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ORIGINAL RESEARCH

(γ,2n) Reaction Cross Section Calculations on Several Structural Fusion Materials

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Abstract In this study, the theoretical photo-neutron cross-sections produced by (γ,2n) reactions for several structural fusion materials such as ^{51}V, ^{55}Mn, ^{58}Ni, ^{90,91,92,94}Zr, and ^{181}Ta have been carried out for incident photon energies up to 40 MeV. Reaction cross-sections as a function of photon energy have been calculated theoretically using the PCROSS and TALYS 1.2 computer codes. TALYS 1.2 default and pre-equilibrium models have been used to calculate the pre-equilibrium photo-neutron cross-sections. For the reaction equilibrium component, PCROSS Weisskopf–Ewing model calculations have been preferred. The calculated results have been compared with each other and against the experimental data in the existing databases EXFOR. Generally, TALYS 1.2 default and pre-equilibrium model cross-section calculations are in good agreement with the experimental data for all reactions along the incident photon energy in this study. Pre-equilibrium option can be recommended, if experimental data are not available or are unlikely to be produced due to the experimental difficulty.

Keywords Photo-neutron cross-section · (γ,2n) Reaction · Structural fusion materials · EXFOR file

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Introduction

The future of controlled thermonuclear fusion reactors is largely dependent on the nuclear reaction cross-section data and the selection of structural fusion materials. The development of fusion materials for the safety of fusion power systems and understanding nuclear properties is important. A special emphasis is being given for the development of the structural materials because the success of the fusion reactors is largely dependent on the development of these materials. The development of adequate structural materials is a major step towards fusion reactors becoming an efficient source of energy, particularly if the promise of an environmentally safe machine is to be realized. The reaction cross-section data have a critical importance on fusion reactor neutronics and development for fusion reactor technology. Photonuclear reaction data are very important for understanding the structure and dynamics of the atomic nucleus. Moreover, photo-induced reaction cross-sections are also of importance for a variety of current or emerging applications like: radiation shielding design and radiation transport analysis, calculations of absorbed dose in the human body during radiotherapy, physics and technology of fission reactors (influence on neutron balance) and fusion reactors (plasma diagnostics and shielding), activation analysis including safeguards and inspection technologies for identification of materials through radiation induced by photonuclear reactions and nuclear waste transmutation [1–5].

The nuclear reaction models are frequently needed to provide the estimation of the reaction cross-sections, especially if the experimental data are not obtained or in cases where it is difficult to carry out the experimental measurements [6–19]. Such predictions can guide the design of the target/blanket configurations and can reduce engineering over design costs. So the cross-section evaluation for materials irradiated by photons attaches special importance to use of systematics of photon-induced reaction cross-section.

In our previous work [20], we investigated (α,xn) neutron-emission spectra of several structural fusion materials. In this study, the theoretical (γ,2n) reaction cross-sections of several structural fusion materials such as ^{51}V, ^{55}Mn, ^{58}Ni, ^{90,91,92,94}Zr, and ^{181}Ta in photon-induced reactions have been investigated. The calculations on the excitation functions of ^{51}V(γ,2n)^{49}V, ^{55}Mn(γ,2n)^{53}Mn, ^{58}Ni(γ,2n)^{56}Ni, ^{90}Zr(γ,2n)^{88}Zr, ^{91}Zr(γ,2n)^{89}Zr, ^{92}Zr(γ,2n)^{90}Zr, ^{94}Zr(γ,2n)^{92}Zr, and ^{181}Ta(γ,2n)^{179}Ta reactions have been carried out for incident photon energies up to 40 MeV. Reaction cross-sections as a function of photon energy have been calculated theoretically using PCROSS [21] and TALYS 1.2 [22, 23] computer codes. TALYS 1.2 default and pre-equilibrium models have been used to calculate the pre-equilibrium photo-neutron cross-sections. For the reaction equilibrium component, PCROSS Weisskopf–Ewing (WE) [24] model calculations have been preferred. The calculated results have been compared with each other and experimental data existing in the EXFOR [25].

