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Calculation of excitation functions of the ^{54,56,57,58}Fe(p, n) reaction from threshold to 30 MeV

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Abstract. The cross-sections for the formation of ^{54,56,57,58}Co in the ^{54,56,57,58}Fe(p, n) reaction from threshold to 30 MeV protons have been theoretically calculated using the TALYS-1.4 nuclear model code, whereby we have studied major nuclear reaction mechanisms, including direct, pre-equilibrium and compound nuclear reaction. Subsequently, the level density and shell damping parameters have been adjusted and at the same time, the odd–even effects are well comprehended. The excitation functions have been compared with experimental nuclear data. It is observed that the theoretical cross-sections match fairly well. Proton-induced reaction cross-sections provide clues to understand the nuclear structure and offers a good testing ground for ideas about nuclear forces. In addition, complete information in this field is very much required for application in accelerator-driven subcritical system.

Keywords. Iron target; level density; shell correction; pairing interaction; excitation function; pre-equilibrium.

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1. Introduction

For a better understanding of the experimental data, it is instructive and advantageous to perform nuclear model calculations and compare the experimental and calculated data. The nuclear data for iron are of particular importance, because of the role of iron as a structural material, is vital for the construction of nuclear reactors, and also in designing accelerator-driven sub-critical system (ADSS). Understanding the nucleon-induced reactions is a crucial step for further development of the theory of nuclear reactions. In addition, complete information in this field is strongly needed in many applications, such as the ADSS, which has been an interesting focus in nuclear physics. In ADSS, the energy ranges considered are: thermal neutron below 0.1 MeV, fast neutron from 0.1 to 20 MeV and high energy region above 20 MeV. The spectrum of these neutrons emanating from the target is considerably lower in the thermal region and high-energy region than the spectrum in the fast neutron [1,2]. The basic idea of ADSS is to use high-intensity proton energy accelerators for the production of intense neutron flux through spallation processes.

The importance of the basic nuclear data cannot be undermined. Basic nuclear data have been evolved for thermal, fast and fusion reactors, and are vital in the research studies involving ADSS concepts [3]. It is a well-known fact that in order to meet the increasing energy requirements of the Indian population, we have to turn to the technique of using thorium for power production, which is being carried out in ADSS.

The upgradation of basic nuclear data is a part of the plan of improving and justifying the use of some simulation tools like computational codes, modelling techniques and computerized data bases.

We need nuclear data for predicting nuclear collision, production of isotopes, formation of gases and heat generation in the ADSS and also for converting fertile to fissile nuclei and for transmutation of radioactive nuclei to stable ones.

In this process, a beam of high-energy protons is directed towards the target, which yields copious neutrons by (p, xn) spallation reaction. A spallation target as a source of neutrons and up to one neutron can be produced per 25 MeV of incident proton, which will then drive the subcritical nuclear reactor. While these projects obviously require large amount of nuclear data for intermediate energy neutrons, the accelerator-driven neutron sources also require better information of proton-induced reactions for the neutrons producing target (Ta, Pb, Bi), as well as for the surrounding structural materials (Al, Fe, Ni, Zr), which form integral part of nuclear reactors.

Fast-reactor components operate at high temperatures (up to 750°C), because of which only special stainless steel can be used in fast reactors [4]. Iron is a good candidate which can be operated at temperature as high as 950°C. Iron is an interesting element also for physical considerations. 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 number of light ions in the interaction with iron [5,6]. 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.

The current results of the theoretical calculation like ALICE-IPPE and STAPRE of proton-induced reactions on natural Fe were calculated from their respective threshold up to 20 MeV [7,8]. The results from these calculations using the above-mentioned codes are higher than the results from experimental data. In all the calculations, standard recommended input data of level density parameters, pre-equilibrium and compound nucleus were used and no other parameter fitting was done [9,10]. Therefore, improved nuclear data libraries for ^{54,56,57,58}Fe(p, n) reactions are needed for applications over incident proton energy range from threshold to 30 MeV. As the set of optical model calculations of Fe is obtained to fit to the experimental data of reaction cross-sections for $^{\mathrm{nat}}$Fe usually require many adjustable parameters, it is imperative that the parameters chosen should be within a reasonable range. In this work, the level density parameters and shell damping factor were adjusted accordingly to get a good fit with the experimental data [11–13]. Studies of excitation curves for the (*p*, *n*) reaction on four stable iron isotopes have revealed an interplay of the compound nucleus and the pre-equilibrium mechanisms, due to their different dependence on the target neutron excess [14]. The shapes and magnitudes of the excitation functions from the reaction thresholds up to 30 MeV are also well reproduced by describing nuclear model calculations using a consistent set of model parameters [15]. The main purpose of this work is to check the predictive power of the nuclear model calculations on the excitation functions and to understand the mechanisms of compound nucleus and pre-equilibrium models starting from reaction threshold to 30 MeV as well as to check the shell effects in the (*p*, *n*) reactions on four stable iron isotopes. In the present calculation, we have computed excitation functions of ^{54,56,57,58}Fe(*p*, *n*) reactions from reaction threshold to 30 MeV and compared these values with the available experimental data.

