NUCL SCI TECH (2017) 28:147
DOI 10.1007/s41365-017-0298-4

Response of multi-step compound pre-equilibrium reaction cross sections for the (*p, n*) reactions to forms of optical model parameters

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Received: 2 March 2017 / Revised: 10 May 2017 / Accepted: 2 June 2017 / Published online: 8 September 2017

Abstract In furtherance to improving agreement between calculated and experimental nuclear data, the nuclear reaction code GAMME was used to calculate the multi-step compound (MSC) nucleus double differential cross sections (DDCs) for proton-induced neutron emission reactions using the Feshbach-Kerman-Koonin (FKK) formalism. The cross sections were obtained for reactor structural materials involving ^{52}Cr(*p, n*)^{52}Mn, ^{56}Fe(*p, n*)^{56}Co, and ^{60}Ni(*p, n*)^{60}Cu reactions at 22.2 MeV incident energy using the zero-range reaction mechanism. Effective residual interaction strength was 28 MeV, and different optical potential parameters were used for the entrance and exit channels of the proton-neutron interactions. The calculated DDCs were fitted to experimental data at the same backward angle of 150°, where the MSC processes dominate. The calculated and experimental data agree well in the region of pre-equilibrium (MSC) reaction dominance against a weaker fit at the lower emission energies. We attribute underestimations to contributions from the other reaction channels and disagreement at higher outgoing energies to reactions to collectively excited states. Contrary to the FKK multi-step direct calculations, contributions from the higher stages to the DDCs are significant. Different sets of parameters resulted in varying levels of agreement of calculated and experimental data for the considered nuclei.

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Keywords Proton-neutron interaction · Multi-step compound theory · Optical model parameters · Structural materials · Nuclear reactor facilities

1 Introduction

The pre-equilibrium reaction is considered as a series of two-body nuclear reactions involving projectiles, having several incident energies, and the target nuclei. The quantum mechanical way of calculating the double differential cross sections of the reactions has been carried out using the Feshbach-Kerman-Koonin (FKK) theory [1]. The two partitions of the pre-equilibrium process in the FKK theory: Multi-step compound (MSC) processes and the multi-step direct (MSD) processes are well documented [2–5]. The FKK theories of pre-equilibrium reactions have been developed into the stage of numerical comparison with experiment [1, 6–9].

The quantum–mechanical theories, just like the phenomenological models, assume that the nucleus is excited by a series of nucleon–nucleon collisions involving the projectile and target nucleons: in a series of steps beginning with the projectile in the continuum. At each stage in the excitation process, the states with at least one particle in the continuum and the states with all particles bound are considered separately. These are formally described by the projection operators P and Q acting on the total wave function, Ψ, with $P + Q = 1$. The set of states P contributes to the MSD process and the complementary set of states Q to the MSC process [10].

Since no interaction potential model explains the nuclear reaction cross sections for the entire energy range, the nucleons-nuclei interactions can be interpreted using

different theoretical models. The average total reaction cross sections can be interpreted using the optical model [11–15]. The scattering cross sections can be well fitted by the optical-model potential with suitably adjusted parameters [16]. The optical model provides the basis for many quantum–mechanical pre-equilibrium and direct reactions cross-sectional calculations for nuclear data evaluation and other applied purposes [17]. The optical-model potential is widely used in the distorted-wave Born-approximation (DWBA) analysis and can perform a simultaneous analysis of elastic scattering and total reaction cross sections [18, 19]. The optical model has been parameterized [20–22] and its energy dependence [23–26] has been investigated. Although the microscopic approach exists, the phenomenological approach to the optical model provides excellent description of nucleon-nucleus elastic scattering for medium and heavy nuclei [27–29].

In this work, the GAMME computer code [30] was used to calculate the MSC emission cross section and double differential cross section for the (*p, n*) nuclear reactions using the FKK theory. The double differential emission cross section calculated at 150° for ^{52}Cr(*p, n*)^{52}Mn, ^{56}Fe(*p, n*)^{56}Co, and ^{60}Ni(*p, n*)^{60}Cu reactions was fitted to experimental data [31]. It is sufficiently accurate to use the zero-range potential because calculations with finite range Gausian and Yukawa interactions gave similar results to those obtained with the zero-range reaction [32, 33]. For this reason, the calculations were carried out using the zero-range form for the residual proton-neutron interaction: and interaction strength of 28 MeV for the reactions. The theoretically calculated values were fitted and compared with the experimental data at 22.2 MeV incident energy from Ref. [31]. Since the MSC pre-equilibrium reaction is known to dominate at the backward angles, the data were fitted at 150° scattering angle.