Calculation Methods

Photo-neutron cross-sections as a function of photon energy have been calculated theoretically using PCROSS code for the WE model and TALYS 1.2 computer code for the default and pre-equilibrium models.

The equilibrium particle emission is described by the WE Model in which angular momentum conservation is neglected. In the process, the basic parameters are binding energies, inverse reaction cross-section, the pairing and the level-density parameters. The reaction cross-section for incident channel a and exit channel b can be written as

$$\sigma_{ab}^{WE} = \sigma_{ab}(E_{inc})\frac{\Gamma_b}{\sum_{b'}\Gamma_{b'}} \tag{1}$$

where E_{inc} is the incident energy. In Eq. (1), Γ_b can be also expressed as

$$\Gamma_b = \frac{2s_b+1}{\pi^2\hbar^2}\mu_b\int d\varepsilon\sigma_b^{inv}(\varepsilon)\varepsilon\frac{\omega_1(U)}{\omega_1(E)} \tag{2}$$

where U, μ_b, s_b are the excitation energy of the residual nucleus, the reduced mass and the spin, respectively. The total single-particle level density is taken as,

$$\omega_1(E) = \frac{1}{\sqrt{48}}\frac{\exp\left[2\sqrt{\alpha(E-D)}\right]}{E-D};\quad \alpha = \frac{6}{\pi^2}g \tag{3}$$

where σ_b^{inv}, E, D and g are the inverse reaction cross-section, the excitation energy of the compound nucleus, the pairing energy and the single particle level density, respectively.

TALYS [22, 23] is a computer code for the prediction and analysis of nuclear reactions that involve photons, neutrons, protons, deuterons, tritons, hellions and alpha particles, in the 1 keV–200 MeV energy range and for target nuclides of masses 12 and heavier. For this, TALYS integrates the optical model, direct, pre-equilibrium, fission and statistical nuclear reaction models in one calculation scheme and thereby gives a prediction for all the open reaction channels. In TALYS, several options are included for the choice of different parameters such as γ-strength functions, nuclear level densities and nuclear model parameters [26].

The γ-ray strength function is obtained from the compilation by Kopecky and Uhl [27] and the nuclear level density is also based on an approach using the Fermi-gas model [28]. The pre-equilibrium reactions were considered by the two component exciton model [29]. The effects of direct like interactions due to complex particles (clusters) were calculated by the phenomenological model of Kalbach [30]. This model performs the pre-equilibrium calculations by taking into account the contributions from the break-up, transfer and knock-out reactions [31]. TALYS contains the ECIS–06 code [32] for optical model and direct reaction calculations. The default optical model potentials were from the compilation of Koning and Delaroche [33].

The pre-equilibrium model of TALYS is the two-component exciton model of Kalbach [34]. In the two-component model, the neutron and proton type of the created particles and holes is explicitly followed throughout the reaction. The exciton model cross-section given as:

$$\frac{d\sigma_k^{EM}}{dE_k} = \sigma^{CF}\sum_{p_\pi=p_\pi^0}^{p_\pi^{eq}}\sum_{p_v=p_v^0}^{p_v^{eq}}\omega_k(p_\pi,h_\pi,p_v,h_v,E_k) \times S_{pre}(p_\pi,h_\pi,p_v,h_v) \tag{4}$$

where $p_\pi(p_v)$is the proton (neutron) particle number and $h_\pi(h_v)$ the proton (neutron) hole number. The initial proton and neutron particle numbers are $p_\pi^0 = Z_p$and $p_v^0 = N_p$, with Zp (Np) the proton (neutron) number of the projectile. Generally, $h_\pi = p_\pi - p_\pi^0$and $h_v = p_v - p_v^0$ so that the initial hole numbers are zero, i.e., $h_\pi^0 = h_v^0 = 0$ for primary pre-equilibrium emission [35].

