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Original Article

Study on (n,p) reactions of ^{58,60,61,62,64}Ni using new developed empirical formulas

Mustafa Yiğit

Department of Physics, Faculty of Arts and Science, Aksaray University, Aksaray, Turkey

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A B S T R A C T

Nuclear fusion seems to be a good choice of energy source in the future. Nickel is one of the crucial structural materials for fusion devices. In this work, the cross section data of ^{58}Ni(n,p)^{58}Co, ^{60}Ni(n,p)^{60}Co, ^{61}Ni(n,p)^{61}Co, ^{62}Ni(n,p)^{62}Co and ^{64}Ni(n,p)^{64}Co reactions were calculated using the nuclear codes ALICE/ASH, EMPIRE 3.2 and TALYS 1.8. In addition, the cross sections were calculated with the empirical formulas obtained in our previous paper at 14–15 MeV. The obtained results were compared with the measured values in the literature, and with the evaluated data files (JEFF-3.3, TENDL-2017, ENDF/B-VIII.0).

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1. Introduction

Fusion is one of the most sustainable energy sources because of environmental and safety advantages. Since fusion does not result in the release of CO_2 or SO_2, it will not contribute to air pollution, acid rain and global warming. Therefore, studies on the energy research and development of fusion process are very crucial. It is known that the design and performance of a fusion power plant are dependent on the properties of the fusion structural components [1–3]. Nickel is one of the crucial structural materials for fusion devices. Thus the nuclear excitation functions of neutron reactions are important for fusion technology. Actually, the correct data on cross sections for hydrogen production in reactor materials through different (n,p) reactions at the energies up to 20 MeV are required. In this context, the cross section data for isotopes produced by fast neutrons are of prime interest for future fusion power plants, the radiation damage effects, the calculation of nuclear transmutation rates, the nuclear heating, etc [4–6]. The development of theoretical calculation schemes of nuclear reactions is vigorously dependent on the understanding of neutron reactions. Accordingly, the theoretical models are mostly needed to provide the neutron cross section predictions, if the experimental values at certain incident energies are not available because of the experimental difficulty. Nuclear reaction codes can be used in obtaining the neutron cross sections [7]. These codes offer a number of nuclear reaction model options. In general, the reaction codes incorporate the different level density models for predicting excitation functions for various reaction channels. Accordingly, the level density models as input parameter in the reaction codes are very important in determining the excitation functions via the nuclear reaction models [8]. The cross sections at certain incident energies can be calculated from the systematics based on the compound and pre-compound emission mechanisms. Especially, at the neutron energies of 14–15 MeV, the use of systematics for obtaining the neutron cross sections plays an important role in nuclear calculations in the field of reaction physics [9–12]. Recently, the theoretical reaction codes such as TALYS, ALICE and EMPIRE based on different nuclear theories have been used to predict neutron-cross sections on nickel isotopes. The (n, 2n) cross sections on ^{58,60,61,62,64}Ni isotopes were calculated using the computer codes ALICE/ASH and TALYS 1.8 by Baldık and Yılmaz [13]. Also, the cross section data for the ^{58,60,61,62,64}Ni(n,p) reactions were estimated using different input parameters in TALYS-1.0 by Lalremruata et al. [5]. In addition, the nuclear cross sections for (n,p) reaction channels induced by neutrons on some nickel isotopes were obtained using the computer code EMPIRE 3.0 by Pandey et al. [4]. In this paper, the cross sections for (n,p) reactions on ^{58,60,61,62,64}Ni target nuclei were calculated up to energy of 20 MeV using different level density models [14–18] in the ALICE/ASH [19], EMPIRE 3.2 [20] and TALYS 1.8 [21]

E-mail address: mustafayigit@aksaray.edu.tr.

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reaction codes. Furthermore, the empirical formulas obtained in our previous work [22] and in the literature [23–25] at the neutron energies of 14–15 MeV were used for predicting the (n,p) reaction cross sections. The obtained present cross section results are discussed and compared with the values taken from EXFOR [26], and with the ENDF/B-VIII.0 [27], JEFF-3.3 [28], TENDL-2017 [29] library data.

