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Excitation Function of (n, p) and (n, α) Reactions for Long-Lived Target and Residual Nuclei Of Importance in Fusion Reactor Technology

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***Abstract*- The cross-sections of ^{50}Cr(n,p)^{50}V, ^{63}Cu(n,p)^{63}Ni, ^{55}Fe(n,p)^{55}Mn, ^{60}Fe(n,p)^{60}Mn, ^{59}Ni(n,p)^{59}Co, ^{60}Ni(n,p)^{60}Co, ^{63}Ni(n,p)^{63}Co, ^{51}Cr(n,α)^{48}Ti, ^{63}Cu(n,α)^{60}Co, ^{55}Fe(n,α)^{52}Cr, ^{58}Ni(n,α)^{55}Fe, ^{59}Ni(n,α)^{56}Fe, ^{63}Ni(n,α)^{60}Fe and ^{50}V(n,α)^{47}Sc reactions have been calculated by using TALYS-1.4 code from threshold to 20 MeV. For the confirmation of pre-equilibrium emissions, the double differential cross-section of outgoing proton and alpha particles is also investigated at 14 MeV. The calculated cross-section data have also been compared with systematics at 14.7 MeV. A good agreement between the calculated results, experimental data as well as systematics is obtained.**

***Keywords*- Cross-sections, double differential cross-section, Pre-equilibrium, systematic, TALYS-1.4.**
PACS Nos 28.52.-s; 28.52.Av; 28.52.Fa; 25.60.Dz

I. INTRODUCTION

The cross-section calculations for long lived target and residual nuclei at ~14 MeV neutrons energy are of great importance for the development of low activation materials in fusion reactors. Cr, Cu, Fe, Ni and V are main constituents suitable for structural and blanket components in fusion reactors. The fast neutron induced reactions such as (n,p) (n,α) on these materials produce some long lived product nuclei. Experimental determinations of cross-sections for long lived radio nuclides involve great difficulty. If the wrong lifetime of the product nuclide is used the experimental cross-section shows incorrect values. Although, in few reactions measured data of activation cross sections at few energies are available but complete excitation function of the reactions is necessary for the development of fusion reactors. Therefore, theoretical investigation is needed to support and extend the experimental cross-sections data for entire incident neutron energies (from threshold to 20 MeV).

TALYS-1.4 which is a recent and versatile nuclear reaction code developed by A.J. Koning et al. [1] has opened up options for calculating cross-sections for various reaction channels.

In the present work, we have calculated (n,p) and (n,α) reactions for long lived target and product nuclei of Cr, Cu, Fe, Ni and V in the energy range from threshold to 20 MeV. The pre-equilibrium emission plays an important role in determining the (n,p) (n,α) reactions cross-section and therefore we have studied the compound nucleus and pre-equilibrium components on these reactions from threshold to 20 MeV neutron energy. The double differential cross-sections (DDX) for outgoing proton and alpha particles at 14MeV neutron energy are also calculated to understand the compound nucleus and pre-equilibrium components.

The main aim of this work is to check the predictive power of TALYS-1.4 to calculate the unknown cross-sections for some important long lived target and product nuclei reactions. This aim was accomplished by the consistency of the calculation method, cross checking of used parameters by the available experimental data, systematic studies and the trend of calculated results for all the range of incident energies.

II. CALCULATIONS

The (n,p) and (n,α) reaction cross-sections of long lived target and product nuclei of Cr, Cu, Fe, Ni and V isotopes from threshold to 20 MeV have been calculated by TALYS-1.4 code. The semi microscopic JLM optical model potential for neutron and proton proposed by Bauge-Delaroche et al., [2] and folding approach of Wanadabe et al., [3] for alpha particle has been taken in the present calculations. The compound nucleus contribution is calculated by Hauser Feshbach model given by Hauser et al., [4]. The Pre-equilibrium contributions are taken into account by invoking two component exciton model with optical model for collision probabilities (Preeqmode 3) using Kalbach systematic given by Kalbach [5] with the particle hole density by Dobes and Betak [6] and Betak and Dobes [7]. The nuclear structure inputs like nuclear masses and discrete energy level densities of the nuclei involved in the calculations are taken from latest compilation available in RIPL given by Capote et al., [8].