The emission rate W_k has been derived by Cline and Blann [36] from the principle of microreversibility, and can easily be generalized to a two-component version [37]. The emission rate for an ejectile k with relative mass μk and spin sk is

$$W_k(p_\pi, h_\pi, p_\nu, h_\nu, E_k) = \frac{2s_k + 1}{\pi^2 \hbar^3} \mu_k E_k \sigma_{k,inv} \times (E_k) \frac{\omega(p_\pi - Z_k, p_\nu - N_k, h_\nu, E^{tot} - E_k)}{\omega(p_\pi, h_\pi, p_\nu, h_\nu, E^{tot})} \quad (5)$$

where $\sigma_{k,inv}$ $(E_k)$is the inverse reaction cross section, again calculated with the optical model, Z_k (N_k) is the charge (neutron) number of the ejectile and E^{tot} is the total energy of the composite system [29]. The details of the other code model parameters and options of TALYS 1.2 can be found in Ref. [22, 23].

Results and Discussion

In the present study, (γ,2n) reaction cross-sections of ^{51}V(γ,2n)^{49}V, ^{55}Mn(γ,2n)^{53}Mn, ^{58}Ni(γ,2n)^{56}Ni, ^{90}Zr(γ,2n)^{88}Zr, ^{91}Zr(γ,2n)^{89}Zr, ^{92}Zr(γ,2n)^{90}Zr, ^{94}Zr(γ,2n)^{92}Zr and ^{181}Ta(γ,2n)^{179}Ta reactions using PCROSS, the default and pre-equilibrium options in the TALYS 1.2 computer codes have been calculated up to 40 MeV photon incident energy. The photo-neutron cross-sections exhibited by (γ,2n) reactions for ^{51}V, ^{55}Mn, ^{58}Ni, ^{90,91,92,94}Zr and ^{181}Ta target nuclei have been plotted as a function of photon energy in Figs. 1, 2, 3, 4, 5, 6, 7 and 8. All experimental values used in this study were taken from the EXFOR library.

The photo-neutron cross-section calculations of ^{51}V(γ,2n)^{49}V reaction have been compared with the experimental data in Fig. 1. The calculated default and pre-equilibrium model photo-neutron cross-sections with TALYS 1.2 code are in good agreement with the experimental data. The PCROSS–WE model calculations are not in agreement with the experimental data in the photon energy region below the 25 MeV. They are higher than the experimental data. They provide good results in the 25–28 MeV incident photon energy region.

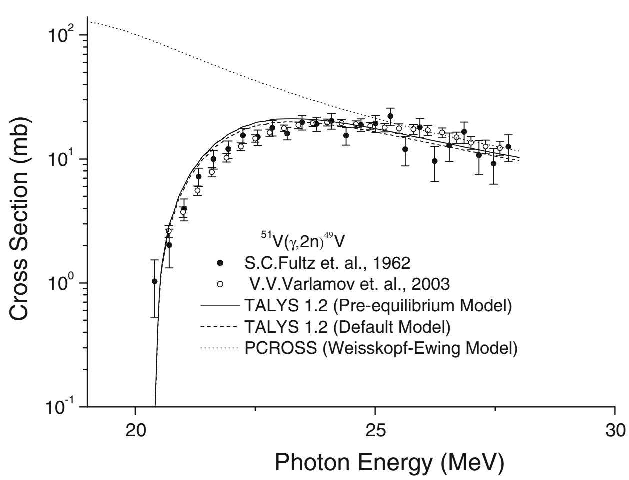

Fig. 1 The comparison of calculated photo-neutron cross-sections of ^{51}V(γ,2n)^{49}V reaction with the experimental EXFOR values reported in Ref. [25]

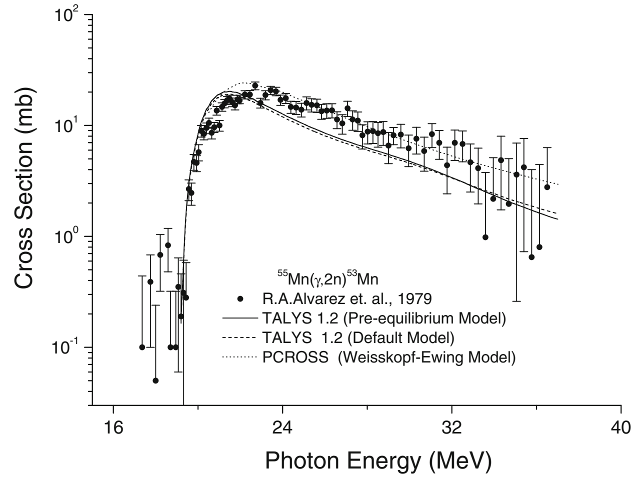

Fig. 2 The comparison of calculated photo-neutron cross-sections of ^{55}Mn(γ,2n)^{53}Mn reaction with the experimental EXFOR values reported in Ref. [25]