2. Theoretical background

2.1. ALICE/ASH code

The ALICE/ASH reaction code [19] which is an advanced version of the ALICE code has been used for the analytical computation of cross sections at the nuclear physics. Especially, this reaction code has been very successful in predicting the nuclear cross sections using the compound and pre-compound emission models. The pre-compound emission spectrum of nucleons in the Geometry Dependent Hybrid (GDH) model [30] is calculated as follows,

$$\frac{d\sigma_v(\varepsilon)}{d\varepsilon} = \pi\lambda\!\!\!^{-}{}^2 \sum_{l=0}^{\infty}(2l+1)T_l P_v(l,\varepsilon) \tag{1}$$

where the term T_l represents the transmission co-efficient for the l–th partial wave. The term $P_v(l,\varepsilon)$ represents decay probability at exit channel energy. The term $\lambda\!\!\!^{-}$ corresponds to the reduced de–Broglie wavelength of incident particle. Different level density models at the ALICE/ASH code [19] can be used at the excitation function calculations. The level density formula at the Fermi gas model with energy-independent level density parameter is given as follows,

$$\rho(\mathrm{U}) \propto (\mathrm{U}-\delta)^{\,-5/4} e^{\left(2\sqrt{a(\mathrm{U}-\delta)}\right)} \tag{2}$$

where the level density parameter is the $a = {}^{\mathrm{A}}\!/\!_{\mathrm{y}}$. The term A is the mass number of nucleus. The term y is a constant. The terms U and δ represent the excitation energy and the pairing correction, respectively [**19**]. The level density formula at the Superfluid nuclear model [16] is given as follows,

$$\rho(\mathrm{U}) = \rho_{\mathrm{qp}}\left(\mathrm{U}'\right)\mathrm{K}_{\mathrm{vib}}\left(\mathrm{U}'\right)\mathrm{K}_{\mathrm{rot}}\left(\mathrm{U}'\right) \tag{3}$$

where the terms $\mathrm{K}_{\mathrm{rot}}(\mathrm{U}')$ and $\mathrm{K}_{\mathrm{vib}}(\mathrm{U}')$ are the rotational and vibrational enhancement factors at effective energy of excitation U'. The $\rho_{\mathrm{qp}}(\mathrm{U}')$ represents the density of quasi particle nuclear excitation [16,19].

2.2. EMPIRE 3.2 code

EMPIRE 3.2 [20] is a reaction code, which is used for analyzing a variety of reactions like compound, pre-compound, direct and fission reactions developed by the nuclear researches. In general, this code is the model code that is widely used for reaction data evaluation works. The projectile particle can be a nucleon, Triton, proton, deuteron, ^{3}He, ^{4}He or ions. The pre-compound emission process in the EMPIRE 3.2 code is given by the Exciton model as follows [31,32],

$$-\mathrm{q}_{\mathrm{t}=0}(\mathrm{n}) = \lambda_+(\mathrm{E},\ \mathrm{n}+2)\tau(\mathrm{n}+2) + \lambda_-(\mathrm{E},\ \mathrm{n}-2)\tau(\mathrm{n}-2)$$

$$-[\lambda_+(\mathrm{E},\ \mathrm{n}) + \lambda_-(\mathrm{E},\ \mathrm{n}) + \mathrm{L}(\mathrm{E},\ \mathrm{n})]\tau(\mathrm{n}) \tag{4}$$

In Eq. (4) $\mathrm{L}(\mathrm{n},\mathrm{E})$ represents the total emission rate integrated over the emission energy for particles and γ-rays. $\mathrm{q}_{\mathrm{t}}(\mathrm{n})$ is the initial occupation probability of compound nucleus for the nuclear state with the excitation number n. Also, the terms $\lambda_-(\mathrm{E},\ \mathrm{n})$ and $\lambda_+(\mathrm{E},\ \mathrm{n})$ are transition rates of nuclear decay to neighbouring states [20]. The pre-compound spectra at this code are given as follows,