The Gilbert and Cameron [9] level densities adjusted to experimental 'a' values and to discrete levels have been used in these calculations. The Gilbert –Cameron formalism splits the excitation energy in two regions. Different functional forms of level densities are applied in each of them. At low excitation energies (below the matching point E_x) the constant temperature formula is used which is:

$$\rho_T(E) = 1/T \exp[(Ex - E_0)/T] \qquad .....(1)$$

Where T is the nuclear temperature, E is the excitation energy Ex= U + Δ^{CTM} with Δ^{CTM} being the pairing correction), and E_0 is an adjustable energy shift. Above U_x the Fermi gas formula is applied which reads:

$$\rho_F(U) = exp\left(2\sqrt{aU}\right)/12\sqrt{2}\sigma(U)a^{1/4}U^{5/4} \qquad .....(2)$$

The level density parameter 'a' and spin cut-off factor $\sigma(U)$ is assumed to be specific energy dependent. In order to check the calculated cross-sections, we have choosen systematics for (n,p) and (n,α) reactions at 14.7 MeV given by R. Doczi et al., [10] and Majdeddin et al., [11].

$$\sigma_{n,p} = 23.659(A^{1/3}+1)^2 \exp\{-23.041(N\text{-}Z/A)+ (N\text{-}Z/A)^2\} \qquad ......(3)$$

$$\sigma_{n,\alpha} = 15.0678(A^{1/3}+1)^2 \exp -27.55\{(N\text{-}Z/A)+ (N\text{-}Z/A)^2\} \qquad ....(4)$$

The double differential cross-section (DDX) for the emission of proton and alpha particles at 14MeV neutrons also have been calculated using above mentioned parameters and nuclear models.

III. Results & Discussion

The calculated cross-sections data together with the experimental values taken from EXFOR data library for all cases of Cr, Cu, Fe, Ni and V are shown in Figs. 1-14. In all the figures, the bell like shape of the excitation curve, which is a characteristic of compound nucleus formation rises abruptly above the reaction threshold and descends due to competitive (n,np), (n,2n) and (n,nα) reactions. The pre-equilibrium contribution increases with neutron energy, appears around ~ 10-20 MeV and enhance the total (n,p) and (n,α) cross-sections. For the confirmation of role of pre-equilibrium emission, we have calculated the double differential cross-section (DDX) for all (n,p) and (n,α) reactions at 14 MeV neutron energy, which are shown for four cases in Figs. 2,5,9 and 10 along-with calculated reaction cross-sections.

The calculated values of (n,p) and (n,α) reaction cross-sections both for long-lived target and residual radionuclide using TALYS-1.4 along with systematics and latest available experimental data near 14 MeV are shown in Table 1. In all cases, our calculated cross-section values are close to available experimental values and systematics except in one case where our calculated value is much lower than systematics and there is no experimental data available for this case.

TABLE-1

ESTIMATED (N,P) AND (N,α) CROSS-SECTIONS FOR LONG-LIVED TARGET AND RESIDUAL NUCLEI AT 14.7±0.2 MeV.

$T_{1/2}$ gives target $T_{1/2}$ / residual $T_{1/2}$ in years (if not stated otherwise).

Reaction	$T_{1/2}$	$\sigma_{systematic}$	σ_{Talys}	σ_{exp}
^{50}Cr(n,p)^{50}V	∞/1.4× 10^{17}	294±50	230.149	381
^{63}Cu(n,p)^{63}Ni	∞/100.1	70±13	56.1014	58.6
^{55}Fe(n,p)^{55}Mn	2.73/∞	145	174.384	-
^{60}Fe(n,p)^{60}Mn	1.5×10^6/51 sec	17	2.9223	-
^{59}Ni(n,p)^{59}Co	7.6×10^4/∞	165	138.869	-
^{60}Ni(n,p)^{60}Co	∞/5.27	148±8	143.81	142.6
^{63}Ni(n,p)^{63}Co	100.1/27.4 sec	34	33.2723	-
^{51}Cr(n,α)^{48}Ti	2.734/∞	60.7	54.683	-
^{63}Cu(n,α)^{60}Co	∞/5.2713	35.26	44.2937	42
^{55}Fe(n,α)^{52}Cr	2.737/∞	63.7	74.4309	-
^{58}Ni(n, α)^{55}Fe	∞/2.737	133	121.515	101.6
^{59}Ni(n, α)^{56}Fe	7.6×10^4/∞	80	99.8923	-
^{63}Ni(n, α)^{60}Fe	100/1.5×10^6	11	8.03701	-
^{50}V(n, α)^{47}Sc	1.7×10^{17}/3.349 days	30.58	39.689	40