The focus of this work is on the response of multi-step compound pre-equilibrium reaction cross sections for the (*p, n*) reactions to some forms of optical model parameters. The (*p, n*) reaction, as a charge exchange reaction, is a powerful spectroscopic tool of nuclear structure physics with spectroscopic characteristics that are closely related to the free interactions between nucleons [34]. The three nuclei considered: Chromium, iron, and nickel are important structural materials in nuclear reactor facilities for nuclear science and engineering studies.

2 Materials and method

2.1 FKK MSC formalism

The MSC pre-equilibrium emission cross section is given by the sum of product of the cross section for the formation of the compound system multiplied by the sum over all stages of the probability of pre-compound emission from the *N*th stage and the probability of reaching the *N*th stage without pre-equilibrium emission. The double differential cross section for pre-equilibrium emission by the MSC process is given by [2]:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E} = \pi\lambda^2 \sum_J (2J+1) \left[\sum_{N=1}^{r}\sum_{\ell s\lambda} C^{\lambda}_{\ell sJ} P_\lambda(\cos\vartheta) \sum_{v=N-1}^{N+1} \frac{\langle \Gamma^{\uparrow \ell sv}_{NJ}\rho^v_s(U)\rangle}{\langle \Gamma_{NJ}\rangle} \prod_{m=1}^{N-1} \frac{\langle \Gamma^{\downarrow}_{mJ}\rangle}{\langle \Gamma_{mJ}\rangle} 2\pi \frac{\langle \Gamma_{1J}\rangle}{\langle D_{1J}\rangle}\right], \tag{1}$$

where $C^{\lambda}_{\ell sJ}$ is the angular momentum coupling coefficient with $\lambda = 0, 2, 4,\ldots$ to ensure the symmetric emission characteristic of quasi-equilibrium processes; $2\pi\langle\Gamma_{1J}\rangle/\langle D_{1J}\rangle$ is the strength function for the initial reaction stage, with $\langle D_{1J}\rangle$ being the average level spacing within the class; the total width $\langle\Gamma_{mJ}\rangle$ is the sum of the total escape width, $\langle\Gamma^{\uparrow}_{mJ}\rangle$; and the damping width, $\langle\Gamma^{\downarrow}_{mJ}\rangle$ referring to emission and internal transitions, respectively; $\rho^v_s(U)$ is the density of states in each final state, *v*, whose excitation energy is *U* and $P_\lambda(\cos\theta)$ are the Legendre polynomials of order zero. Also, ℓ, *s,* and *J* are the orbital, spin, and total angular momentum quantum numbers, respectively.

The escape and damping widths are written in the factorized form as:

$$\left\langle \Gamma^{\uparrow \ell sv}_{nJ}(U)\rho^v_s(U)\right\rangle = X^{\uparrow \ell sv}_{nJ}(U)Y^{\uparrow v}_s(U), \tag{2}$$

$$\left\langle \Gamma^{\downarrow}_{nJ}(E)\right\rangle = X^{\downarrow N+2}_{nJ}Y^{\downarrow N+2}_{n}(E). \tag{3}$$

To calculate the *X* and *Y* functions, the density of a *p*-particle, *h*-hole configuration at an excitation energy is required. According to Ref. [35], the state density is expressed as:

$$\omega(p,h,E) = \frac{g^n}{p!h!(n-1)!}\sum_{i=1}^{p}(-1)^i \binom{p}{i} H\left(E-\Delta-E_{\mathrm{pp}}-iB\right)\left(E-\Delta-A^*_{\mathrm{ph}}-iB\right)^{n-1}, \tag{4}$$

where $g = 6a/\pi^2$ is the single-particle spacing, with *a* being the level density parameter; Δ is the pairing energy and *B* is the binding energy. The step function *H* ($E-\Delta-E_{\mathrm{pp}}-iB$) is unity for $(E-\Delta-E_{\mathrm{pp}}-iB) > 0$, and zero otherwise. A_{ph} and α_{ph} account for Pauli blocking and are given by:

$$A_{\mathrm{ph}} = \frac{p^2+h^2+p-3h}{4g}, \tag{5}$$

$$\alpha_{\mathrm{ph}} = \frac{p^2+h^2+p-h}{2g}. \tag{6}$$

The angular momentum distribution of states at excitation energy is represented by a Gaussian function with a spin cutoff [1]:

$$R_n(J) = \frac{(2J+1)}{\pi^{1/2} n^{3/2}} \exp\left[\frac{-\left(J+\frac{1}{2}\right)}{n\sigma^2}\right]. \quad (7)$$

Thus, the total density of states of spin, J, is given by $\rho(p, h, E, J) = \omega(p, h, E)R_n(J)$.

