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ORIGINAL PAPER

Theoretical cross-sectional calculation of some structural fusion material on (n, α)-induced reactions

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Abstract: ^{27}Al, ^{51}V, ^{52}Cr, 55Mn, ^{56}Fe and ^{58}Ni nuclei are some structural fusion substances. The neutron incident energy around 14–15 MeV is adequate to excite the nucleus for the reactions such as (n, p), (n, d), (n, 2n), (n, t), and (n, α). For fusion reactor technology, the reaction cross-sectional data have a critical importance in fusion reactors and development. Neutron irradiation produces considerable modifications in the mechanical and physical properties of each of the structural fusion material systems raising feasibility questions and design limitations. In this paper, for some structural fusion materials (n, α) reactions such as ^{52}Cr(n, α)^{49}Ti, ^{51}V(n, α)^{48}Si, ^{27}Al(n, α)^{24}Na, ^{58}Ni(n, α)^{55}Fe, ^{56}Fe(n, α)^{53}Cr and ^{55}Mn(n, α)^{52}V were done up to 40 MeV incident neutron energy. In the calculations, the equilibrium and pre-equilibrium impacts have been used. Calculations have been carried out with TALYS 1.9 and EMPIRE 3.2 (Malta) nuclear model codes. Results from performed calculations have been compared with the experimental nuclear reaction data, ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2 evaluated data.

Keywords: (n, α) cross section; Nuclear reactions; TALYS 1.9 nuclear model code; EMPIRE 3.2 (Malta) nuclear model code

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1. Introduction

Nuclear fusion, sometimes referred to as thermonuclear fusion, is a process where two light atomic nuclei come together to form a heavier nucleus [1]. Nuclear fusion can be one of the most attractive sources of energy from the viewpoint of safety and minimal environmental impact. The development of fusion materials for the safety of fusion power systems and understanding nuclear properties is important. The success of fusion power system is dependent on the performance of the first wall, blanket or divertor systems. So, the performance of structural materials for fusion power systems, understanding nuclear properties systematic and working out of (n, α) reaction cross sections are very important. Neutron scattering cross sections and neutron emission differential data have a critical importance on fusion reactors. In fusion reactor structures, a serious damage mechanism has been gas production in the metallic resulting from diverse nuclear (n, p) and (n, a) reactions above a certain threshold energy. [2–10] The experimental cross sections are available in EXFOR for neutron-induced reactions. 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.

Nuclear data are required to explain reaction mechanisms and to develop more nuclear models. Also neutron cross sections around 14 MeV are important from the viewpoint of fusion reactor technology, especially for the calculation of nuclear transmutation rates, nuclear heating and radiation damage to the materials used in the construction of the core and inner walls of the reactor.

In the present work, neutron incident reaction cross sections for some structural fusion materials such as ^{27}Al(n, α)^{24}Na, ^{51}V(n, α)^{48}Sc, ^{52}Cr (n, α) ^{49}Ti, ^{55}Mn(n, α)^{52}V, ^{56}Fe (n, α) ^{53}Cr, and ^{58}Ni(n, α)^{55}Fe have been calculated up to 40 MeV by using the equilibrium and pre-equilibrium models. Calculations have been carried out with TALYS

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1.9 and EMPIRE 3.2 (Malta) nuclear model codes. Results from performed calculations have been compared with the experimental nuclear reaction data, ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2 evaluated data.

2. Theoretical calculations methods of nuclear reaction cross sections

The elementary pre-equilibrium differential cross section for the emission of a particle k with emission energy E_K can then be expressed in terms of s, the composite-nucleus formation cross section σ^{CF}, and an emission rate W_k [11–20]:

$$\frac{d\sigma_k^{\mathrm{PE}}}{dE_K} = \sigma^{CF} \sum_{p_\pi=p_\pi^0}^{p_\pi^{\max}} \sum_{p_\upsilon=p_\upsilon^0}^{p_\upsilon^{\max}} W_k(p_\pi, h_\pi, p_\upsilon, h_\upsilon, E_k)\tau(p_\pi, h_\pi, p_\upsilon, h_\nu) P(p_\pi, h_\pi, p_\upsilon, h_\nu) \quad (1)$$

where the factor P represents the part of the pre-equilibrium population that has survived emission from the previous states and now passes through the (p π, h π, p υ, h υ) configurations, averaged over time. $p_\pi^0 = Z_p$ and $p_\upsilon^0 = N_p$ are the initial proton and neutron particle numbers, respectively, with Z_p (N_p) the proton (neutron) number of the projectile. $h_p^0 = h_\upsilon^0 = 0$ and $h_\nu = p_\nu - p_\nu^0$, for any exciton state in the reaction process; so that the initial hole numbers are $h_p^0 = h_\nu^0 = 0$ for primary pre-equilibrium emission. Particle emission only occurs from n = 3 (2p1 h) and higher exciton states [21–35].