$$\frac{\mathrm{d}\sigma_{\mathrm{a,b}}}{\mathrm{d}\varepsilon_{\mathrm{b}}}(\varepsilon_{\mathrm{b}}) = \sigma^{\mathrm{r}}_{\mathrm{a,b}}(\mathrm{E}_{\mathrm{inc}})\mathrm{D}_{\mathrm{a,b}}(\mathrm{E}_{\mathrm{inc}}) \times \sum_{\mathrm{n}} \mathrm{W}_{\mathrm{b}}(\mathrm{E},\mathrm{n},\varepsilon_{\mathrm{b}})\tau(\mathrm{n}) \tag{5}$$

where the term $\sigma^{\mathrm{r}}_{\mathrm{a,b}}(\mathrm{E}_{\mathrm{inc}})$ is the (a,b) nuclear reaction cross section and $\mathrm{D}_{\mathrm{a,b}}(\mathrm{E}_{\mathrm{inc}})$ is the depletion factor. $\mathrm{W}_{\mathrm{b}}(\mathrm{E},\mathrm{n},\varepsilon_{\mathrm{b}})$ denotes the emission probability of a particle of type b (or γ-ray) with energy ε_{b} from a nuclear state with excitation energy E and exciton n of compound nucleus [20].

2.3. TALYS 1.8 code

The TALYS code 1.8 [21] is the reaction model code that is widely used for the analysis of nuclear structure and nuclear reaction experiments. The reactions produced by neutrons, protons, gammas, deuterons, tritons, ^{3}He and ^{4}He can be simulated by this code in the 1 keV–200 MeV energy range. Reaction models, which are used in the TALYS 1.8 can be categorized into optical, direct, compound, pre-compound and fission models [21]. In this computer code, the Hauser–Feshbach model [33] to account for the evaporation peak of the nuclear spectrum of a nuclear reaction has been employed to define compound emission, binary and multiple processes. The nuclear cross section for pre-compound particle emission process in the TALYS code 1.8 is given as follows,

$$\frac{d\sigma_k^{PE}}{dE_k} = \sigma^{CF} \sum_{p_\pi=p_\pi^0}^{p_\pi^{max}} \times \sum_{p_\upsilon=p_\upsilon^0}^{p_\upsilon^{max}} W_k(p_\pi,h_\pi,p_\upsilon,h_\upsilon,E_k)\tau(p_\pi,h_\pi,p_\upsilon,h_\upsilon)P(p_\pi,h_\pi,p_\upsilon,h_\upsilon) \tag{6}$$

where the term σ^{CF} is the cross section for the compound-nucleus formation calculated via the optical model. The terms $h_\pi(h_\upsilon)$ and $p_\pi(p_\upsilon)$ represent the proton (neutron) hole number and the proton (neutron) particle number, respectively. The term τ is the average lifetime for the exciton state. Also, the terms E_k and W_k correspond to the emission energy and the emission rate of a particle k. The term P denotes the part of the pre-compound population for the emission to survive the previous states and passes through the $(p_\pi, h_\pi, p_\upsilon, h_\upsilon)$ configuration, averaged over time. The initial neutron and proton particle numbers are $p_\upsilon^0 = N_p$ and $p_\pi^0 = Z_p$, respectively with $Z_p(N_p)$ the proton (neutron) number of incoming particle [21,33].

2.4. Cross section formulas

The nuclear data of reaction cross section for different energies have been needed for describing nuclear structure, binding energy and excited nuclear states [10]. Furthermore, the data on cross sections are necessary for both developing more advance nuclear model and explaining the particle emission process from a nuclear reaction [10,12]. So, the empirical formulas have been used in obtaining the cross sections. In recent years, many researchers have widely studied and suggested the empirical formulas for various reaction channels [9–11,22–25]. In our previous paper [22], we presented an empirical systematic for predicting the (n,p) cross sections at 14–15 MeV. According to previous report [22], the cross section formulas including isotopic effects in the (n,p) reactions at 14–15 MeV are given as follows,

$$\sigma(n,p) = 49.478\left(A^{1/3}+1\right)^2 exp[-32.079s] \qquad \text{for target nuclei with even} - A$$

$$\sigma(n,p) = 44.893\left(A^{1/3}+1\right)^2 exp[-31.349s] \qquad \text{for target nuclei with odd} - A \tag{7}$$

where the s are the asymmetry parameters [22].