2. Nuclear models

Using TALYS-1.4 nuclear reaction code, the excitation function of the (*p*, *n*) reaction on four stable iron isotopes, viz, ^{54}Fe, ^{56}Fe, ^{57}Fe and ^{58}Fe were calculated and plotted. In general, the main reasons for using TALYS-1.4 [16,17] are: (1) It is a nuclear physics tool that can be used for the analysis of nuclear reaction experiments. The interplay between experiment and theory gives us insight in the fundamental interaction between particles and nuclei, and precise measurements enable us to constrain our models. In return, when the resulting nuclear models are believed to have sufficient predictive power, they can give an indication of the reliability of measurements. (2) TALYS-1.4 is a computer code consisting of a variety of nuclear reactions such as direct, compound, pre-equilibrium and fission reactions developed by the nuclear research and consultancy group (NRG) [18]. (3) TALYS-1.4 provides accurate simulations of nuclear reactions involving neutrons, γ-rays and light ions with $Z \leq 2$ (protons, deuterons, tritons, ^{3}He and α-particle). (The code supports a wide energy range, between 1 keV and 200 MeV, and target masses between 12 and heavier elements). (4) The authors used TALYS-1.4, which should enable evaluation of all nuclear reactions beyond resonance range. Numerous nuclear models are available in TALYS-1.4; (5) Several parameters can be adjusted in TALYS-1.4 depending upon the needs or requirements of the user and all these parameters remain within the physically acceptable limits.

3. Parameters adjusted in this work

The evaluation of the cross-sections is one of the main tasks in the field of low-energy nuclear reactions. These reactions are described by different models which depend on the incident energy of the projectile. The most widely investigated range of energies is 0–200 MeV. In this range, one can distinguish three classes of reactions depending on the time required for production. The fastest are called direct reactions and the slowest are the reactions giving rise to a compound nucleus formation. Between these extreme processes, there are the pre-equilibrium reactions [19]. To calculate the cross-sections using the compound nucleus model as well as the pre-equilibrium models, one of the most important ingredients is the level density; it is an important characteristic of the nucleus, as it allows one to explore the mechanism of nuclear excitations, information about the structure of the excited nuclei. In our calculations, the energy dependence of the level-density parameter plays a very important role in which the energy-dependent factor is one of the commonly used level-density parameter [20]. This notion is connected to the fact that the typical spacing of the first excited nuclear levels in medium and heavy nuclei is of the order of a tenth or some tenths of MeV for low excitation energies, but become very densely spaced, when these energies increase, so that a quick individual description is no longer feasible. For the calculation of level densities, several models have been employed [21].

The calculation of theoretical cross-section in the energy region from threshold to 30 MeV was performed using TALYS-1.4 nuclear reaction code, taking into account the compound and precompound nuclear processes, in the framework of the Hauser–Feshbach theory [22] and the exciton model [23], respectively. The calculation of level densities of the nuclei involved within the generalized superfluid model (GSM) developed by Ignatyuk *et al* [24], takes care of superconductive pairing correlations, shell effects and collective enhancement of the level density of the nucleus in a consistent way according to the Bardeen–Cooper–Schrieffer theory [25]. The superfluid model has predicted the existence of two energetic regions with entirely different characteristics depending on the critical temperature $T_{\rm c}$ of the phase transition from superfluid to normal state. The condensation energy, the critical energy of phase transition and the effective excitation energy are connected with the correlation function Δ_0 through the following equations:

$$T_{\rm c} = 0.567\Delta_0, \tag{1}$$

where $\Delta_0 = 12/\sqrt{A}$ is the systematic value of pairing correlation function. For $T < T_{\rm c}$ or $(U' < U_{\rm c})$, where U' is the effective excitation energy and $U_{\rm c}$ is the critical energy, the nucleus is in the superfluid phase, since the nucleons are paired and for this reason, the ground-state energy is reduced by the condensation energy $E_{\rm co}$ with respect to the energy which the same nucleus would have in an independent particle model. For $T \geq T_{\rm c}$ or $(U' \geq U_{\rm c})$, the nucleus is in the normal phase, where the pairing disappears and the system behaves like an independent particle, so that the effective excitation energy can be defined as

$$U' = U - E_{\rm co}, \tag{2}$$

where U is the true excitation energy of the compound nucleus. The level-density parameter is considered constant in the superfluid phase of the nucleus and the level density follows the simple parametrizations of the Fermi gas model [26] with a shift in the excitation energy by

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

where $E_{\rm co}$ is the condensation energy characterizing the decrease of the ground-state energy of the Fermi gas because of the correlation interaction and χ is the parity index of the nuclei given by

$$\chi = \delta_{N,{\rm par}} + \delta_{Z,{\rm par}}, \tag{4}$$

$\delta_{K,\mathrm{par}}$ is equal to 1 if K is even and 0 if K is odd. This effect is called odd–even effect. In addition to the energy needed to excite the fermions, certain energy is required because the fermions have the tendency to form pairs. Therefore, Δ_0 is the energy required to break the nucleon pairs, so that the final state of the nucleus is analogous to a gas of independent particles. The level-density parameter λ varies with energy according to the equation:

$$\lambda = \tilde{\lambda}\left[1 + \frac{\delta\varepsilon_0}{U' - E_{\mathrm{co}}} f(U' - E_{\mathrm{co}})\right], \tag{5}$$

where $\tilde{\lambda}$ is the asymptotic value of λ at high excitation energy and $\delta\varepsilon_0$ is the shell correction of the nuclear binding energy. The normal phase behaviour of λ [27] was determined by the dimensionless function $f(U')$. Equation (2) contains a shell damping factor γ through $f(U')$ that simulates the damping of the shell effects in the shell corrections, and subsequently causes the shell effect to disappear at high energies. The attenuation and disappearance of the shell effects with increasing excitation energy are modelled by the function

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

The following systematical 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 [28] represents the asymptotic parameter that has been used.

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

where A is the mass number, α and β are global parameters that have been determined to give the best average level density description over a whole range of nuclides. U is the value of the excitation energy that was approximated by the following eq. (9) [29]:

$$U = \lambda_{\mathrm{c}} T_{\mathrm{c}}. \tag{9}$$

As for the semiempirical level-density parameter λ_{c}, its calculation has been proposed by Gilbert–Cameroon [30]. To a certain extent, the GSM resembles the constant temperature model (CTM), which differentiates between a low-energy and a high-energy regions. Thus, the total level density is given by

$$\rho(U, J) = \frac{1}{\sqrt{2\pi\sigma}} \frac{\sqrt{\pi}}{12} \frac{\exp[2\sqrt{\lambda U}]}{\lambda^{1/4} U^{5/4}}. \tag{10}$$

Essentially, $\rho(U)$ denotes the level density for the nuclear state. σ is the spin cut-off parameter defined by

$$\sigma^2 = 0.0139 \frac{A^{5/3}}{\tilde{\lambda}} \sqrt{\lambda U}. \tag{11}$$

The parameters $\delta\varepsilon_0$, $\gamma_{1,2}$, α and β introduced in eqs (5), (7) and (8), were adjusted in this work to achieve the best prediction within TALYS-1.4. Thus, by introducing the level-density parameter λ and by adjusting the above-mentioned parameters, the calculated cross-sections were found to be in good agreement with the experimental data. The optical model potentials for neutron and proton used in the TALYS-1.4 calculation is the global parametrizations of Koning and Delaroche [31].

