

Calculation of pre-equilibrium effects in neutron-induced cross section on ^{65}Cu

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Abstract. Copper is one of the constituents of alloys for structural components and a dosimetry material. In this study, we calculated the proton emission spectra and the excitation function produced by (n, xp) and (n, p) reactions respectively by using the Exciton model predictions combined with the Kalbach angular distribution systematics and the Hybrid Monte-Carlo Simulation (HMS). The sensitivity studies on the input parameters from optical model, level density, spin cut-off parameter and mean free path have been investigated for our calculations with the code EMPIRE and the code TALYS. The proton emission spectra and the excitation function for ^{65}Cu nucleus were discussed and found in good agreement with the available experimental data.

1. Introduction

The calculations of proton emission spectra and of the excitation function produced by (n, xp) and (n, p) reactions are indispensable for the design of nuclear devices. The development of high quality nuclear data of copper is particularly important due to its role as an important structural material in many accelerator-driven system designs. Natural copper consists of two isotopes, that is ^{63}Cu (69, 17%) and ^{65}Cu (30, 83%). Recently, the calculations of proton emission spectra and of the excitation function produced by $^{63}\text{Cu}(n, xp)$ and $^{63}\text{Cu}(n, p)^{63}\text{Ni}$ reactions [1], respectively, are used in the framework of preequilibrium models with the new version of the EMPIRE 3.2 code [2].

The main purpose of this work is to investigate the sensitivities on the preequilibrium models and those on the input parameters from Reference Input Parameter Library (RIPL-3) [3] calculations as optical model, level density and level density a -parameter calculations of proton emission spectra and of the excitation function produced by $^{65}\text{Cu}(n, xp)$ and $^{65}\text{Cu}(n, p)^{65}\text{Ni}$ reactions, respectively, using TALYS 1.8 [4] and EMPIRE 3.2 [2] codes. The input parameters of spin cut-off, M2constant, M2limit and M2shift from the squared matrix element of the TALYS [4], Exact NR (nonrelativistic), Fermi gas densities, default damp rate in HMS, single particle level density g , adjustable partial level density, adjustable pairing shift for adjustment of the Fermi gas level density and mean free path have been taken in account but they affect weakly the calculations.

2. Theoretical models formula

The phenomenological pre-equilibrium mechanism as defined by Griffin [5] is the exciton model. Two versions

of the exciton model are implemented in TALYS [4]: the default is the two-component model in which the neutron or proton particles and holes are followed throughout the reaction. The pre-equilibrium differential cross section for the emission of a particle k with emission energy E_k can be expressed in terms of the lifetime of exciton state $(p_\pi, h_\pi, p_\nu, h_\nu)\tau$, the composite nucleus formation cross section σ_{CF} , and an emission rate W_k

$$\frac{d\sigma_k^{\text{PE}}}{dE_k} = \sigma_{CF} \sum_{p_\pi=p_\pi^0}^{p_\pi^{\text{max}}} \sum_{p_\nu=p_\nu^0}^{p_\nu^{\text{max}}} W_k(p_\pi, h_\pi, p_\nu, h_\nu, E_k) \tau(p_\pi, h_\pi, p_\nu, h_\nu) \times P(p_\pi, h_\pi, p_\nu, h_\nu,) \quad (1)$$

where the factor P represents the part of the pre-equilibrium population that has survived emission from the previous states and passes through the $(p_\pi, h_\pi, p_\nu, h_\nu)$ configurations, averaged over time. The lifetime τ of exciton state $(p_\pi, h_\pi, p_\nu, h_\nu)$ in Eq. (1) is defined as the inverse sum of the total emission rate and the various internal transition rates

$$\tau(p_\pi, h_\pi, p_\nu, h_\nu) = \left[\begin{array}{l} \lambda_{\pi}^+(p_\pi, h_\pi, p_\nu, h_\nu) + \lambda_{\nu}^+(p_\pi, h_\pi, p_\nu, h_\nu) + \\ \lambda_{\pi\nu}^0(p_\pi, h_\pi, p_\nu, h_\nu) + \lambda_{\nu\pi}^0(p_\pi, h_\pi, p_\nu, h_\nu) + \\ W(p_\pi, h_\pi, p_\nu, h_\nu) \end{array} \right]^{-1} \quad (2)$$