3. Results

Cross section prediction with nuclear reaction codes is quite important for a better understanding of the experimental measurements. The ALICE/ASH, EMPIRE 3.2 and TALYS 1.8 reaction codes were used for the calculations of excitation function of the (n,p) reactions on some nickel isotopes. The Back-shifted Fermi Gas model (BSFGM) [15] and Constant Temperature model + Fermi Gas model (CTM + FGM) [17], the Generalized Superfluid model (GSFM) [18] in the TALYS 1.8 code, and the Enhanced Generalized Superfluid model (EGSM) [14] in the EMPIRE code, and the Superfluid nuclear model (SFM) [16] and Fermi gas model (FGM) in the ALICE/ASH code were used in the present calculations. Thereby, the newly calculated cross sections are given in Figs. 1–5 together with the results of the experimental literature data as well as with evaluated data files (JEFF-3.3, ENDF/B-VIII.0, TENDL-2017). The numerical values of the calculated cross sections for (n,p) reactions at the neutron energies around 14.5 MeV are given in Table 1.

The nuclear excitation functions for the ^{58}Ni(n,p)^{58}Co reaction are given in Fig. 1. The evaluated values from JEFF-3.3, ENDF/B-VIII.0 and TENDL-2017 are in excellent agreement with the experimental data except for a few data points. Furthermore, the cross section data of Filatenkov [34], Ikeda et al. [38] and Pavlik et al. [39] are in good agreement with the FGM and CTM + FGM calculations for the reaction ^{58}Ni(n,p)^{58}Co. Also, the cross section data predicted using CTM + FGM level density generally agree well with the experimental measurements of Mannhart and Schmidt [35], Zhou et al. [36], Semkova et al. [37] and Paulsen and Widera [40] except for a few data points. The data calculated via SFM level density using the code ALICE/ASH shows acceptable agreement with the cross section values reported by Barry [42]. The calculation results obtained using SFM level density show acceptable agreement with the measurements of Buczko et al. [41] in the energy region of 5.38–9.6 MeV. At higher incident energies, however, the data of Buczko et al. [41] are in reasonable agreement with the CTM + FGM calculations. The cross section predicted using the formula of Levkovskii [25] is in acceptable agreement with the experimental data at the energies of 14–15 MeV.

The calculated and measured excitation functions for the ^{60}Ni(n,p)^{60}Co reaction are shown in Fig. 2. The theoretical calculations obtained using FGM level density by the ALICE/ASH code agree well with the cross section values measured by Greenwood [46], Doczi et al. [50], Tingyan et al. [48], Filatenkov [34], Konno et al. [44], Meadows et al. [47] and Osman and Habbani [49] for the investigated reaction. In addition, these cross section measurements are in very good agreement with the evaluated excitation functions from JEFF-3.3, ENDF/B-VIII.0 and TENDL-2017. The excitation function results from the BSFGM, FGM, SFM, CTM + FGM and the evaluated data files agree satisfactorily well with the cross section results of Sudar et al. [43] and Wagner et al. [45]. The cross section value of 140.81 mb calculated using our cross section