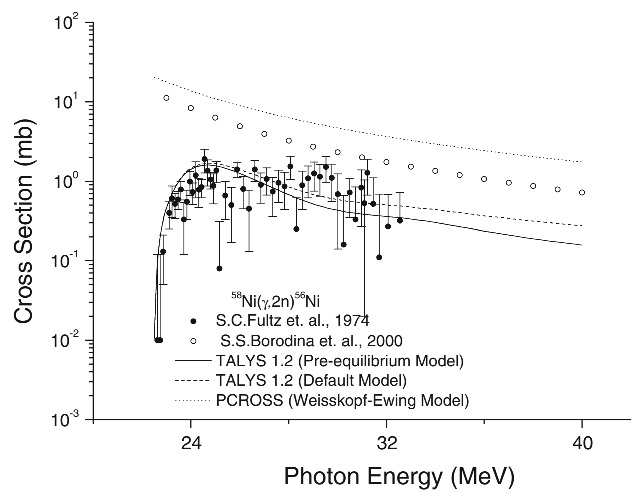

Fig. 3 The comparison of calculated photo-neutron cross-sections of ^{58}Ni(γ,2n)^{56}Ni reaction with the experimental EXFOR values reported in Ref. [25]

^{55}Mn(γ,2n)^{53}Mn reaction cross-section calculations have been compared with the experimental data in Fig. 2. PCROSS–WE, TALYS 1.2 default and pre-equilibrium model results are harmony with the experimental data in the photon energy region 20–38 MeV. The equilibrium PCROSS–WE model calculations are in better agreement than TALYS calculations. The photo-neutron cross-section calculations of ^{58}Ni(γ,2n)^{56}Ni reaction have been compared with the experimental data in Fig. 3. Although TALYS 1.2 default and pre-equilibrium model calculations are in good agreement with the experimental values of Borodina et al. [38], PCROSS–WE model calculations show a

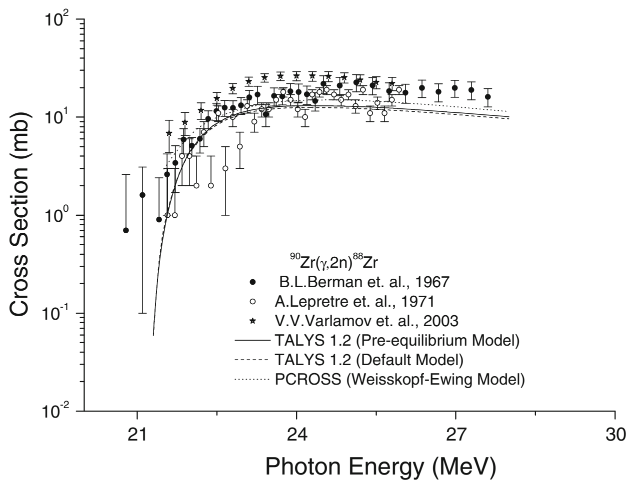

Fig. 4 The comparison of calculated photo-neutron cross-sections of $^{90}Zr(\gamma,2n)^{88}Zr$ reaction with the experimental EXFOR values reported in Ref. [25]