In the one-component exciton model as implemented in PCROSS module of EMPIRE [2], the phenomenological pre-equilibrium mechanism as defined by Griffin [5] is based on the solution of the master equation [6] proposed by Cline [7] and Ribansky et al. [8]. The pre-equilibrium spectra in this model are given as:

$$\frac{d\sigma_{a,b}}{d\epsilon_b}(\epsilon_b) = \sigma_{a,b}^r(E_{inc}) D_{a,b}(E_{inc}) \times \sum_n W_b(E, n, \epsilon_b) \tau(n) \quad (3)$$

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The next pre-equilibrium model described in EMPIRE [2] is the Hybrid Monte-Carlo Simulation (HMS) formulated by Blann [9]. This model calculates double-differential emission spectra [double- differential HMS (DDHMS)] using linear momentum densities.

The phenomenological Gilbert-Cameron Model [10], the basic relations of the Fermi Gas Model, the Generalized Superfluid Model (GSM) level density [11], the microscopic level density Hartree-Fock-Bogoliubov model (HFBM) of Goriely et al., [12] and the Back Shifted Fermi Gas Model [13] as included in RIPL-3 [3], are used in this work.

3. Results and discussions

The calculated double-differential cross sections for the $^{65}\text{Cu}(n, xp)$ nuclear reaction at 9- and 11-MeV incident neutron energies, the proton emission spectra at 14.8 MeV, the calculated total cross section in neutron energy range from 9.0 to 15.0 MeV and the excitation function for the $^{65}\text{Cu}(n, p)^{65}\text{Ni}$ reaction in the neutron energy range up to 41 MeV are illustrated in Fig. 1 through 5. We used a statistical model that is an advanced implementation of the Hauser-Feshbach theory [14] to describe the equilibrium emission from the compound nucleus. The local and global nucleon optical models of Koning and Delaroche [15] have been used for neutrons and protons for all the calculations by using TALYS [4].

At 9-MeV incident neutron energy and for different emission angles (30° , 60° and 120°), the double-differential cross sections calculated are shown in Fig. 1. In the framework of exciton model at one component [5] using PCROSS of EMPIRE [2] combined with Kalbach angular distribution systematics [16], the optical model parameters of Delaroche et al. have been used for neutrons [17] and for protons, the optical model parameters of Xiaohua Chonghai have been chosen [18]. The HFBM level density [12] used consists in using single-particle level schemes obtained from constrained axially symmetric Hartree-Fock-Bogoliubov method (HFBM). However, choosing the level density models and the number of discrete levels may fail, we may be forced to adjust the level density parameters themselves. These are done with the ROHFBA input parameter (HFB pseudo a -parameter to adjust numerical HFB level densities for nucleus), and set to -0.920 in ^{65}Cu . In the framework of HMS [9] model using DDHMS module of EMPIRE [2], we choose the same level density HFBM [12] and we use the ROHFBP input parameter (HFB pairing-like parameter to shift in energy numerical HFB level densities for nucleus), that is set to -5.000 in all nuclei. The optical models for neutrons and protons are the same as those used in PCROSS of EMPIRE [2]. In the framework of exciton model at two components using TALYS [4], the GSM level density [11] is chosen. As the shell effects are taken into account, the changes on the level density a -parameter affect the fit and set to 5.1 in ^{65}Cu . At 9-MeV incident neutron energies, the results using the level density a -parameter of the GSM level density [11] by using TALYS [4] for $^{65}\text{Cu}(n, xp)$ reaction are closer to experiment [19] than those used with the a -parameter of HFBM level density by using the PCROSS and DDHMS modules of EMPIRE [2].