For calculating the excitation functions, we used two different nuclear reaction program codes. "Exciton" and "two-component exciton" models were used in TALYS 1.9, EMPIRE 3.2 (Malta) nuclear reaction program code for pre-equilibrium reaction systematics, respectively [12, 13].

In the two-component exciton model, which is the default model for TALYS reaction cross-sectional computations, the holes and particles are followed throughout the reaction. The notation for the following equation gives the numbers of particles which could be proton or neutron and holes as pπ(pν) and hπ(hν), respectively. From this, the proton exciton number is defined as $n_\pi = p_\pi + h_\pi$ and the neutron exciton number as $n_\upsilon = p_\upsilon + h_\upsilon$ which give us to construct the charge-independent particle number as $p = p_\pi + p_\upsilon$, the exciton number as $n = n_\pi + n_\upsilon$ and the hole number as $h = h_\pi + h_\upsilon$.

EMPIRE uses the Exciton [14] model PCROSS module for the reaction in cross-sectional computations of pre-equilibrium reactions. A unified model is used by the exciton model that is the solution of a key equation that was previously represented by Cline [15] and Ribansky [16].

3. Results and discussions

In the present work, for some structural fusion materials (n, α) reactions such as ^{27}Al(n, α)^{24}Na, ^{51}V(n, α)^{48}Sc, ^{52}Cr (n, α)^{49}Ti, ^{55}Mn(n, α)^{52}V, ^{56}Fe (n, α)^{53}Cr, and ^{58}Ni(n, α)^{55}Fe have been calculated up to 40 MeV incident neutron energy. Results from performed calculations have been compared with the experimental nuclear reaction data, ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2 evaluated data. A reasonable agreement with theoretical excitation functions and experimental was obtained. It can be said that at least this work helps to show the way to the later experimental studies and contributes to the new studies on (n, α) reaction cross sections . The results can be concluded and summarized as follows:

3.1. Excitation function of ^{27}Al(n, α)^{24}Na reaction

Figure 1 shows the calculated excitation functions for the nuclear reactions ^{27}Al(n, α)^{24}Na in comparison with the experimental nuclear reaction data, ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2 evaluated data. The experimental cross-sectional datasets are between 3.5 and 40 MeV, and the data around 9 E 17 MeV show big discrepancies. The TALYS 1.9 follows the trend of the experimental nuclear reaction data. The pre-equilibrium spectra calculations of emitted (α) for ^{27}Al nuclei are in reasonable agreement with experimental nuclear reaction data and with ENDF/B-VIII.b4, JEFF-3.2 and JENDL-4.0 files (evaluations international libraries). Generally, there is a good agreement between the cross sections calculated with TALYS 1.9 and the experimental nuclear reaction data. The results of

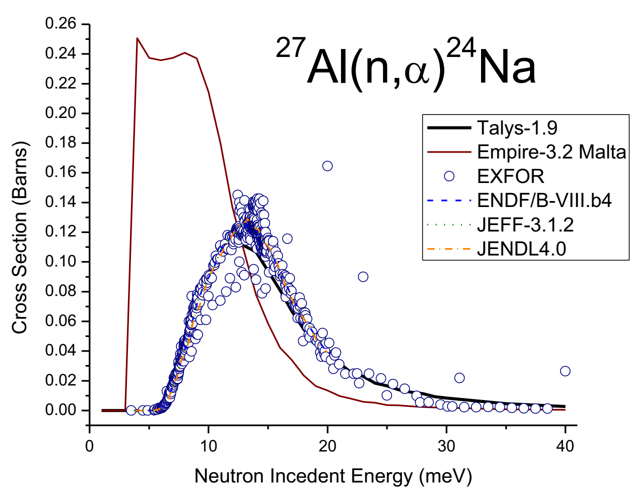

Fig. 1 Excitation curves of ^{27}Al(n, p)^{24}Na reaction calculated by TALYS 1.9 and EMPIRE 3.2 (Malta) along with the experimental values, and evaluated nuclear data files ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2. The experimental values reported in Ref. (EXFOR) [36]