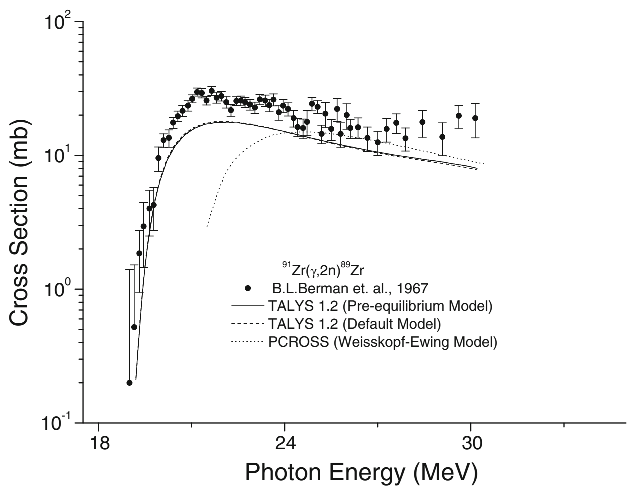

Fig. 5 The comparison of calculated photo-neutron cross-sections of $^{91}Zr(\gamma,2n)^{89}Zr$ reaction with the experimental EXFOR values reported in Ref. [25]

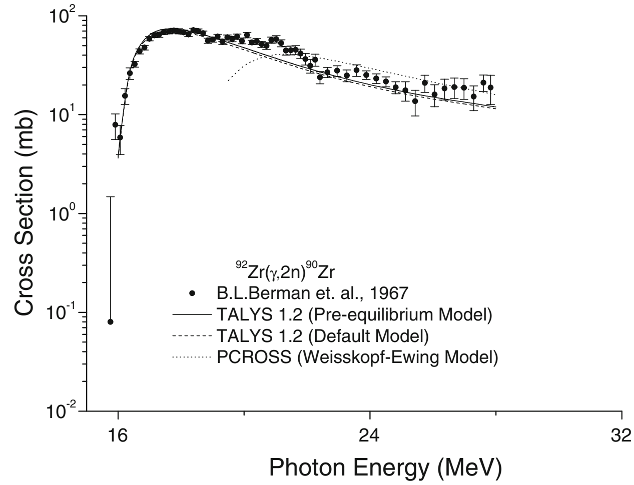

Fig. 6 The comparison of calculated photo-neutron cross-sections of $^{92}Zr(\gamma,2n)^{90}Zr$ reaction with the experimental EXFOR values reported in Ref. [25]

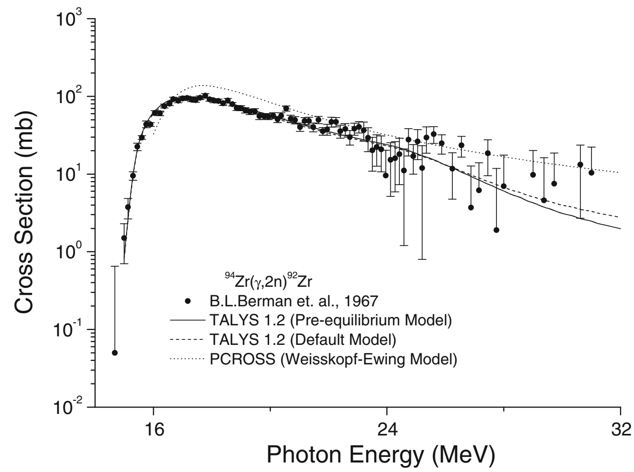

Fig. 7 The comparison of calculated photo-neutron cross-sections of $^{94}Zr(\gamma,2n)^{92}Zr$ reaction with the experimental EXFOR values reported in Ref. [25]

similar structure with the experimental values of Fultz et al. [39] but they are higher than the experimental values. The calculated results of (γ,2n) reactions for $^{90,91,92,94}Zr$ target nuclei have been compared with the experimental data in Figs. 4, 5, 6 and 7. TALYS 1.2 default and pre-equilibrium model calculations in Figs. 4, 5, 6 and 7 are in the good agreement with the experimental data. PCROSS-WE model calculations are shown to have a good agreement with the experimental data in Figs. 4, 5, 6 and 7 at the energy regions 21–28 MeV for the $^{90}Zr(\gamma,2n)^{88}Zr$, 24–30 MeV for the $^{91}Zr(\gamma,2n)^{89}Zr$, 20–28 MeV for the $^{92}Zr(\gamma,2n)^{90}Zr$ and 16–31 MeV for the $^{94}Zr(\gamma,2n)^{92}Zr$ reactions. The comparisons of the calculated photo-neutron cross-sections of $^{181}Ta(\gamma,2n)^{179}Ta$ reaction is given in Fig. 8. TALYS 1.2 default and pre-equilibrium model results are in agreement with the experimental data in the photon energy region 14–25 MeV. The PCROSS–WE model calculations are in harmony with the experimental data in the photon energy region above the 18 MeV.

