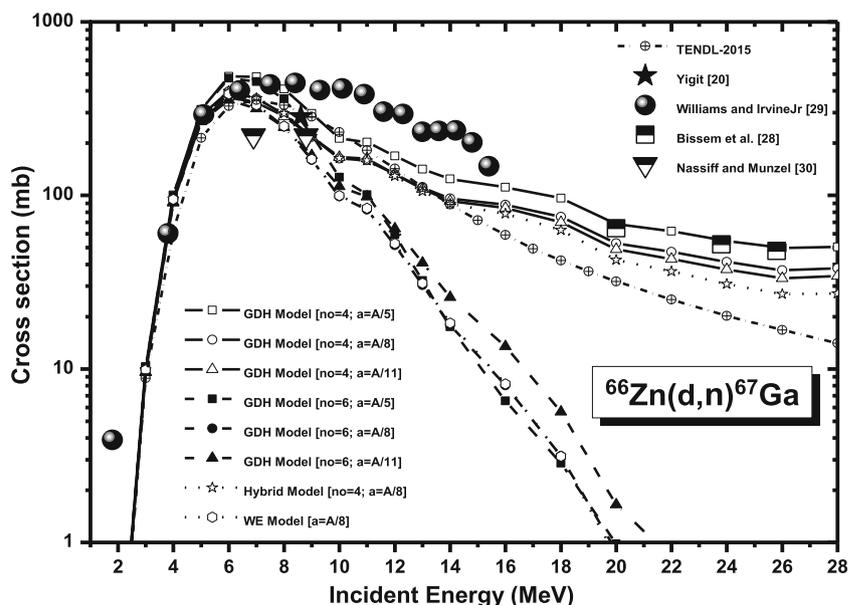


Fig. 4 Cross section values of the $^{66}\text{Zn}(d, n)^{67}\text{Ga}$ nuclear reaction with the data reported Williams and Irvine Jr [29], Bissem et al. [28], Nassiff and Munzel [30], and Yiğit [20]



obtained using the empirical formula of Yiğit [20] is 300.7 mb at 8.6 MeV deuteron energy. There is no experimental data on the cross section at this energy. The cross section point of Yiğit [20] is higher than the other cross section calculations.

3.1.4 $^{66}\text{Zn}(d, n)^{67}\text{Ga}$ nuclear reaction

The experimental data and model calculations for the $^{66}\text{Zn}(d, n)^{67}\text{Ga}$ nuclear reaction are shown in Fig. 4 up to the deuteron energy of 28 MeV. The model-based excitation functions have maximum cross sections about projectile energies of 5–9 MeV. The nuclear model calculations are in acceptable agreement with the

experimental results of Williams and Irvine Jr [29] up to the maximum energy region of excitation functions. The pre-equilibrium GDH model calculations estimated by the initial exciton number $n_0 = 4$ give a reasonable estimate of three data points reported by Bissem et al. [28] at the energy range of 20–25.8 MeV. The cross section value calculated using the empirical formula of Yiğit [20] is 284.45 mb at the deuteron energy of 8.6 MeV. In addition, the cross section value of Yiğit [20] is quite compatible with the TENDL library and the data of Nassiff and Munzel [30].

Fig. 5 Cross section values of the $^{45}\text{Sc} (d, 2n) ^{45}\text{Ti}$ nuclear reaction with the data reported by Hermanne et al. [31] and Yiğit [21]