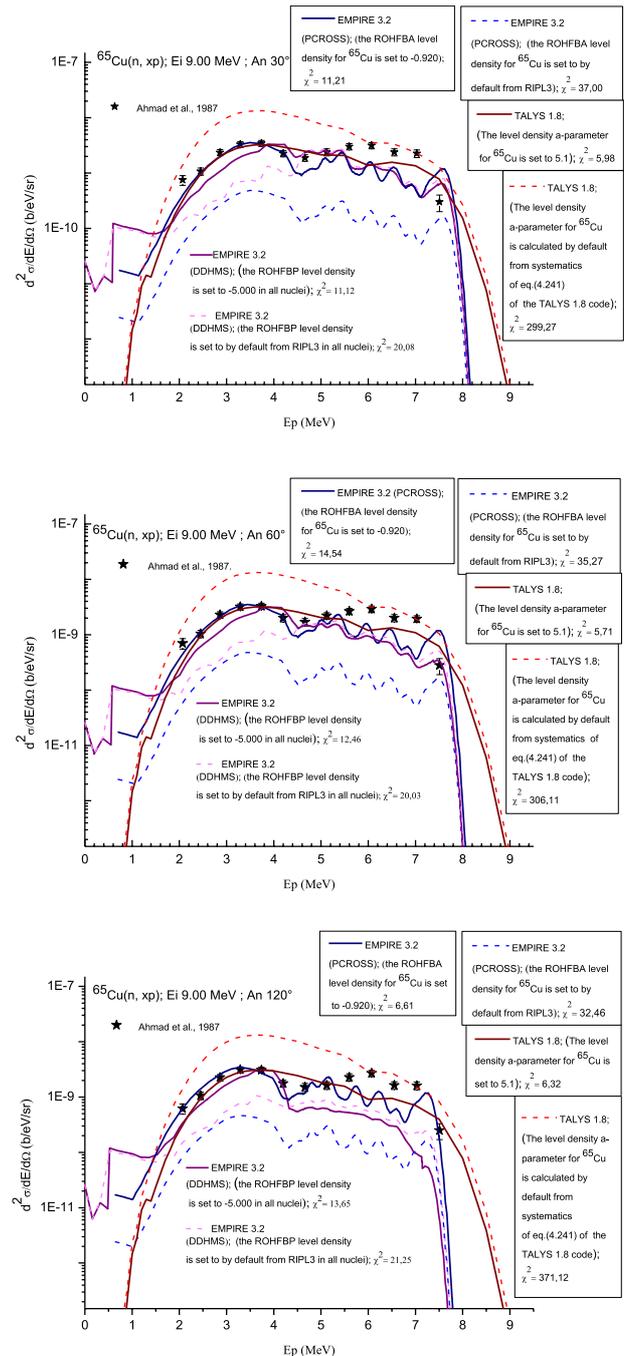


Figure 1. Effect of the level density a -parameter on the proton emission spectrum for $^{65}\text{Cu}(n, xp)$ reaction at 9-MeV incident neutron energy and at different emission angles (continuous and dashed lines) compared to the experimental data [19] (solid stars).

At 11-MeV incident neutron energy and for different emission angles (30° , 60° , 105° and 130°), the optical models for neutrons and protons are the same as those used at 9-MeV incident neutron energies. The HFBM level density [12] is used and the ROHFBA input parameter is set to -0.61 in ^{65}Cu in both PCROSS and DDHMS of EMPIRE [2]. The GSM level density [11] is chosen by using TALYS [4] and the level density a -parameter is set to 5.2 in ^{65}Cu . As shown in Fig. 2, the results using the a -parameter of HFBM level density by using PCROSS and DDHMS of EMPIRE [2] for $^{65}\text{Cu}(n, xp)$ reaction are closer