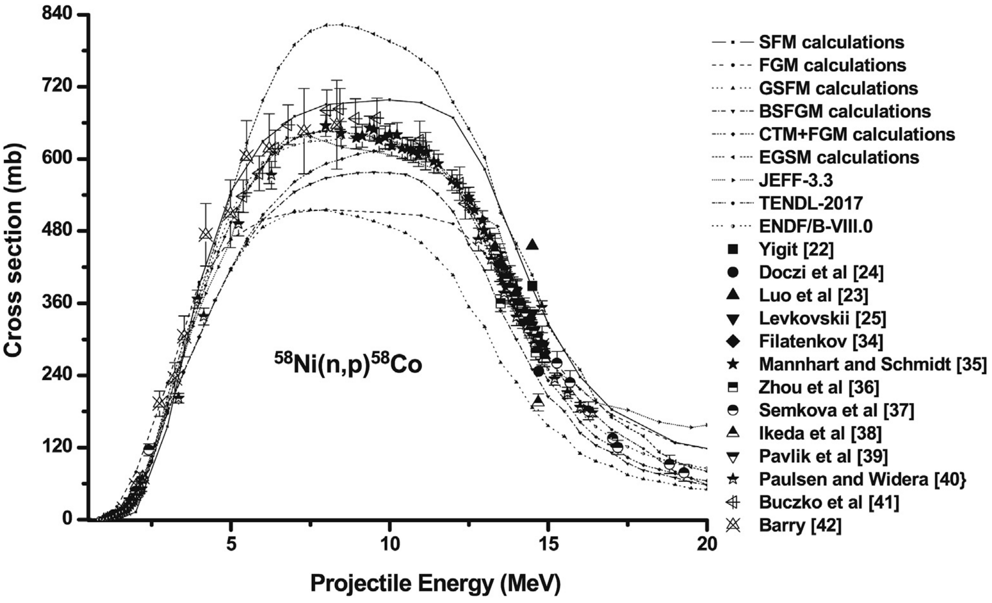

Fig. 1. Excitation function predictions using the nuclear codes and empirical formulas for the ^{58}Ni(n,p)^{58}Co reaction and comparison with the existing measurements.

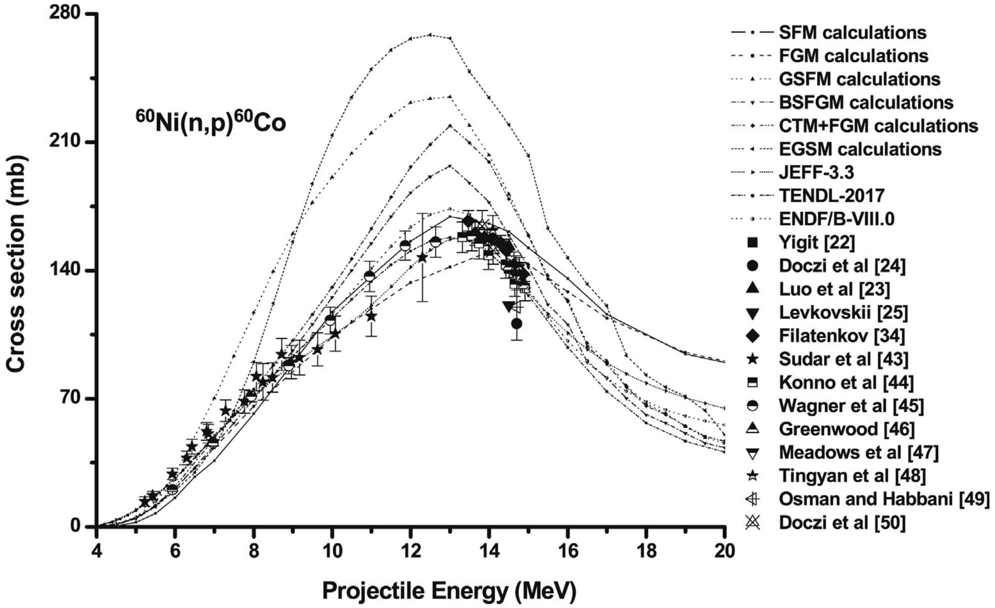

Fig. 2. Excitation function predictions using the nuclear codes and empirical formulas for the ^{60}Ni(n,p)^{60}Co reaction and comparison with the existing measurements.