In general all figures show that, although a few calculated data with TALYS 1.2 code follow the experimental ones from above or below as parallel, generally all the compared data are in agreement with each other. TALYS 1.2 default and pre-equilibrium model cross-section calculations are the best agreement with the experimental data for all reactions along the incident photon energy in this study. PCROSS–WE model calculations show a similar structure with experimental data except for $^{51}V(\gamma,2n)^{49}V$ reaction. As one can see in the figures, the good agreement between the calculations and experimental values shows

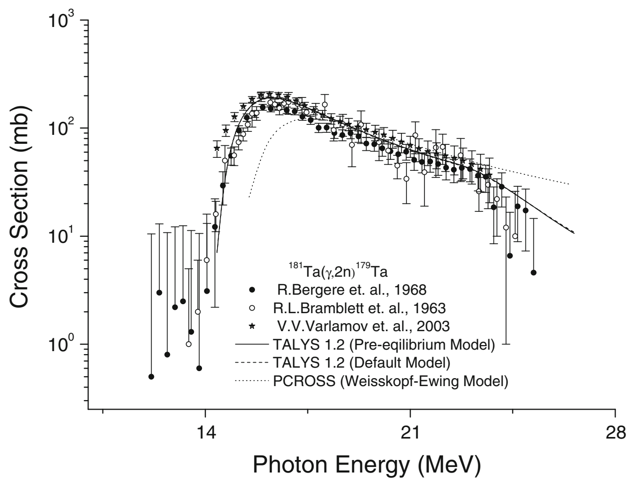

Fig. 8 The comparison of calculated photo-neutron cross-sections of ^{181}Ta(γ,2n)^{179}Ta reaction with the experimental EXFOR values reported in Ref. [25]

that TALYS is able to reproduce reasonably the cross-sections in this case even without any tuning of the parameters.

Also, the agreement with the theoretical results obtained with TALYS 1.2 using the default and pre-equilibrium parameters proves again the prediction strength of the code. Besides, TALYS 1.2 code will give more information for nuclear reaction researchers.

Summary and Conclusions

In this study, the theoretical photo-neutron cross-sections of several structural fusion materials such as ^{51}V, ^{55}Mn, ^{58}Ni, ^{90,91,92,94}Zr, and ^{181}Ta in (γ,2n) reactions have been calculated up to 40 MeV incident photon energies using PCROSS and the TALYS 1.2 computer codes. TALYS 1.2 default and pre-equilibrium models have been used to calculate the pre-equilibrium photo-neutron cross-sections. For the reaction equilibrium component, PCROSS–WE model calculations have been preferred. The calculated results have been also compared with the available experimental values in literature. The results can be summarized and concluded as follows:

1. (γ,2n) reaction cross-sections calculated with TALYS 1.2 code are mostly in agreement with the experimental data.
2. Both TALYS 1.2 default and pre-equilibrium model calculations are in good harmony with each other for all reactions in this study.
3. Generally, PCROSS–WE model calculations show a similar structure with experimental data except for ^{51}V(γ,2n)^{49}V reaction.
4. The good agreement between the calculations and experimental values shows that TALYS is able to reproduce reasonably the cross-sections in this case even without any tuning of the parameters.
5. The agreement with the theoretical results obtained with TALYS 1.2 using the default and pre-equilibrium parameters proves again the prediction strength of the code.
6. TALYS 1.2 pre-equilibrium option can be recommended, if experimental data are not available or are unlikely to be produced due to the experimental difficulty.

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