2.2 Method of calculation

In this work, it was assumed that the target consisted of a core to which the neutron was bound in a shell model state. The projectile was captured into a state of the residual nucleus, and the neutron was ejected through a residual nucleon–nucleon interaction. The level density parameter a and the pairing energy were obtained from the table of Ref. [36]. The cross section for pre-equilibrium emission from each stage is proportional to the square of modulus of the radial matrix element:

$$I = \left(\frac{4}{3}\pi r_0^3\right) V_0 \frac{1}{4\pi} \int_{r=0}^{\infty} R_1(r)R_2(r)R_3(r)R(r)\frac{\mathrm{d}r}{r^2}, \quad (8)$$

where $R_{1,2}(r)$ are the radial wave functions for the initial bound states, and $R_3(r)$ and $R(r)$ are those of the bound and unbound states, respectively. The distorted wave functions for the projectile, ejectiles, and competing ejectiles were calculated using Beccheti and Greenlees (BG) [37] and Wilmore and Hodgson (WH) [38] optical potentials for neutrons which are applicable to $A > 40$ and is determined on the basis of data up to 24 MeV. For protons, the BG and Patterson et al. (P) [39] optical potentials were used. The harmonic oscillator wave functions were used for the bound nucleons. A two-body residual interaction of zero range given by Ref. [4] was adopted:

$$V(r_1, r_2) = V_0\left(\frac{4}{3}\pi r_0^3\right)\delta(r_1, r_2), \quad (9)$$

where V_0 is the residual interaction strength, and $r_0 = 1.20$ fm is the Bohr radius

The GAMME code is a nuclear reactions code for calculating the MSC double differential cross section using the FKK theory [2]. Being made up of five major subroutines, GAMME is flexible and can be adapted for different nuclear reactions. The input file contains information on the projectile particle, target nucleus, ejectile of interest, and the competing ones. On the basis of the equations and philosophy of pre-equilibrium nuclear interactions, GAMME calculated the MSC double differential cross sections for the first three stages of the pre-equilibrium reaction, the evaporation stage and the sum of the cross sections.

3 Results and discussion

The experimental data were in the laboratory system. For consistency reasons and ease of comparison, the double differential cross sections contained in the experimental data were transformed into the center-of-mass (CM) system in which the calculated cross sections were obtained. The outgoing angles and energies were changed to reflect the transformation. Linear interpolation was carried out between the cross sections and the outgoing energies of the emitted neutron particles for both the calculated and experimental data at 150°.

3.1 Performance of the GAMME code

The GAMME code was written for single particle emission calculations using the MSC FKK formalism and has been successfully used for the calculation of the double differential cross sections for the ^{52}Cr(*p, n*)^{52}Mn, ^{56}Fe(*p, n*)^{56}Co, and ^{60}Ni(*p, n*)^{60}Cu reactions. In carrying out the calculations, the input file was used to generate the MSC double differential cross sections for the pre-equilibrium chain—first three stages of the excitation process, the evaporation or residual stage, and the sum of these cross sections for each of the reactions. The pre-equilibrium stages after the third do not contribute appreciably to the MSC cross section and were absorbed into the residual stage [2] to avoid complications without an appreciable effect on the final calculated results.

The reaction cross-sectional contributions from the first stage were between 30% for Fe (BG optical potential parameters) and 51% for Ni (BG–WH optical potential parameters). For the second stage, the contributions were between 22% for Fe (BG optical potential parameters) and 26% for Ni (combination of BG–WH and that of WH–P). The third stage contributed between 12.5% for Cr and 15% for Ni with the same BG optical potential parameter. The evaporation stage contributed between 10% for Ni (BG–WH optical potential parameters) and 34% for Fe with the optical potential parameters of BG.

It was observed that though the contributions of the first stage to the calculated double differential cross section are appreciable, the contributions from the second, third, and the evaporation stages are also significant, at least for the FKK MSC calculations on the targets considered and at the incident energy. Therefore, the contributions must be added to that of the first stage for a better fit to the experimental data. This is depicted in Fig. 1 where sums of these contributions were in better agreement with the experimental data. This is unlike in the FKK MSD calculations where the contributions from the first stage alone are about 80% of the calculated double differential cross