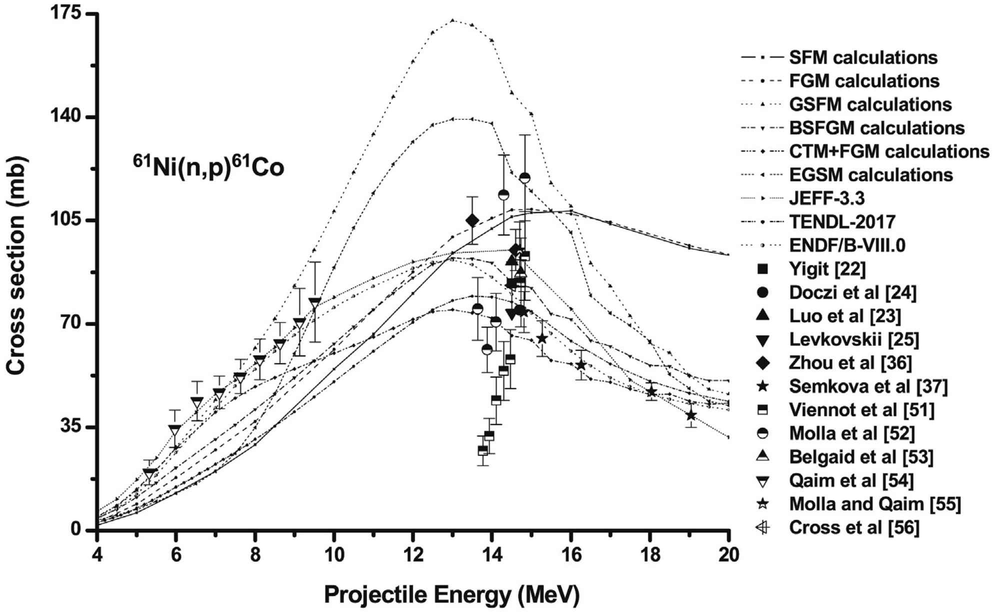

Fig. 3. Excitation function predictions using the nuclear codes and empirical formulas for the ^{61}Ni(n,p)^{61}Co reaction and comparison with the existing measurements.

systematic [22] is in very good agreement with the measurement (142±2.13 mb) of Greenwood [46] at the neutron energy of 14.5 MeV. The obtained data (111.03 mb) via the formula of Doczi et al. [24] is in reasonable agreement with the experimental value (120±18 mb) reported by Osman and Habbani [49] at14.7 MeV.

The excitation functions for the ^{61}Ni(n,p)^{61}Co nuclear reaction are shown in Fig. 3. The cross section results from the JEFF-3.3, ENDF/B-VIII.0, CTM + FGM and GSFM show acceptable agreement with the measurement reported by Qaim et al. [54] within uncertainty limits. The shape of excitation functions measured by Viennot et al. [51] and Molla et al. [52] is different from the data calculated using nuclear models. The excitation function reported by Molla and Qaim [55] in the energy range of 13.64–14.83 MeV is in good agreement with the cross section values of the ENDF/B-VIII.0 and CTM + FGM. The cross sections calculated using the empirical formulas are quite consistent with the measurements of Semkova et al. [37], Zhou et al. [36], Molla and Qaim [55], Belgaid et al. [53] and Cross et al. [56] at the neutron energies near 14.5 MeV. Especially, the value of 83.76 mb calculated using our cross section systematic [22] at 14.5 MeV is in very good agreement with the measurement (83±8 mb) reported by Cross et al. [56].

Fig. 4 shows the cross section calculations and measurements for the reaction ^{62}Ni(n,p)^{62}Co. The cross sections, which are calculated using EGSM level density have higher values than the other excitation functions at maximum cross section region. The cross sections reported by Ercan et al. [57] and Ribansky et al. [58] have very large discrepancies with the measurements of Maslov et al. [59] and Cross et al. [56] at the neutron energies near 14 MeV.