The excitation function of ^{50}Cr(n,p)^{50}V is shown in Fig.1. There is only one experimental point present at 14.1 MeV and our calculated value is lower than the experimental point but is in accordance with the systematics. Further experimental measurements are recommended for this reaction.

The excitation curve for $^{63}Cu(n,p)^{63}Ni$ reaction with direct, pre-equilibrium and compound components is shown in Fig. 2 and our calculated values are in good agreement with the experimental data and systematics. We have also shown the double differential cross-section (DDX) for $^{63}Cu(n,xp)$ reaction at 14 MeV incident neutron energy in Fig.2, in which (n,p) channel is dominant than other channels. So the double differential cross-section (DDX) is mainly due to the $^{63}Cu(n,p)^{63}Ni$ reaction.

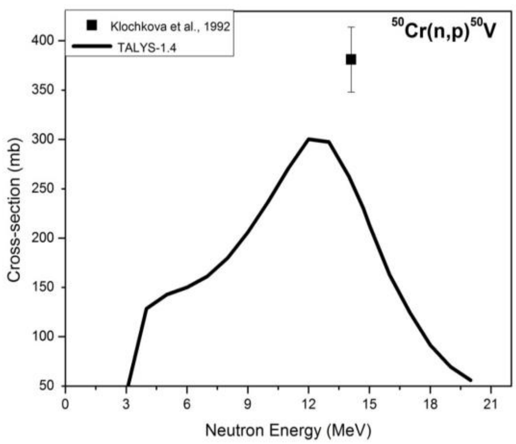

Fig. 1. Excitation function of the $^{50}Cr(n,p)^{50}V$ reaction.

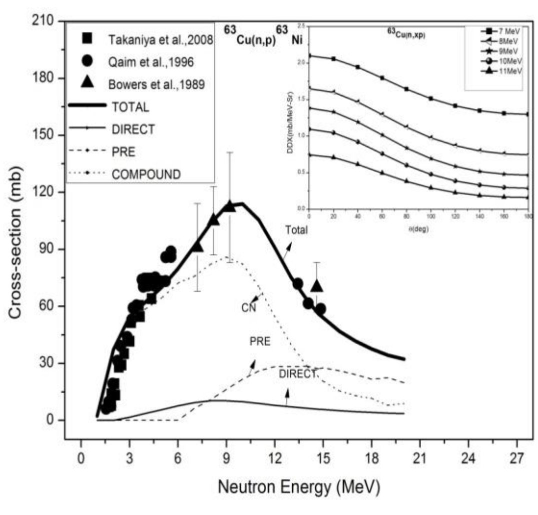

Fig. 2. Excitation function of the $^{63}Cu(n,p)^{63}Ni$ reaction alongwith double differential cross-sections (DDX) with angle of emission for 7,8,9,10 and 11 MeV proton particles emitted through $^{63}Cu(n,xp)$ reaction at 14MeV neutrons.

The excitation curve for $^{55}Fe(n,p)^{55}Mn$ and $^{60}Fe(n,p)^{60}Mn$ are shown in Figs. 3 and 4, respectively. There is no experimental data available because the targets $^{55}Fe(t_{1/2}=$ 2.73years) and $^{60}Fe(t_{1/2}=$ 1.5×10^{6}years) are radioactive and products have unsuitable half-lives $^{55}Mn(t_{1/2}=\infty)$ $^{60}Mn(t_{1/2}=$ 51sec) leading to difficulty in using activation technique measurements of cross-sections for these reactions. The systematic value for $^{55}Fe(n,p)^{55}Mn$ is comparable to calculated values but for $^{60}Fe(n,p)^{60}Mn$ reaction the calculated value is lower than systematic values.