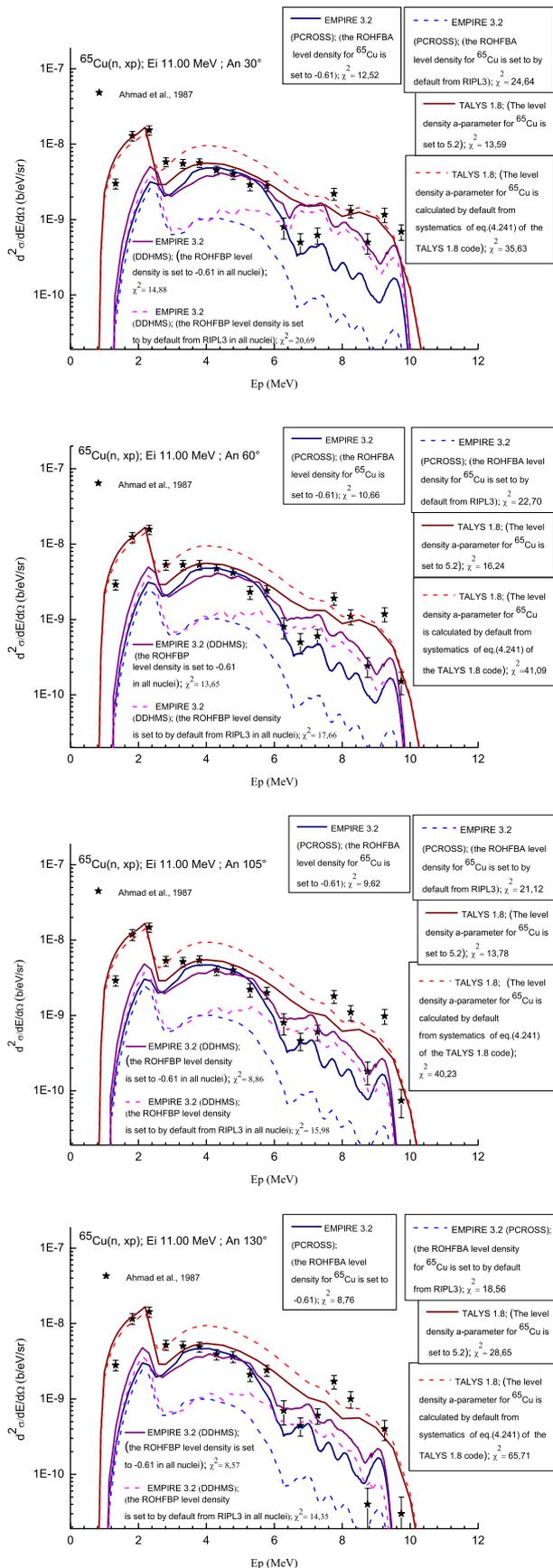


Figure 2. Effect of the level density a -parameter on the proton emission spectrum for $^{65}\text{Cu}(n, xp)$ reaction at 11-MeV incident neutron energy and at different emission angles (continuous and dashed lines) compared to the experimental data [19] (solid stars).

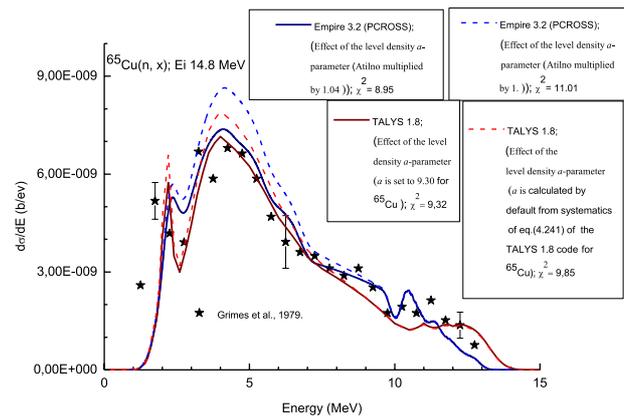


Figure 3. Effect of the level density a -parameter on the proton emission spectrum for $^{65}\text{Cu}(n, xp)$ reaction at 14.8 MeV incident neutron energy (continuous and dashed lines) compared to the experimental data [22] (solid stars).

to experiment [20] than those used with the level density a -parameter of the GSM level density [11] of TALYS [2].

Figure 3 shows the proton emission energy spectra at 14.8 MeV neutron energy. The optical model parameters of Varner et al., have been used for neutrons [20] and for protons, the optical model parameters of Kailas et al., have been chosen [21]. The G.C level [10] density is chosen by using PCROSS of EMPIRE [2]. As the collective enhancements are taken into account, the changes on the level density a -parameter affect the fit and has been multiplied by 1.04. This level density a -parameter for the G.C Model [10] cannot be read as a single input entry. This is done with the Atilno input parameter. The Fermi gas model level density is chosen by using TALYS [4], and the presence of shell effects at low energy and their disappearance at high energy, the level density a -parameter is set to 9.30. The shape and magnitude of the level density a -parameter for the G.C model [10] by using PCROSS of EMPIRE [2] are closer to experiment [23] when compared to the level density a -parameter of the Fermi gas model using TALYS [4].