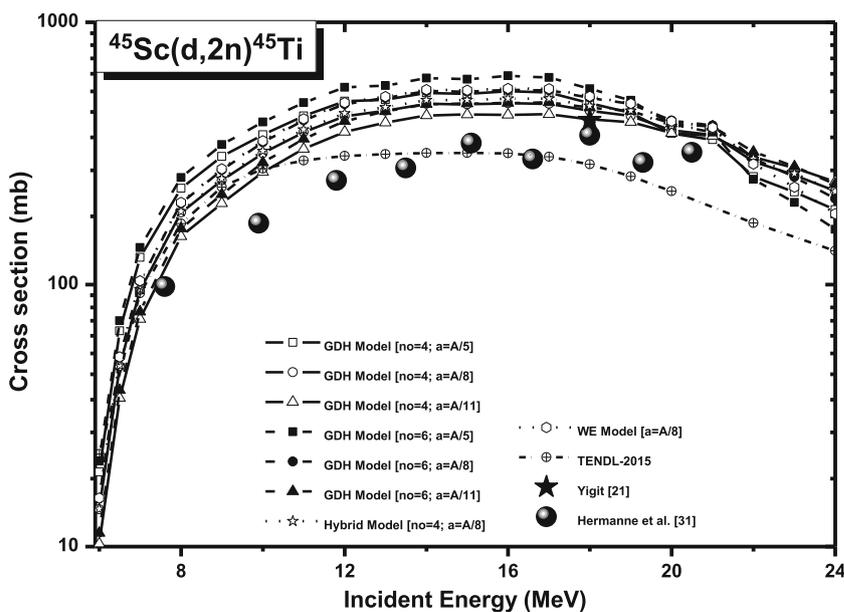
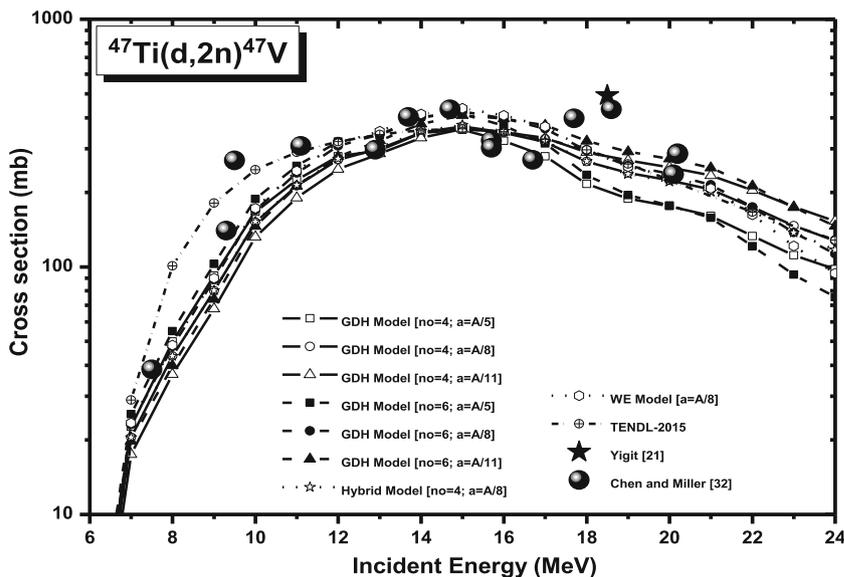


Fig. 6 Cross section values of the $^{47}\text{Ti} (d, 2n) ^{47}\text{V}$ nuclear reaction with the data reported by Chen and Miller [32] and Yiğit [21]



3.2 (d, 2n) nuclear reactions

3.2.1 $^{45}\text{Sc}(d, 2n) ^{45}\text{Ti}$ nuclear reaction

Figure 5 gives the comparison of the calculated nuclear cross sections and measured data for the $^{45}\text{Sc} (d, 2n) ^{45}\text{Ti}$ reaction up to the incident energy of 24 MeV. The shape of excitation function measured by Hermanne et al. [31] have an acceptable harmony with the cross section results calculated using the level density parameter $\alpha = A/11$ and initial exciton number $n_0 = 4$, and TALYS-based TENDL-2015 library data. Nuclear cross sections for the investigated reaction, $^{45}\text{Sc} (d, 2n) ^{45}\text{Ti}$, have maximum position in the deuteron energy range of 14–18 MeV. In addition, the

cross section calculated via the formula of Yiğit [21] gives satisfactory agreement with the measured data of Hermanne et al. [31]. The modification using the initial exciton number and the level density parameter in pre-equilibrium model calculations causes little changes on cross sections.