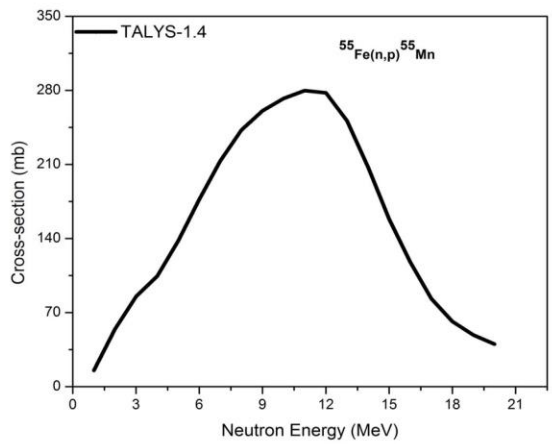

Fig.3. Excitation function of the $^{55}Fe(n,p)^{55}Mn$ reaction.

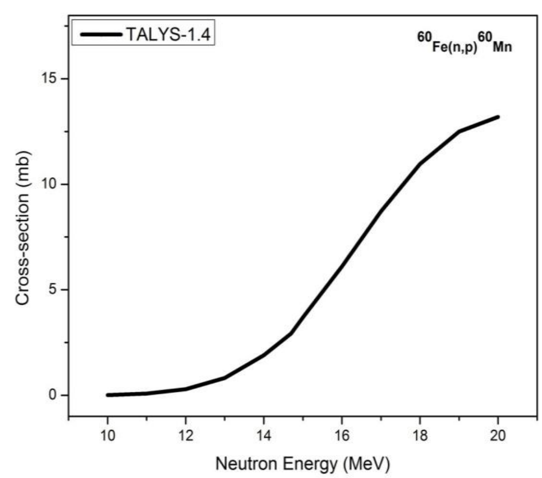

Fig.4. Excitation function of the $^{60}Fe(n,p)^{60}Mn$ reaction.

The component wise excitation curve for $^{59}Ni(n,p)^{59}Co$ along-with double differential cross-section (DDX) for $^{59}Ni(n,xp)$ reaction at 14 MeV incident neutrons energy are shown in Fig. 5. There is no experimental data available because target nuclei $^{59}Ni(t_{1/2}=7.6\times10^{4})$ is radioactive and product nuclei $^{59}Co(t_{1/2}=\infty)$ is stable.

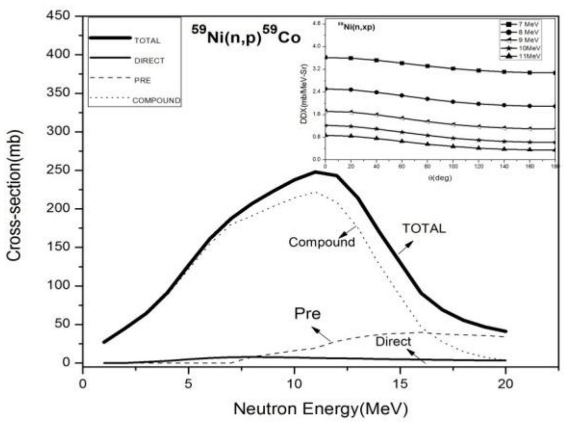

Fig.5. Excitation function of the $^{59}Ni(n,p)^{59}Co$ reaction alongwith double differential cross-sections (DDX) with angle of emission for 7,8,9,10 and 11MeV proton particles emitted through $^{59}Ni(n, xp)$ reaction at 14MeV neutrons.

The excitation curve for $^{60}Ni(n,p)^{60}Co$ and $^{63}Ni(n,p)^{63}Co$ are shown in Figs. 6 and 7, respectively. For $^{60}Ni(n,p)^{60}Co$ reaction, there is lot but discrepant experimental data available and our calculated values are in a good agreement with recent experimental data as well as systematics whereas for $^{63}Ni(n,p)^{63}Co$ reaction, no experimental data is available because target $^{63}Ni(t_{1/2}=100$ years) nuclei is radioactive.