4. Results and discussions

The calculated cross-section data for proton-induced reactions on Fe isotopes are presented in table 1. The mass dependence of the calculated nuclear level-density parameter is shown in figure 1. The level density and the pairing energy in ^{57}Fe shown in table 1 are higher than other Fe isotopes because of the unpaired neutron in ^{57}Fe. Generally, the level density of even–even nuclei is lower than that of odd–even, which in turn is lower than that of odd–odd nuclei because fermions have the tendency to form pairs and therefore, before exciting the fermions of the nucleus, pairs have to be broken, which requires additional energy. Also, the difference in nuclear level density is associated with the shift in pairing correlations in odd-A nuclei such as ^{57}Fe, which is the only stable isotope of iron with non-zero nuclear spin ($I = 1/2$), in which the odd neutron undergoes an $E2$ process through ($5/2 \rightarrow 3/2$), ($5/2 \rightarrow 1/2$) and ($3/2 \rightarrow 1/2$) transitions. In ^{57}Fe, the unpaired neutron weakens the binding energy by 2–3 MeV. The nuclei of the other three isotopes of iron are more stable and difficult to be excited as they are closed shell nuclei. As the nucleus is heated up, the shell effect disappears and this is manifested on the level density of nuclei. At low temperature, nucleons are paired off. The consequence of this pairing effect is the energy gap between the ground state and the lowest two quasiparticle states.

In this study, proton-induced reactions on natural Fe with energy up to 30 MeV have been calculated as part of a systematic investigation of excitation functions. The cross-sections were calculated for the production of ^{54,56,57,58}Co. The excitation curve for ^{54}Fe(p, n)^{54}Co is given in figure 2. Experimental data are not available for ^{54}Fe(p, n)^{54}Co. Here, the cross-section for ^{54}Fe(p, n)^{54}Co calculated using GSM is compared with that obtained from the CTM generated by default parameters.

The calculated results for ^{56}Fe(p, n)^{56}Co, ^{57}Fe(p, n)^{57}Co and ^{58}Fe(p, n)^{58}Co reaction cross-sections are in good agreement with experimental data [7,8,32–41] taken from EXFOR as shown in figures 3–5. The computed cross-section together with the experimental data are plotted. The latter was retrieved from exchange format EXFOR database [42]. The Levkovskij data shown in figures 3–5 were corrected according to the new cross-section data measured by Takács *et al* [43] of the $^{\mathrm{nat}}$Mo(p, x)^{96}Tc monitor reaction used by Levkovskij, i.e. by a factor 0.76 ($\sim$190.8 mb/250 mb). The excitation functions for ^{56}Fe(p, n)^{56}Co are shown in figure 3. Except for data by Levkovskij [32] and Jenkins *et al* [34], the experimental data agree well with the result of TALYS-1.4 calculations. The excitation function of ^{57}Fe(p, n)^{57}Co shown in figure 4 and that of ^{58}Fe(p, n)^{58}Co

Table 1. Parameters adjusted in the calculation.

Nucleus	λ (MeV^{-1})	$\tilde{\lambda}$ (MeV^{-1})	γ (MeV^{-1})	P_s (MeV)	E_{sh} (MeV)	E_s (MeV)	E_{co} (MeV)	T_c (MeV)
^{54}Fe(p,n)^{54}Co	5.668	6.114	0.148	0.000	−1.021	13.378	3.103	1.090
^{56}Fe(p,n)^{56}Co	6.691	6.695	0.149	0.000	−0.010	11.197	3.173	1.002
^{58}Fe(p,n)^{58}Co	7.778	7.779	0.190	0.000	−0.001	10.045	2.332	0.796
^{57}Fe(p,n)^{57}Co	8.548	8.558	0.280	1.550	−0.010	7.646	2.332	0.796

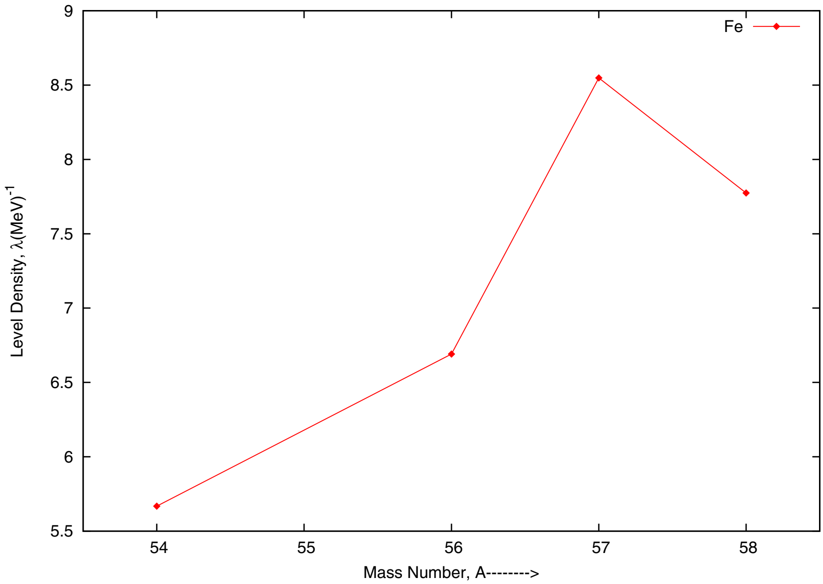

Figure 1. Mass dependence of the calculated nuclear level density parameter.

shown in figure 5 have approximately the same shape. Except for a few scattered points of Levkovskij data at the lower energy region and Antropov *et al* [39] data, the experimental data and the result of TALYS-1.4 calculations are found to be in good agreement.