3.2.2 $^{47}\text{Ti} (d, 2n) ^{47}\text{V}$ nuclear reaction

Figure 6 presents the comparison of the model-based nuclear cross sections and experimental data for the $^{47}\text{Ti} (d, 2n) ^{47}\text{V}$ reaction up to the projectile energy of 24 MeV. The TALYS-based TENDL library data and the obtained cross section results using ALICE-ASH code are in good agreement with the experimental data of Chen and Miller

Fig. 7 Cross section values of the $^{48}\text{Ti}(d, 2n)^{48}\text{V}$ nuclear reaction with the data reported by WestJr et al. [33], Chen and Miller [32], Burgus et al. [34], and Yiğit [21]

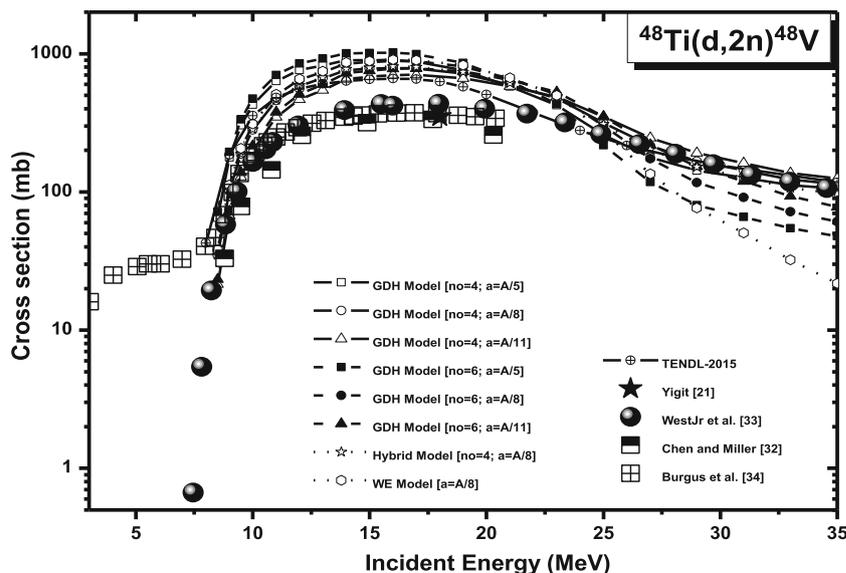
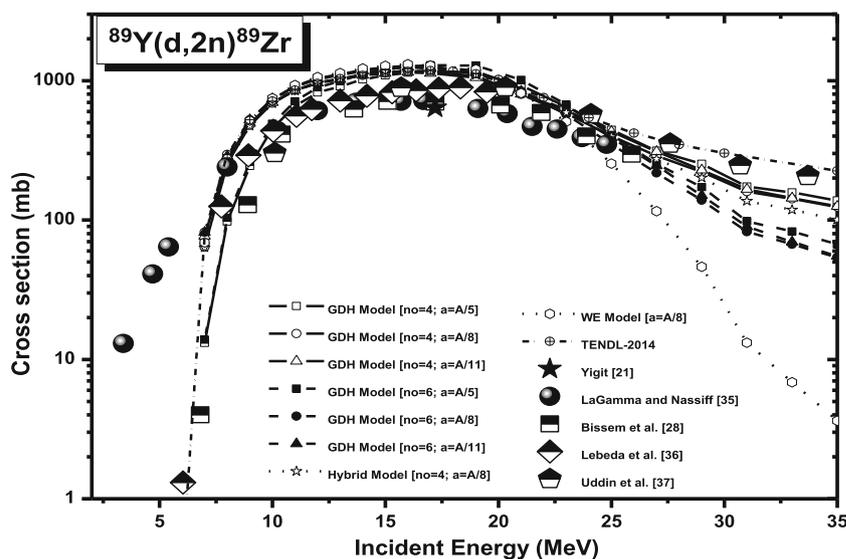


Fig. 8 Cross section values of the $^{89}\text{Y}(d, 2n)^{89}\text{Zr}$ nuclear reaction with the data reported by LaGamma and Nassiff [35], Bissem et al. [28], Lebeda et al. [36], Uddin et al. [37], and Yiğit [21]



[32]. From Fig. 6, it can be seen that the excitation functions calculated using the nuclear equilibrium and pre-equilibrium models have approximately the same spectral structure. The cross section value calculated using the formula included non-elastic and Coulomb effects of Yiğit [21] is 492.9 mb. The cross section point of Yiğit [21] is higher than the experimental data of 432 mb reported by Chen and Miller [32]. The excitation functions via different nuclear models seem to have a peak around 15 MeV, whereas the experimental data of Chen and Miller [32] have a dispersed structure.