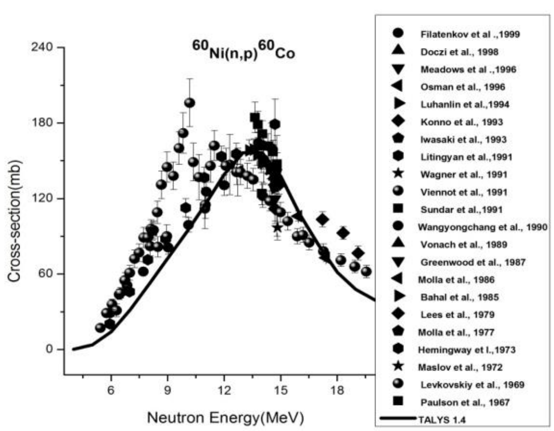

Fig.6. Excitation function of the $^{60}Ni(n,p)^{60}Co$ reaction.

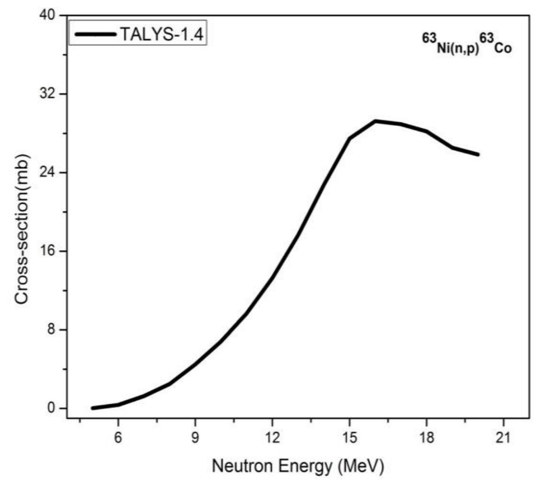

Fig.7. Excitation function of the $^{63}Ni(n,p)^{63}Co$ reaction.

The excitation curve for $^{51}Cr(n,\alpha)^{48}Ti$ reaction is shown in Fig. 8. No experimental data is available for this reaction due to the large half life of target $^{51}Cr(t_{1/2}=2.73$ years) nuclei and production of stable product $^{48}Ti(t_{1/2}=\infty)$ nuclei but our calculated value at 14.7 MeV is close to the systematics.

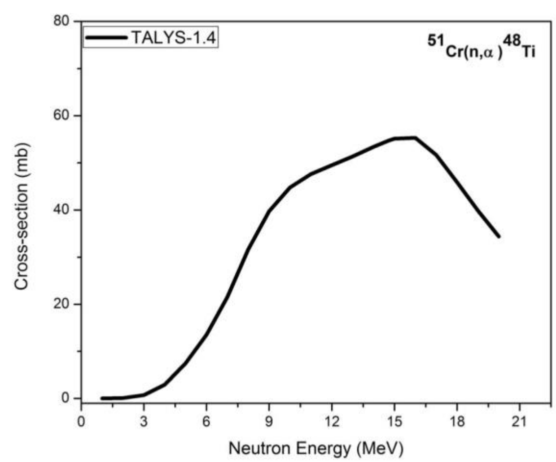

Fig. 8. Excitation function of the $^{51}Cr(n,\alpha)^{48}Ti$ reaction.

The excitation curve for $^{63}Cu(n,\alpha)^{60}Co$ reaction with direct, pre-equilibrium and compound contribution along-with double differential cross-section (DDX) for $^{63}Cu(n,x\alpha)$ reaction at 14 MeV incident neutron energy for emitted alpha particles are shown in Fig. 9.

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For this reaction, our calculated cross-section value is in good agreement with experimental data upto 16 MeV energy and between 16-20 MeV our values are somewhat higher than experimental values. However, our calculated value at 14 MeV is in close agreement with latest experimental value as well as systematics.

