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Study of Excitation Functions of (p, n) Reactions for ^{56}Fe and ^{57}Fe Target from Threshold to 30 MeV

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Abstract: The theoretical calculation of the cross section for formation of ^{56,57}Co in (p, n) reaction from ^{56,57}Fe target have been studied from reaction threshold to 30 MeV using TALYS-1.4 nuclear model reaction code whereby we have studied major nuclear reaction mechanisms, including direct, pre-equilibrium and compound nuclear reactions. These calculations were carried out by adjusting the effective imaginary potential, level density and shell damping parameters. It is observed that an excellent agreement between the theoretical calculated and experimental data is obtained with minimal effort on parameter fitting. We have also observed that there is significant contribution of pre-equilibrium emission in (p, n) reaction cross-section of ^{56}Fe and ^{57}Fe. The systematic increase in (p, n) cross-sections with increasing neutron number in reactions induced by protons on ^{56}Fe and ^{57}Fe is explained in terms of compound and pre-equilibrium mode.

Keywords: Iron target; Level density; shell correction; pairing interaction; Excitation function; Pre-equilibrium.

1. INTRODUCTION

The nuclear data for iron is particularly important due to the latter's role as an important structural material for the construction of nuclear reactors in many Accelerator Driven Sub-critical System (ADSS) designs. An alloy of iron is exceptionally strong and is used as a structural material for the construction of nuclear reactors. The common materials suitable for the reactor structures are stainless steel with Cr, Fe and Ni as main constituent, since these elements possess a high resistance to mechanical stress, stability to radiation and high

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temperature, as well as low neutron absorption. Fast reactor components operate at high temperatures (up to 750°C) and neutron irradiations, and only special stainless steels can comply with these requirements. Iron is one of the good candidates which can be operated at high temperature at 950^{0}C [8]. Stainless steel is the main off-core structural material for thermal reactors and is an essential material for fast neutron reactors. Iron is also an interesting element for physical considerations. It's most abundant isotope ^{56}Fe, is the third most tightly bound nuclide, with a binding energy per nucleon of 8.790 (± 0.03) MeV/A. Studies of excitation functions of charged particle-induced reactions like protons and α particles are of considerable significance for testing nuclear models as well as for practical applications. Bombardment of Fe target with protons open a number of reaction channels, out of which the neutron exit channel in the (p, n) reaction of iron is of interest for this discussion as neutrons produced in an ADSS spallation target can produce subsequently a large quantity of light-ions in the interaction with iron [4, 5]. The (p, n) reaction transforms the target nucleus to isotopes with one more proton in its ground or an excited state. Once the outgoing neutron energy is measured, we can determine the excitation energy of the residual nucleus of cobalt isotopes from the reaction kinematics.

2. NUCLEAR MODELS AND CALCULATIONS

The nuclear reaction model calculations performed include the direct-interaction, pre-equilibrium and compound nucleus contributions. The calculation of excitation functions for (p, n) reactions from threshold to 30 MeV for ^{56}Fe and ^{57}Fe were calculated using Talys-1.4 nuclear model code [1] with minimal effort on parameters fitting such as level density parameter and 'Shell damping factor' has been adjusted. The nuclear level densities of the nuclei involved in the calculations were treated within the generalized super fluid model (GSM), which takes into account pairing correlation and shell effects. Within the GSM the level density $\rho(U)$ is treated separately in two energy regions depending on the nuclear temperature T. Where the critical temperature value T_c is given by

$$T_c = 0.567\Delta_0 \tag{1}$$

And $\Delta_0 = 12/\sqrt{A}$ is the pairing correlation function. For $T < T_c$ or $(U' < U_c)$ the nucleus is in the normal phase. The shift in the excitation energy given by

$$E_{co} = \left(\frac{3}{2\pi^2}\right)\lambda_c\Delta_0^2 - \chi\Delta_0 \tag{2}$$

Where, Eco is the condensation energy and χ is the parity index of the nuclei given by

$$\chi = \delta_{N,par} + \delta_{Z,par} \tag{3}$$

$\delta_{K,par}$ is equal to 1 if K is even and 0 if K is odd

The level-density parameter λ varies with energy according to the equation.

$$\lambda = \tilde{\lambda}\left[1 + \frac{\delta\varepsilon_0}{U^{'} - E_{co}} f(U' - E_{co})\right] \tag{4}$$

Where, $U^{'} = U + n\Delta_0$ and

$$U = \lambda_c T_c \tag{5}$$

$U^{'}$ is the effective excitation energy and U is the true excitation energy of the compound nucleus.

n = 0, 1, 2 for even-even, even-odd and odd-odd nuclei respectively. $\tilde{\lambda}$ is the asymptotic value of λ at high excitation energy and $\delta\varepsilon_0$ is the shell correction of the nuclear binding energy.

The attenuation and disappearances of the shell effects with increasing excitation energy are modeled by the function

$$f(U) = \frac{(1 - \exp(-\gamma U))}{U} \tag{6}$$

The following systematically formula for the damping parameter is used

$$\gamma = \frac{\gamma_1}{A^{1/3}} + \gamma_2 \tag{7}$$

The parameters of $\gamma_{1,2}$ can be adjusted, within normal limits. In this work, the Ignatyuk formula represents the asymptotic parameter has been used.

$$\tilde{\lambda} = \alpha A + \beta A^{2/3} \tag{8}$$

Finally the level density is therefore given by

$$\rho(U,J) = \frac{1}{\sqrt{2\pi\sigma}} \frac{\sqrt{\pi}}{12} \frac{\exp[2\sqrt{\lambda U}]}{\lambda^{1/4} U^{5/4}} \tag{9}$$

Table 1: Parameters adjusted in the calculation are 'λ' is the level density parameter, $\tilde{\lambda}$ is asymptotic level density parameter, γ are the shell damping factors, '$\delta\varepsilon_0$' is the shell correction, '*w*' the adjusted value of the imaginary potential of Koning and Delaroche.