3.2.3 $^{48}\text{Ti}(d, 2n)^{48}\text{V}$ nuclear reaction

The calculated and experimental excitation curves for the considered nuclear reaction are presented in Fig. 7 up to

the incident energy of 35 MeV. The experimental cross section data reported by Chen and Miller [32], West Jr. et al. [33], and Burgus et al. [34] give similar results to each other in the 10–20 MeV energy range for this nuclear reaction, whereas these data exhibit lower cross section structure from the theoretical results. The excitation functions have a maximum structure in the 12–20 MeV energy range. TALYS-based TENDL data and the pre-equilibrium model calculations ($n_0 = 4$) are in very good agreement with the cross section data of WestJr et al. [33] at projectile deuteron energies above 23 MeV. The measured data of Chen and Miller [32], West Jr et al. [33], and Burgus et al. [34] agree with the cross section obtained using the systematic of Yiğit [21].

3.2.4 $^{89}\text{Y}(d, 2n)^{89}\text{Zr}$ nuclear reaction

The calculated excitation functions and experimental data of LaGamma and Nassiff [35], Bissem et al. [28], Lebeda et al. [36], and Uddin et al. [37] are presented in Fig. 8 up to the projectile deuteron energy of 35 MeV for the investigated nuclear reaction. The experimental data reported by LaGamma and Nassiff [35], Lebeda et al. [36], and Bissem et al. [28] for the considered reaction have an acceptable harmony with the nuclear cross section values calculated using the pre-equilibrium and equilibrium models by the ALICE–ASH code. The TALYS-based TENDL data are in agreement with the cross section results measured by Uddin et al. [37] except for the incident energy of 10.1 MeV. The results of LaGamma and Nassiff [35] and Bissem et al. [28] agree with the cross section value obtained using the formula of Yiğit [21]. The section data calculated by the WE model give minimum values above the incident deuteron energy of 25 MeV.

4 Conclusion

In this study, the excitation functions of some (d, n) and (d, 2n) nuclear reactions produced by the deuteron particle on the fusion structural materials such as chromium, nickel, zinc, scandium, titanium, and yttrium were investigated by using the different initial exciton numbers and level density parameters via the pre-equilibrium and equilibrium models. The obtained excitation functions were also compared with the experimental results and TENDL library data, and the cross section values were calculated using the formulae of Yiğit [20, 21]. The excitation functions for the (d, n) nuclear reactions have maximum position in the deuteron energy of 4–9 MeV, whereas the maximum cross section values for the (d, 2n) nuclear reactions are reached in the energy range of 14–20 MeV. The cross section values predicted by the empirical formula of Yiğit [21] for the (d, 2n) nuclear reactions give an acceptable agreement with the measured data. On the other hand, the calculated cross section results of Yiğit [20] are not very consistent with the measured data for the $^{50}\text{Cr}(d, n)^{51}\text{Mn}$ and $^{58}\text{Ni}(d, 2n)^{59}\text{Cu}$ nuclear reactions. It seemed that the calculated excitation functions change very little with the variation of the nuclear level density parameters. Generally, the calculated cross section data via the pre-equilibrium model (initial exciton number $n_0 = 4$) for the investigated nuclear reactions have an acceptable harmony with the available experimental data. Especially, selecting the initial exciton number of $n_0 = 4$ in the pre-equilibrium models for cross section calculations of (d, n) nuclear reactions appears to be good. So, the initial exciton number is an important parameter of the pre-equilibrium process. We hope that the

obtained results in this paper will stimulate future experimental cross section investigations of deuteron–nuclei interaction.

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