EMPIRE 3.2 (Malta) give unacceptable results between 0 and 13 MeV and strongly underestimate between 15 and 26 MeV. The estimation of EMPIRE 3.2 (Malta) is acceptable between 28 and 38 MeV.

3.2. Excitation function of $^{51}V(n, \alpha)^{48}Sc$ reaction

Figure 2 shows the calculated excitation curve for the nuclear reactions $^{51}V(n, \alpha)^{48}Sc$ in comparison with the experimental nuclear reaction data, ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2 evaluated data. The experimental cross-sectional datasets are between 2.96 and 38.5 MeV. The theoretical investigation using TALYS 1.9 & EMPIRE 3.2(Malta) indicates the emitted alpha spectra, and the compound contribution is dominant by the pre-equilibrium contribution which mainly comes from the high-energy emitting alphas and the low-energy emitting alphas. The theoretical investigation using TALYS 1.9 & EMPIRE 3.2(Malta) follows the trend of the experimental nuclear reaction data, but EMPIRE 3.2(Malta) strongly overestimates above 11 MeV, while TALYS 1.9 overestimates over 16 MeV. The equilibrium calculations of the TALYS 1.9 and EMPIRE 3.2(Malta) are mostly in good agreement with the experimental nuclear reaction data and with ENDF/B-VIII.b4 and JENDL-4.0.files (evaluations international libraries).

3.3. Excitation function of $^{52}Cr(n, \alpha)^{49}Ti$ reaction

Figure 3 shows the calculated excitation curve for the nuclear reactions $^{52}Cr(n, \alpha)^{49}Ti$ in comparison with the experimental nuclear reaction data, ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2 evaluated data. The experimental nuclear reaction data are rather few for $^{52}Cr(n, \alpha)^{49}Ti$ reactions. When there are more experimental values for these reactions, more reliable results can be obtained. The evaluated nuclear data files ENDF/B-VIII.b4, JEFF-3.2 and JENDL-4.0 show significant discrepancies in energy between 0 and 40 MeV. The results of the theoretical nuclear reaction model calculations follow the trend of the experimental values, but the estimation of TALYS 1.9 is much better.

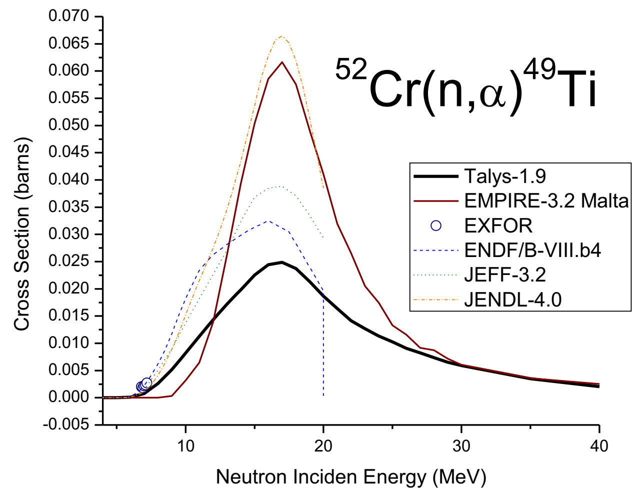

Fig. 3 Excitation curves of $^{52}Cr(n, \alpha)^{49}Ti$ reaction calculated by TALYS 1.9 and EMPIRE 3.2 (Malta) along with the experimental values, and evaluated nuclear data files ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2. The experimental values reported in Ref. (EXFOR) [36]