The calculated total cross section in the neutron energy range from 2.0 to 15.5 MeV is shown in Fig. 4. By using PCROSS of EMPIRE [2], the local and global nucleon optical models of Koning and Delaroche [15] have been used for neutrons and protons. The level density of G.C [10] is used in PCROSS of EMPIRE [2] while the BSFG Model [13] is used in TALYS [4]. The expression for the total BFM level density is given from Eq. (4.280) of TALYS [4]. Figure 4 shows that the G.C [10] and BSFG Models [13] affect strongly the shape of the curve compared to the Fermi gas model level density.

Figure 5 shows the calculated total cross section in neutron energy range up to 41.0 MeV. The HFBM level density [12] and the BSFG Model [13] are used in PCROSS of EMPIRE [2] and TALYS [4] respectively. The optimum incident neutron energy range for producing the ^{65}Ni nucleus is 12 to 13 MeV by using TALYS [4] and 13 to 14 MeV by using EMPIRE [2]. The maximum cross-section values are obtained by ~ 13 MeV in both codes, and the results using the BSFG Model [13] of TALYS [4] are closer to experiment [25] than those

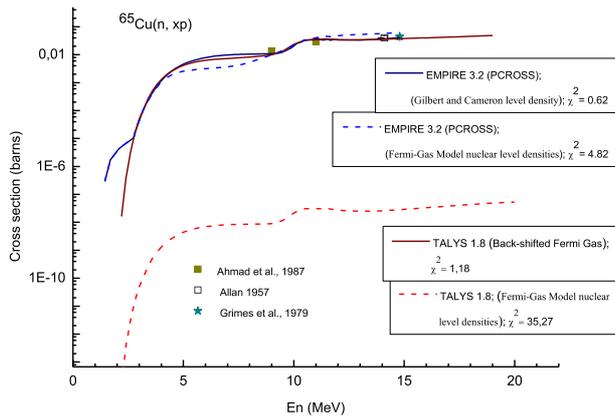


Figure 4. Comparison between calculated total cross section with G.C level density [11], BSGF [14] and Fermi Gas Model nuclear level density (continuous and dashed lines) for $^{65}\text{Cu}(n, xp)$ reaction to the experimental data [19,22,23] in neutron energy range from 9.0 to 15.0 MeV using the Exciton Model.

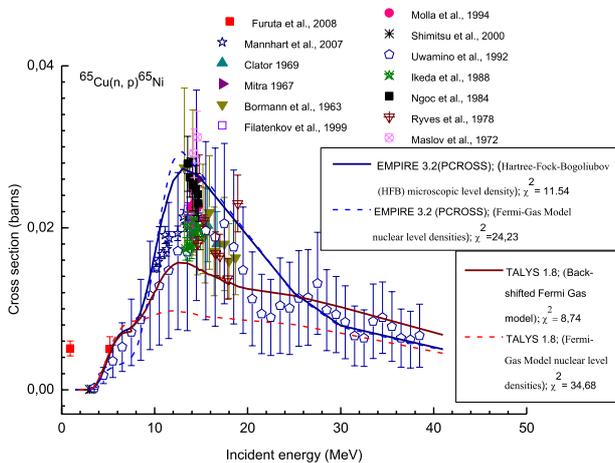


Figure 5. Comparison between calculated total cross section with HFBM [13], BSGF [14] and Fermi Gas Model nuclear level density (continuous and dashed lines) for $^{65}\text{Cu}(n, p)$ reaction to the experimental data [24] in neutron energy range up to 41.0 MeV using the Exciton Model [5].

used with the HFBM level density [12] in PCROSS of EMPIRE [2].

4. Conclusion

We have analyzed the calculated double-differential cross sections, the angle-integrated calculations, the calculated proton emission cross section of (n, xp) reactions and the excitation function of (n, p) on the ^{65}Cu target using the pre-equilibrium models and the level density models with the level density a -parameter modified of EMPIRE [2] and TALYS [4]. Our results show that the lower χ^2 value gives a significantly better fit when compared to the experimental data [19,22–24].

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