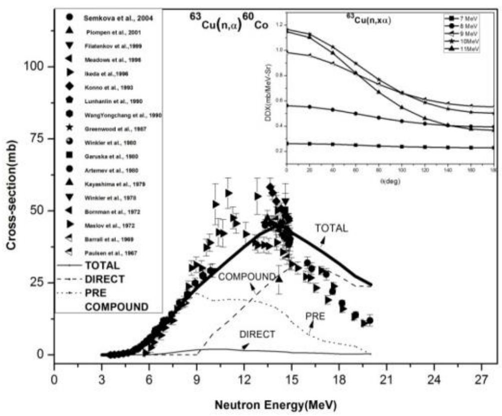

Fig. 9. Excitation function of the $^{63}Cu(n,\alpha)^{60}Co$ reaction alongwith double differential cross-sections (DDX) with angle of emission for 7,8,9,10 and 11 MeV alpha particles emitted through $^{63}Cu(n, x\alpha)$ reaction at 14 MeV neutrons.

For $^{55}Fe(n,\alpha)^{52}Cr$ reaction, we have also shown direct, pre-equilibrium and compound contribution along-with double differential cross-section (DDX) for alpha particles emitted through $^{55}Fe(n,x\alpha)$ reaction at 14 MeV incident neutron energy in Fig. 10. There is no experimental data.

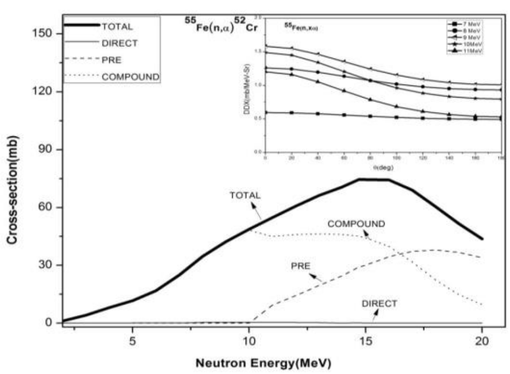

Fig. 10. Excitation function of the $^{55}Fe(n,\alpha)^{52}Cr$ reaction alongwith double differential cross-sections (DDX) with angle of emission for 7,8,9,10 and 11 MeV alpha particles emitted through $^{55}Fe(n, x\alpha)$ reaction at 14MeV neutrons.

This is also due to the radioactive target $^{55}Fe(t_{1/2} = 2.737$ year) nuclei and the stable product $^{52}Cr(t_{1/2}=\infty)$ nuclei, however, the systematic value is in good agreement with calculated value.

The excitation curve for $^{58}Ni(n,\alpha)^{55}Fe$ is shown in Fig.11. The calculated values are in a good agreement with the experimental data and systematics.

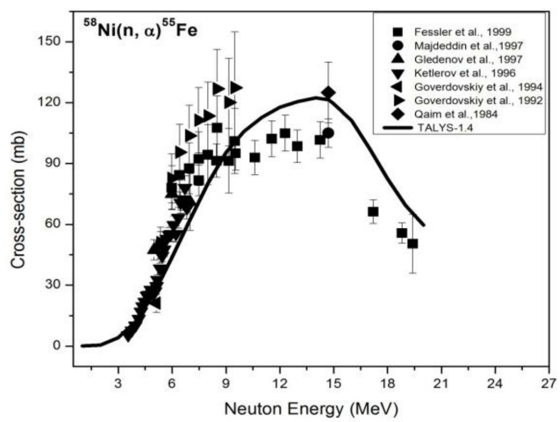

Fig. 11. Excitation function of the $^{58}Ni(n,\alpha)^{55}Fe$ reaction.

The excitation functions of $^{59}Ni(n,\alpha)^{56}Fe$ and $^{63}Ni(n,\alpha)^{60}Fe$ are shown in Fig.12 and 13 respectively. The target nuclei for these reactions are radioactive with large half lives $^{59}Ni(t_{1/2} = 7.6 \times 10^4$ years) and $^{63}Ni(t_{1/2} = 100$ years). So there is no experimental data available for these reactions, but at 14.7 MeV our calculated values are close to the systematics.

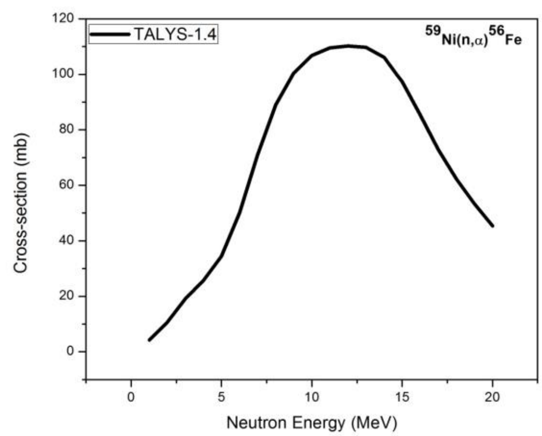

Fig.12. Excitation function of the $^{59}Ni(n,\alpha)^{59}Fe$ reaction.