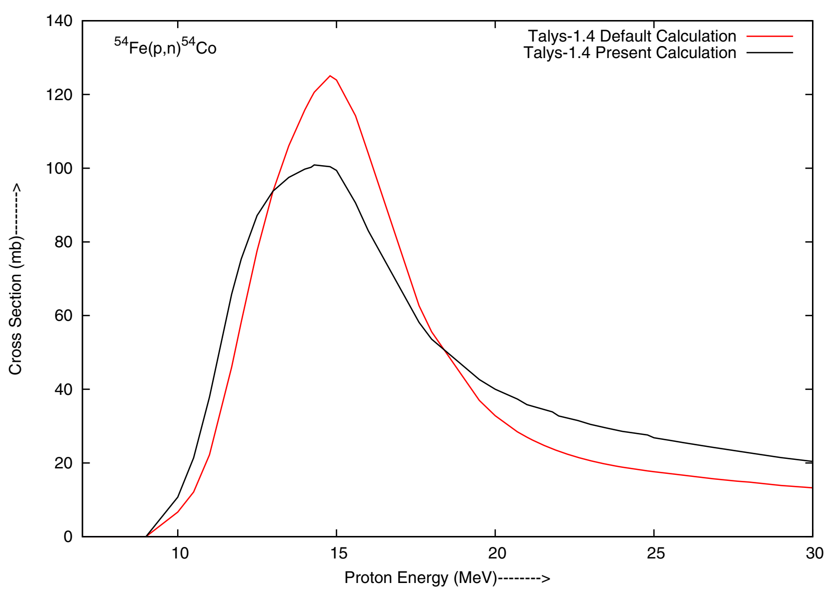

Figure 2. Excitation function for ^{54}Fe(p, n)^{54}Co reaction. Experimental data are not available for ^{54}Fe(p, n)^{54}Co reaction.

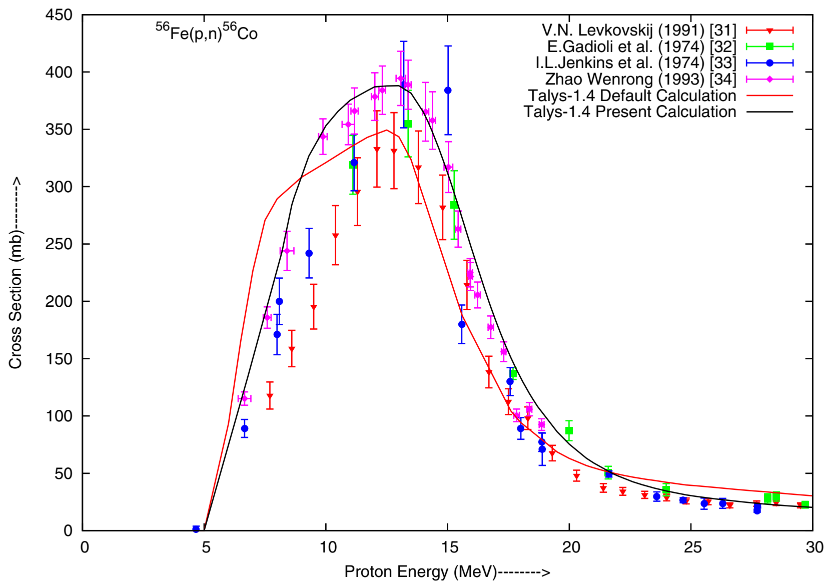

Figure 3. Excitation function for ^{56}Fe(p, n)^{56}Co reaction. The black solid line represents TALYS-1.4 calculation. The datapoints represent experimental data taken from EXFOR (2011) database.