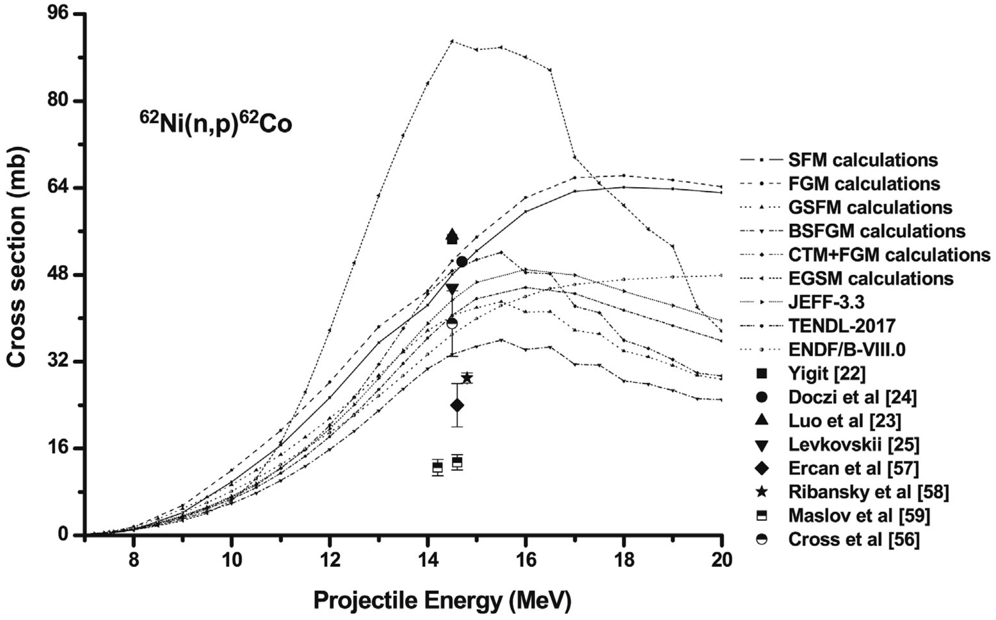

Fig. 4. Excitation function predictions using the nuclear codes and empirical formulas for the ^{62}Ni(n,p)^{62}Co reaction and comparison with the existing measurements.

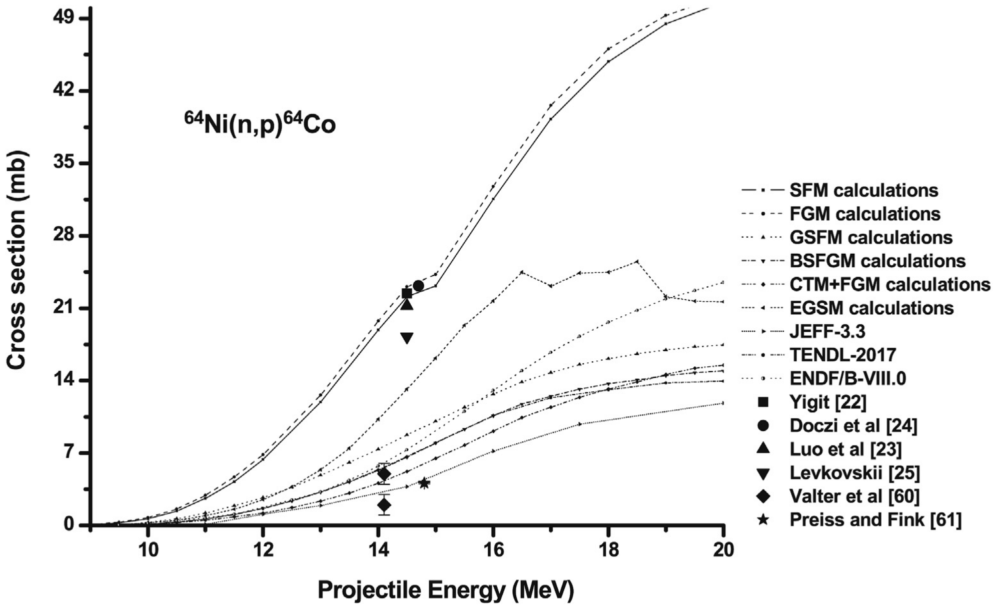

Fig. 5. Excitation function predictions using the nuclear codes and empirical formulas for the ^{64}Ni(n,p)^{64}Co reaction and comparison with the existing measurements.

Particularly, two cross section values measured by Maslov et al. [59] are too lower than the other values. The value calculated from the cross section systematic of Levkovskii [25] is in good agreement with the cross section data of 39±6 mb reported by Cross et al. [56] at 14.5 MeV. In addition to the cross section value of Cross et al. [56] within the experimental error bar shows acceptable agreement with the cross sections obtained using the ALICE/ASH and TALYS 1.8 calculations, and with the evaluated values from ENDF/B-VIII.0, JEFF-3.3 and TENDL-2017.