Nucleus	λ **MeV-1**	$\tilde{\lambda}$ **MeV-1**	γ **MeV-1**	$\delta\varepsilon$**0** **MeV**	**w** **MeV**
56Fe(p,n)	6.691	6.695	0.149	-0.010	1.012
57Fe(p,n)	8.548	8.558	0.280	-0.010	1.030

The optical model potentials for neutron and proton used in the TALYS-1.4 calculation is the global parameterizations of Koning and Delaroche [7]. In this work, in order to achieve the best prediction of the cross section the parameters, $\delta\varepsilon_0, \gamma_{1,2}$, α and β were adjusted.

3. RESULTS AND DISCUSSIONS

In this study proton induced reactions on ^{56}Fe and ^{57}Fe target with energy from threshold up to 30 MeV have been calculated as a part of a systematic investigation of excitation functions. In comparison with experimental data the calculated cross section of ^{56}Fe (p, n)^{56}Co given in Figure-1 and ^{57}Fe(p, n)^{57}Co plotted in Figure-2 are in good agreement with experimental data taken from EXFOR. The latter was retrieved from Exchange Format EXFOR database [11,3]. The Levkovskij data showing in Figure-1 and Figure-2 were renormalized according to new cross- section data measured by Takács et al. [2] of the ^{nat}Mo (p, x)^{96}Tc monitor reaction used by Levkovskij.

Calculation carried out by Talys-1.4 nuclear model reaction code indicates that the emission of neutrons from nuclear systems at excitation energies beyond a few MeV is caused by the pre-equilibrium contribution of the system in a time much shorter than the time for evaporation from an equilibrated compound nucleus. The broad peak on low energy side can be accounted for compound nucleus contribution. As the composite nucleus proceeds towards statistical equilibrium the projectile energy and momentum are shared between more and more particles after successive interaction. At the initial stages when the number of interactions is small the energy available to each degree of freedom is comparatively large. Consequently, the particles emitted at these stages will carry more energy than those emitted from equilibrated compound nucleus. This is indirectly indicated by the high-energy tails of the excitation function which signify a less rapid fall for the cross section than predicted by the compound nucleus model. Thus the emitted neutrons

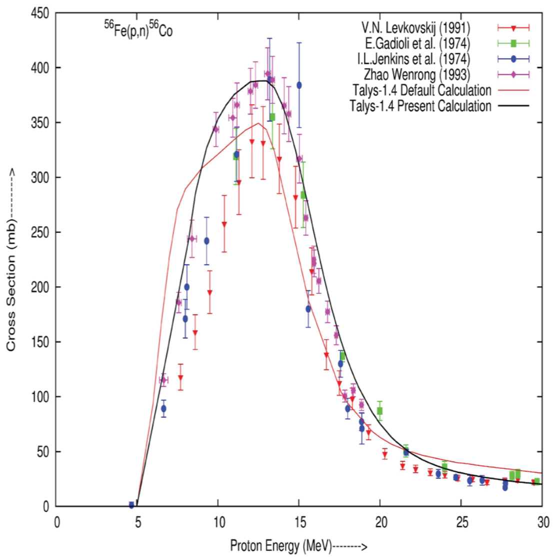

Figure 1: Excitation function for ^{56}Fe (p, n) ^{56}Co.

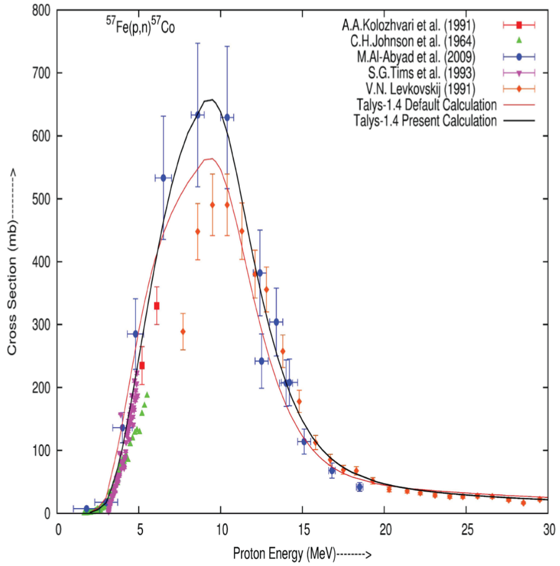

Figure 2: Excitation function for ^{57}Fe (p, n) ^{57}Co.

spectra the compound nucleus contribution is dominated by lower energy region of emitted neutrons and the pre-equilibrium contribution mainly comes from the higher energy region.

CONCLUSIONS

The excitation function of $^{56,57}Fe$ (p, n) reaction over proton energy ranging from threshold to 30 MeV have been analyzed using TALYS-1.4 nuclear model reaction code whereby generalized super fluid model (GSM) have been employed. It has been observed that the theoretical calculation cross sections match fairly well with the available experimental data, taken from EXFOR database. It is concluded that by choosing the appropriate level density parameter and by adjusting the value of the effective imaginary potential and shell damping parameters [3,6,10,11] one can predict (p, n) reaction cross-sections for $^{56,57}Fe$ from threshold to ~30 MeV closer to the available experimental data. These cross-sections increase with the increase in the neutron number and the compound contribution decreases with the increase in the neutron number for (p, n) reaction of ^{56}Fe and ^{57}Fe. The above observations established the significance contribution of the imaginary potential and the shell damping parameters and subsequently the importance of the statistical model and the shell model in understanding the compound nucleus reaction and pre-equilibrium model.

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