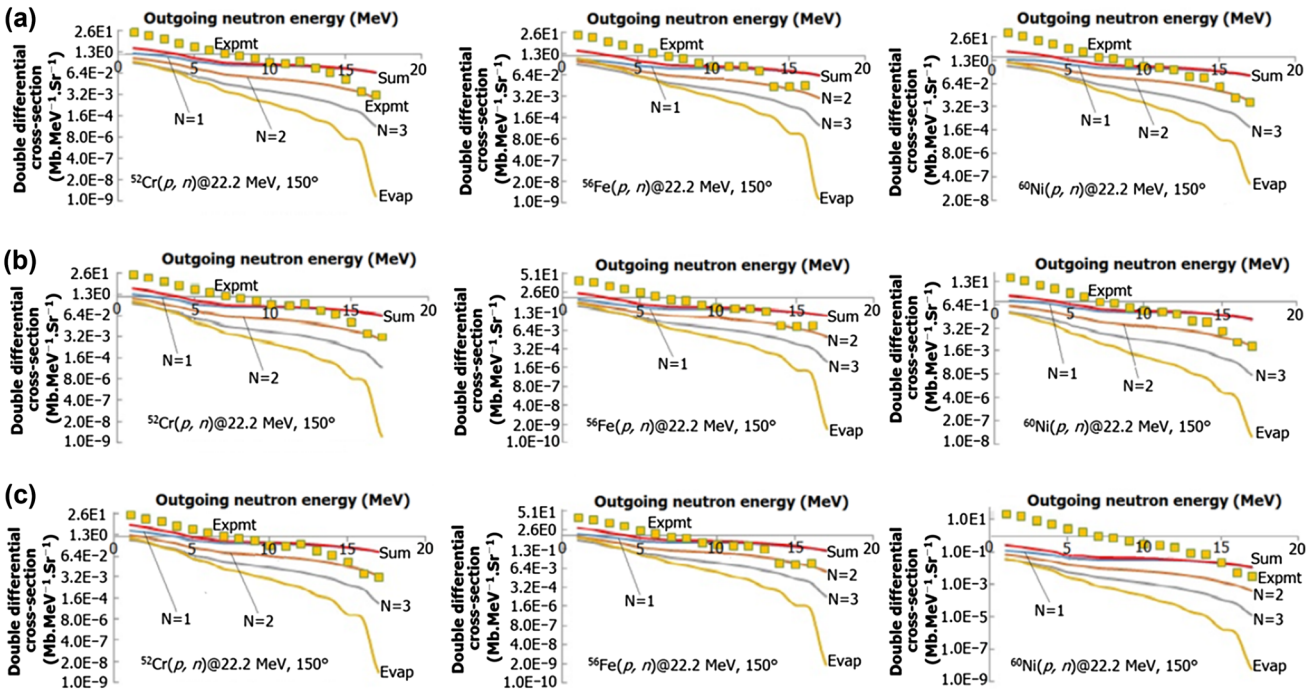

Fig. 1 (Color online) FKK MSC calculations for ^{52}Cr(p, n) ^{52}Mn, ^{56}Fe(p, n) ^{56}Co, and ^{60}Ni(p, n) ^{60}Cu reactions at 22.2 MeV using optical model parameters by **a** the Beccheti and Greenlees [37], **b** Beccheti and Greenlees [37] and Wilmore and Hodgson [38], **c** Wilmore and Hodgson [38] and Patterson et al. [39] for the first three stages of the pre-equilibrium reaction, the evaporation stage and the sum of the cross sections compared with the experimental data of Biryukov et al. [31]. The double differential cross section (Mb·MeV^{-1}·Sr^{-1}) is plotted against the outgoing particle energy (MeV)

section and contributions from higher stages can be neglected with no significant effect on the results [5].

3.2 Comparison of the calculated results with the experimental data

The calculated and experimental double differential cross-sectional data are compared in Fig. 1. In doing this, it is important to note that the experimental spectrum is a combination of four different processes: the compound nucleus (CN), MSC, direct, and MSD reactions. The GAMME code only calculates the MSC contributions by considering the cross sections at the backward angles where MSC and CN are believed to be dominant [4]. Some degree of deviations was observed between the calculated and experimental data, especially at the lower outgoing energy regions of the spectra for the three nuclei considered. This is in agreement with the reported dominance of the compound nucleus reactions at energy regions below 10 MeV and pre-equilibrium reactions between 10 and 15 MeV [4]. The reaction channel, CN, responsible for the underestimation at lower energies was not included in the FKK theory for which the GAMME code used in this work is based. At higher emission energies, there are significant contributions to the double differential cross sections from reactions to low energy collective excited states and/or direct nuclear reaction (DNR). Since the MSD and direct reaction channels for such contributions were not captured in the theory, it is, therefore, believed to be responsible for the level of disagreement between theory and experiment data at higher emission energies.