The nuclear cross sections calculated using the TALYS 1.8, EMPIRE 3.2, ALICE/ASH and empirical formulas for the reaction ^{64}Ni(n,p)^{64}Co are plotted Fig. 5 in together with the measured data, which are obtained from EXFOR. There are only two experimental measurements reported by Valter et al. [60] and Preiss and Fink [61] for the ^{64}Ni(n,p)^{64}Co reaction. From Fig. 5, we can see that the empirical predictions calculated using the cross section formulas of Yigit [22], Luo et al. [23], Doczi et al. [24] and Levkovskii [25] are higher than the cross sections obtained by Valter et al. [60] and Preiss and Fink [61]. The theoretical calculations estimated using the code ALICE/ASH with SFM and FGM level densities are in agreement with the estimations obtained from the empirical formulas of Yiğit [22], Luo et al. [23] and Doczi et al. [24] for the ^{64}Ni(n,p)^{64}Co reaction at the energies near 14.5 MeV. On the other hand, the experiment value of 4.1±0.05 mb measured by Preiss and Fink [61] at 14.8 MeV is in good agreement with the evaluated values from JEFF-3.3. Also, two cross section values measured by **Valter et al.** [60] at 14.1 MeV are quite different in magnitude from each other. These cross section values are in good agreement with

Table 1
The calculated cross sections of the (n,p) reactions on^{58}60·61·62^{,64}Ni at neutron energies around 14.5 MeV.

		Energy (MeV)	Cross sections (in mbarn)				
			^{58}Ni(n,p)^{58}Co	^{60}Ni(n,p)^{60}Co	^{61}Ni(n,p)^{61}Co	^{62}Ni(n,p)^{62}Co	^{64}Ni(n,p)^{64}Co
Nuclear Models	**GSFGM**	14.5	185.77	181.63	148.17	40.49	8.59
	CTM + FGM	14.5	282.78	178.95	66.03	48.70	5.21
	BSFGM	14.5	250.03	159.08	83.98	33.34	6.60
	EGSM	14.5	406.39	219.49	121.13	91	13.16
	SFM	14.5	384.6	161.1	106.32	48	22.13
	FGM	14.5	309.15	148.39	108.53	50.56	23.06
Evaluated data libraries	**ENDF/B-VIII.0**	14.5	298.35	145.63	79.98	37.01	7.329
	JEFF-3.3	14.5	299.3	139.38	95	43.37	3.74
	TENDL-2017	14.5	312.41	139.37	77.45	40.50	6.64
Cross section formulas	**Yiğit (2018)**	14.5	388.34	140.81	83.76	54.54	22.43
	Levkovskii (1964)	14.5	343.68	120.98	73.66	45.58	18.26
	Luo et al. (2008)	14.5	455.51	153.03	91.13	55.19	21.23
	Doczi et al. (1997)	14.7	246.75	111.03	74.71	50.4	23.16

the CTM + FGM calculations.

4. Conclusions

The cross sections of ^{58,60,61,62,64}Ni(n,p) reactions are calculated in the energy range from reaction threshold to 20 MeV. The overall trend of the cross sections calculated using the code ALICE/ASH for the ^{58,60}Ni(n,p)^{58,60}Co reactions is satisfactory. The cross sections calculated using the different level density models have the different magnitude from each other. So, the prediction of (n,p) cross sections is very sensitive to the selection of the level density model at the maximum region of cross sections. In the cross section calculations made by TALYS 1.8 computer code, the theoretical predictions with CTM + FGM level density usually give a better agreement than the BSFGM and GSFM level densities. Moreover, the discrepancies between the experimental and the calculated data can be, due to the level densities of the residual nuclei, which can vary the cross sections with the choice of reaction codes and their input parameters. The present results suggest that the prediction of cross sections via the empirical systematics for the investigated reactions except for ^{64}Ni(n,p)^{64}Co reaction is a powerful method for determining the cross sections.

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