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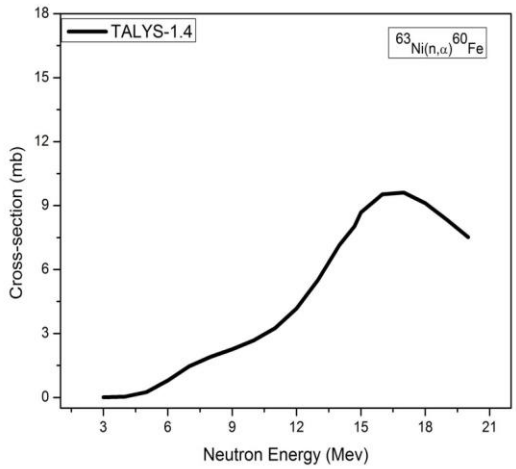

Fig.13. Excitation function of the $^{63}Ni(n,\alpha)^{60}Fe$ reaction.

For $^{50}V(n,\alpha)^{47}Sc$ reaction, there is only one experimental value available as shown in Fig. 14. Our calculated value is in good agreement with the experimental value and systematics.

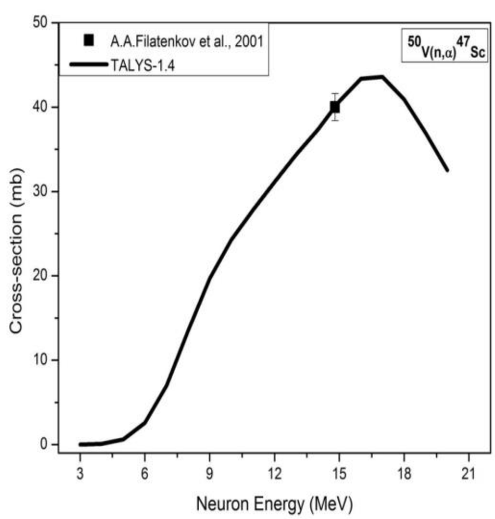

Fig. 14. Excitation function of the $^{50}V(n,\alpha)^{47}Sc$ reaction.

The observation from all the excitation curves indicates that the proton and alpha emission is governed by the compound nucleus model in the lower energy domain and shows a pre-equilibrium tail as incident neutron energy increases.

Our calculations shows that for nuclei Z~20-30 the pre-equilibrium contribution is 10-45% in (n,p) and 30-60% in (n,α) reactions cross-sections at 14 MeV. The variation in double differential cross-section (DDX) with the angle of emission of proton and alpha particles is not close to isotropic distribution and therefore confirms the dominancy of pre-equilibrium contribution as energy increases. Hence the effect of pre-equilibrium emission must be taken into account.

IV. CONCLUSION

We have analyzed the (n,p) and (n,α) reactions cross-sections of long lived target and residual nuclei of Cr, Cu, Fe, Ni and V which are main constituents of structural and blanket materials of fusion reactors with recent code TALYS-1.4. It is concluded that the Gilbert Cameron formalism for level density calculations and JLM optical potential for neutron and proton and Wanadabe optical model potential for alpha particle along-with two component exciton pre-equlibrium model are quite suitable in predicting (n,p) and (n,α) reaction cross-sections for nuclides (Z~20-30) from threshold to 20 MeV. The consistency of calculated results with experimental data and systematics (at 14.7 MeV) demonstrate the predictive power of TALYS-1.4 code to predict the cross-section for the isotopes (Z=20-30) where target and product nuclei have a large half life and no experimental data is available. There is a significant contribution of pre-equilibrium emission in (n,p) and (n,α) reactions cross-section as confirmed by double differential cross-section(DDX) at 14 MeV neutron energy. This is an important step to the validation of nuclear model with good predictive power.

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