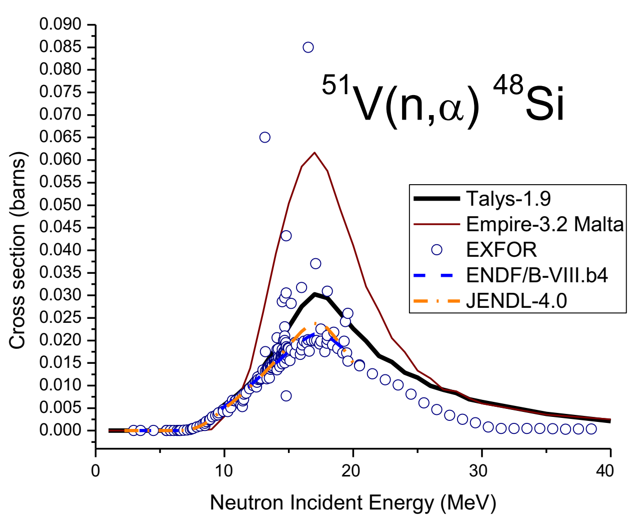

Fig. 2 Excitation curves of $^{51}V(n, \alpha)^{48}Sc$ reaction calculated by TALYS 1.9 and EMPIRE 3.2 (Malta) along with the experimental values, and evaluated nuclear data files ENDF/B-VII.b4, JENDL-4.0. The experimental values reported in Ref. (EXFOR) [36]

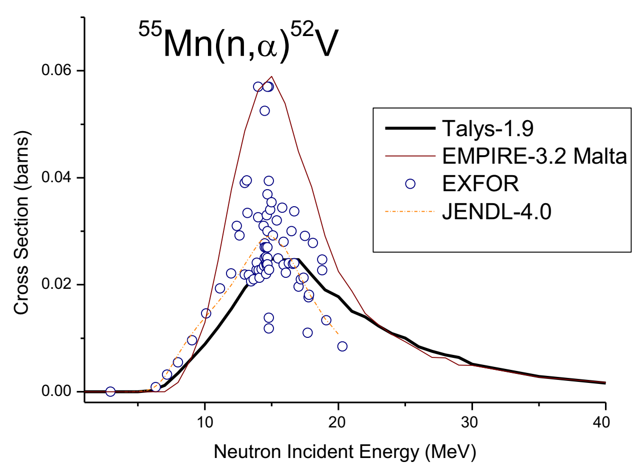

Fig. 4 Excitation curves of $^{55}Mn(n, \alpha)^{52}V$ reaction calculated by TALYS 1.9 & EMPIRE 3.2 (Malta) along with the experimental values, and evaluated nuclear data files ENDF/B-VII.b4. The experimental values reported in Ref. (EXFOR) [36]

3.4. Excitation function of $^{55}Mn(n, \alpha)^{52}V$ reaction

Figure 4 presents the excitation curve of $^{55}Mn(n, \alpha)^{52}V$ nuclear reaction. The experimental nuclear reaction data are between 2.96 and 19 MeV, and the data around 12 *E* 19 MeV show very large discrepancies. The equilibrium results based on the Hauser–Feshbach formalism give lower results than experimental cross-sectional data. The pre-equilibrium calculations with exciton model give the lowest outcomes. The pre-equilibrium spectra calculations using TALYS 1.9 are mostly in good agreement between 13 and 15 MeV with experimental cross-sectional data, while EMPIRE 3.2 (Malta) overestimates between 13 and 20 MeV. The results of the theoretical nuclear reaction model calculations follow the trend of the experimental cross-sectional data, but the estimation of TALYS 1.9 is much better.

3.5. Excitation function of ^{56}Fe (n, $\alpha)^{53}Cr$ reaction

Figure 5 presents the excitation curve of ^{56}Fe (n, $\alpha)^{53}Cr$ nuclear reaction. The experimental nuclear reaction data are rather few for ^{56}Fe (n, $\alpha)^{53}Cr$ reactions. When there are more experimental values for these reactions, more reliable results can be obtained. The results of the theoretical nuclear reaction model calculations follow the trend of the experimental cross-sectional data, but the estimation of TALYS 1.9 is much better.

3.6. Excitation function of $^{58}Ni(n, \alpha)^{55}Fe$ reaction

Figure 6 presents the excitation curve of $^{58}Ni(n, \alpha)^{55}Fe$ nuclear reaction. The experimental nuclear reaction data are rather few for ^{56}Fe (n, $\alpha)^{53}Cr$ reactions. When there are more experimental cross-sectional data for these reactions, more reliable results can be obtained. The excitation functions obtained using TALYS 1.9 & EMPIRE 3.2 (Malta) exhibit very similar trends with each other, but the estimation of TALYS 1.9 is much better. The evaluated nuclear data files ENDF/B-VIII.b4 and JENDL-4.0 show significant discrepancies in energy between 0 and 40 MeV.