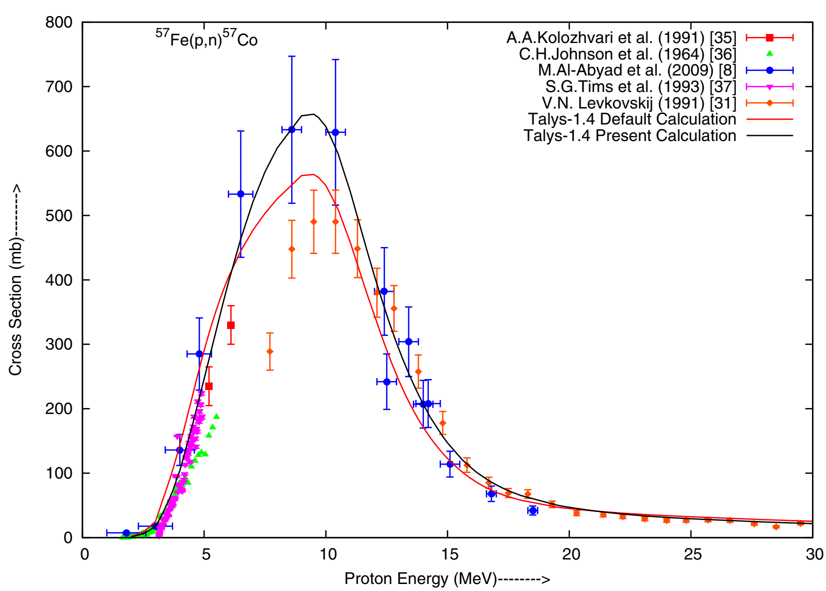

Figure 4. Excitation function for ^{57}Fe(p, n)^{57}Co reaction. The black solid line represents TALYS-1.4 calculation. The datapoints represent experimental data taken from EXFOR (2011) database.

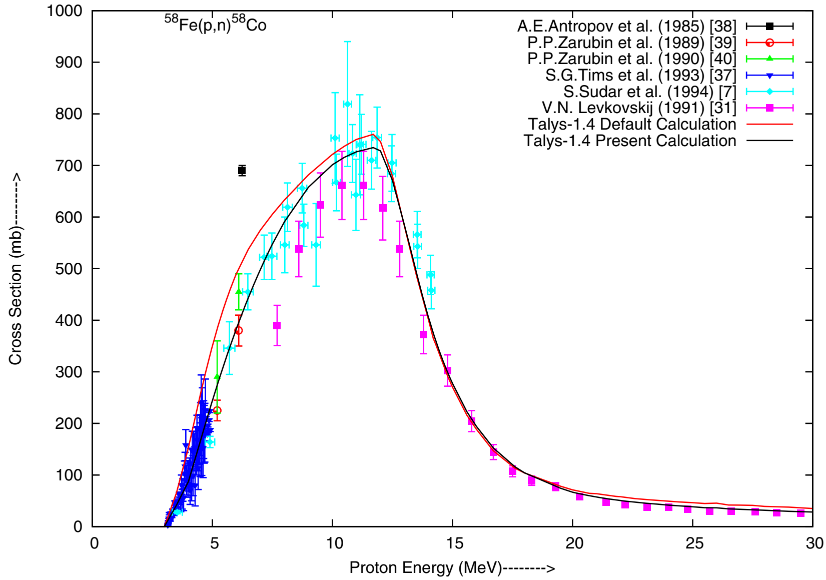

Figure 5. Excitation function for ^{58}Fe(p, n)^{58}Co reaction. The black solid line represents TALYS-1.4 calculation. The datapoints represent experimental data taken from EXFOR (2011) database.

Investigation carried out by TALYS-1.4 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 the low-energy side is due to the 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, in the emitted neutron spectra the compound nucleus contribution is dominated mainly by lower energy region of emitted neutrons, and the pre-equilibrium contribution comes from the higher energy region.

5. Conclusions

We have analysed the excitation functions of ^{54,56,57,58}Fe(p, n) (which are good construction materials for nuclear reactors) reaction over proton energy ranging from threshold to 30 MeV with TALYS-1.4 nuclear reaction code using generalized superfluid model (GSM). It is concluded that by adjusting the value of effective imaginary potential as input parameters and by choosing the appropriate level density parameter as well as the shell damping parameters [13–15], one can predict (*p*, *n*) reaction cross-sections for four stable isotopes of iron from threshold to ∼30 MeV closer to the available experimental data, taken from EXFOR database [44]. We have also observed that there is significant contribution of the effective imaginary potential and pre-equilibrium emission in (*p*, *n*) reaction cross-section of all four stable Fe isotopes. 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.

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