Figure 1 shows the consistent pattern in the shapes of the spectra between 1.0 and 9.0 MeV energy regions for the three nuclei considered and for the various optical potential parameters used. This consistency could be due to the relative closeness of the atomic masses of the nuclei considered or due to the same interaction strength, V_0 used for the theoretical calculations. Between 9.0 MeV and 13 MeV is the MSC dominant region, depicting the strong agreement between the calculated and experimental results.

Comparing the calculated and experimental results, vis-à-vis the different optical-model potentials (Fig. 1), there were no appreciable visible differences between the spectra obtained except in Fig. 1c where the combination of W–H and P parameters was used for the ^{60}Ni nucleus.

3.3 Sensitivity of the calculated results to optical-model potentials

In Fig. 2, only the sum of contributions from various stages was fitted to the experimental data while considering the sensitivity of the calculated double differential cross

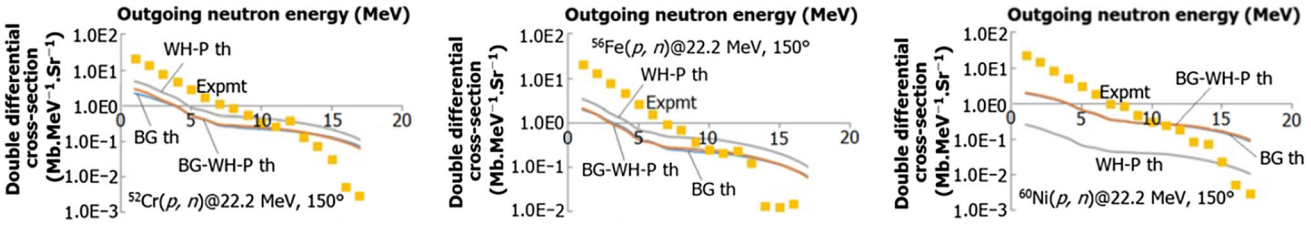

Fig. 2 (Color online) FKK MSC calculations for ^{52}Cr(*p, n*)^{52}Mn, ^{56}Fe(*p, n*)^{56}Co, and ^{60}Ni(*p, n*)^{60}Cu reactions at 22.2 MeV using optical model parameters in Refs. [37–39] compared with the experimental data of Biryukov et al. [31]

sections to the different optical-model potential parameters. The optical-model potential parameters (OMP) were those of proton—the projectile and neutron—the emitted particle employed in the calculations.

From Fig. 2, the calculated cross sections, reflecting the sum of the first three stages and the evaporation stage, are relatively insensitive to the OMP for the three nuclei. We observed a total agreement in the spectra originating from the B–G and those of B–G and W–H OMP. Only the combination of the OMP of W–H and P showed some degree of sensitivity of the calculated double differential cross sections to the optical parameters. This implies that the OMP of B–G and that of W–H could be used on either chromium or iron nucleus without any significant difference in the cross-sectional data. The idea of combination of OMP implies different sets of OMP for the entrance and exit channels. The combination of B–G and W–H implies B–G for protons (entrance channel) and W–H for neutrons (exit channel). For W–H and P, we mean W–H for neutrons and P for protons representing the exit and entrance channels, respectively.

4 Conclusion

The nuclear reaction code GAMME has been used to calculate the multi-step compound nucleus double differential cross section for proton-induced neutron emission nuclear reactions using the Feshbach-Kerman-Koonin (FKK) formalism. These cross sections were obtained for ^{52}Cr(*p, n*)^{52}Mn, ^{56}Fe(*p, n*)^{56}Co, and ^{60}Ni(*p, n*)^{60}Cu at 22.2 MeV incident energy using the zero-range reaction mechanism.

A good agreement was obtained between the calculated and experimental data in the region of pre-equilibrium multi-step compound reaction channel dominance. Underestimations observed at the lower emission energies were due to the contributions from the other reaction channels, which were not included in the FKK theory. The disagreement at higher outgoing energies was attributed to reactions to collectively excited states and DNR. This study showed that for the FKK MSC calculations on the considered targets and incident energy, the contributions from the second, third, and the evaporation stages to the double differential cross section are significant unlike in the FKK MSD calculations where the contributions from the first stage are most important, and other higher stages contributions are negligibly small.

While the calculated results obtained from the parameters of B–G and the combination of those of B–G and W–H showed a good agreement with the experimental data in the energy region of interest, the results obtained from the combination of W–H and P parameters deviated from the experimental data in the same energy region for ^{60}Ni nucleus. The parameters of B–G and W–H used on either chromium or iron yielded similar cross-sectional data.

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