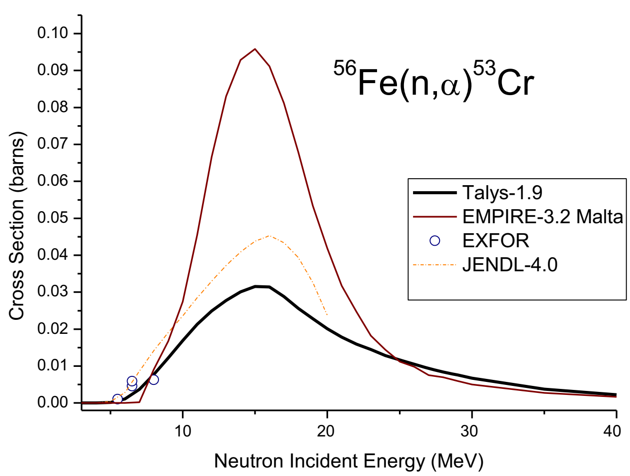

Fig. 5 Excitation curves of ^{56}Fe (n, $\alpha)^{53}Cr$ reaction calculated by TALYS 1.9 & EMPIRE 3.2 (Malta) along with the experimental values, and evaluated nuclear data files JENDL-4.0. The experimental values reported in Ref. (EXFOR) [36]

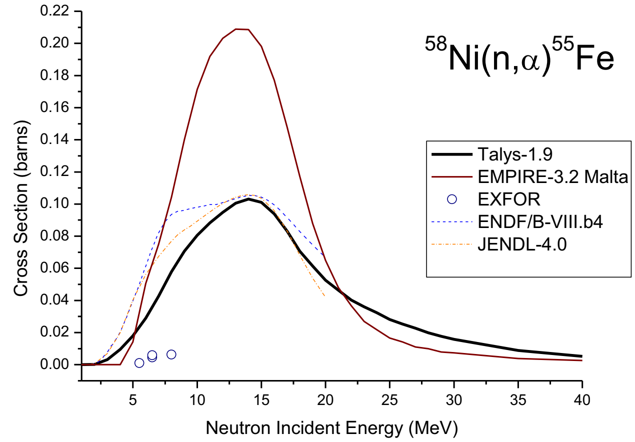

Fig. 6 Excitation curves of $^{58}Ni(n, \alpha)^{55}Fe$ reaction calculated by TALYS 1.9 & EMPIRE 3.2 (Malta) along with the experimental values, and evaluated nuclear data files ENDF/B-VII.b4, JENDL-4.0. The experimental values reported in Ref. (EXFOR) [36]

4. Conclusions

In the present work, for some structural fusion materials (n, α) reactions such as $^{27}Al(n, \alpha)^{24}Na$, $^{51}V(n, \alpha)^{48}Sc$, ^{52}Cr (n, $\alpha)^{49}Ti$, $^{55}Mn(n, \alpha)^{52}V$, ^{56}Fe (n, $\alpha)^{53}Cr$, and $^{58}Ni(n, \alpha)^{55}Fe$ have been calculated. Results from performed calculations have been compared with the experimental nuclear reaction data, ENDF/B-VII.b4, JENDL-4.0 and JEFF-3.2 evaluated data. The calculation results have been compared with the available experimental data, and the conclusions can be drawn as follows:

1. In general, the alpha emission spectrum of neutron bombardment of ^{27}Al, ^{51}V, ^{52}Cr, ^{55}Mn, ^{56}Fe, and ^{58}Ni is in agreement with the experimental data for the TALYS 1.9 models and EMPIRE 3.2 (Malta) Exciton model results.
2. The results of the theoretical nuclear reaction model calculations follow the trend of the experimental points, but the calculation of TALYS 1.9 is much better.
3. More theoretical and experimental works are needed, as a result, because the measurements of the investigated (n, α) reaction cross sections in the literature are not very large.

4. In the present study, the different nuclear reaction program codes used show rather important differences both in shape and in size.

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