EVALUATION OF NEUTRON INDUCED CROSS SECTION DATA USING EMPIRE 3.2.2 AND TALYS 1.8 CODES

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Abstract

The cross sections of ^{67}Zn,^{92,96}Mo,^{208}Pb(n,p) and ^{70}Zn,^{100}Mo(n,2n) reactions have been evaluated using statistical nuclear model codes EMPIRE 3.2.2 and TALYS 1.8 at the neutron energy range from reactions threshold to 20 MeV. The variation in cross section with different optical model potential, level density models, and nuclear reaction models have been investigated at neutron energy 14.5 MeV. In this work, the pre-equilibrium emission contribution in the total cross section has also been verified in the neutron energy of 14.5 MeV. The calculated results were also compared with the experimental data being taken from EXFOR database.

Introduction

The need of precise and accurate neutron induced cross section data is very important in nuclear technologies, such as designing of nuclear reactors, accelerator driven subcritical systems (ADS), transmutation of nuclear waste and medical applications (production of radioisotopes, radiotherapy) etc. The neutron induced reaction cross section data in the fast neutron energy region ~ 14 MeV for the structural material (Zinc and Molybdenum) has many applications in fusion and fission reactors. Similarly, neutron induced cross section data of Lead is also important for shielding materials. The reactions induced by fast neutrons such as, (n, 2n) and (n, p) were used to study the neutron multiplicity and charge particle emission in reactor structure wall that causes micro-structural defects. This neutron data can be generated experimentally by using the neutron activation technique (NAA) over the neutron energy range. For those isotopes where the experimental measurements are not feasible, the cross section data can be generated by using standard nuclear models.

This neutron induced cross section data obtained from theoretical models are important for the study of nuclear reaction mechanism and it can be used by evaluators to interpolate or extrapolate data for the energy range where the data does not exists. EMPIRE and TALYS are two such computer codes based on the statistical model which are used to estimate the cross section data on the basis of three major nuclear reactions mechanism i.e., direct reaction (DR), pre-equilibrium emission (PE) and compound nucleus (CN) decay. Thus the mechanism of the nuclear reactions changes with the incident neutron energy.

In order to study the different reaction mechanisms, the EMPIRE and TALYS model codes were used with different parameters which are defined at particular energy range and elements [1–2].

EMPIRE Calculations

Empire is a modular nuclear reactions code, comprising various nuclear theoretical models in order to estimate the probability of the emitted particles such as photons, nucleons, deuterons and tritons etc., in the energy range up to several hundred MeV.

In the EMPIRE code, the direct reaction is calculated with default spherical optical model that uses the ECIS06 code and which have been used to calculate the particle transmission coefficient. In this calculation, the OM potential parameter has used which is proposed by A.J Koning and J.P. Delaroche [3].The Statistical Hauser-Feshbach model is used for the calculation of the compound nucleus decay. For pre-equilibrium emission, the exciton model (PCROSS code) has been used which describes particle and gamma-emission and also calculate pre-equilibrium emission with default mean free path multiplier PCROSS 1.5.

The contribution from all three mechanisms make total cross-section and maximum contribution comes from the CN decay with an addition of some pre-equilibrium mechanism. The effect of pre-equilibrium contribution increases with increase in incident energy.

Cross section is very sensitive to the level density parameters and EMPIRE incorporated four level density models to calculate them which are as follow:

(i) LEVDEN 0 is the EMPIRE-specific level densities (EGSM RIPL-3) and it is a default model used in EMPIRE, adjusted to RIPL- 3 experimental D_{obs} and to discrete levels. This is Enhanced Generalized Super fluid Model (EGSM). The model uses super fluid model below critical excitation energy and the Fermi gas model above.

(ii) LEVDEN 1 is the Generalized Super fluid Model (GSM, Ignatyuk et al.), adjusted to RIPL-2 experimental D_{obs} and to discrete levels which use constant temperature model below critical energy (Ucrt) and Fermi gas model above critical energy (depend on the compound nucleus excitation energy).

(iii) LEVDEN 2 is Gilbert-Cameron level densities (parameterized by Ijinov et al), which adjusted to RIPL-2 experimental D_{obs} and to discrete levels recommended for CN exited up to about 20 MeV.

(iv) LEVDEN 3 is the RIPL-3 microscopic HFB level densities (where D_{obs} is neutron resonance spacing).

The calculations have been done with the all four choices to check how the cross section is changing with different level density models at 14.5 MeV.

Apart from PCROSS model, the cross section has also been calculated for multi-step direct and multi-step compound (MSD/MSC) pre-equilibrium model.

For emission of charged particle or photons (gamma-ray) the exciton model (PCROSS code) is considered while for the neutron emission a combination of MSD/MSC model is preferred. The required parameters for the nuclear models to calculate the excitation functions have been taken from the RIPL-3 library. The RIPL-3 includes the nuclear masses, discrete levels and decay schemes, neutron resonances, optical model parameters, level densities, gamma-ray strength function and fission barriers [4].

TALYS Calculations

TALYS is another computer code for the analysis and prediction of nuclear reactions. The objective of this code is to reproduce the nuclear reactions that involve neutrons, photons, protons, deuterons, tritons, and ^{3}He particles in the energy range of 1 keV – 200 MeV and for target nuclides of mass 12 and heavier. To achieve this, TALYS code implements a suite of nuclear reaction models into a single code system. This enables us to evaluate nuclear reactions from the unresolved resonance range up to intermediate energies.

TALYS generate nuclear data for all open reaction channels, on a user-defined energy and angle grid, beyond the resonance region. In the present study, calculations have been done with the default set of input parameters, where only we have changed the different level density models and pre-equilibrium models.

In TALYS six level density models are defined for calculating level density parameters, which are as follows:

1. ldmodel 1 Constant temperature and Fermi gas model
2. ldmodel 2 (default) Back-shifted Fermi gas model
3. ldmodel 3 Generalised super fluid model
4. ldmodel 4 Microscopic level densities (Skyrme force) from Goriely's tables
5. ldmodel 5 Microscopic level densities (Skyrme force) from Hilaire's combinatorial tables
6. ldmodel 6 Microscopic level densities (temperature dependent HFB, Gogny force) from Hilaire's.

The calculations have been performed using the optical model potential as proposed by A.J Koning [1]. For the contribution of pre-equilibrium emission in total reaction cross section, the Exciton (preqmode 2) (default) and MSD/MSC models (preqmode 4) were used. The pre-equilibrium contribution in (n, p) and (n, 2n) reaction cross sections have also been performed with and without including the pre-equilibrium channel.

Results and Discussion

From the available options of the level density models , OM potential in the EMPIRE 3.2.2 code, the cross section for the reaction ^{67}Zn(n,p)^{67}Cu, ^{92}Mo(n,p)^{92m}Nb, ^{96}Mo(n,p)^{96}Nb, ^{208}Pb(n,p)^{208}Tl and ^{70}Zn(n,2n)^{69m}Zn, ^{100}Mo(n,2n)^{99}Mo have been evaluated over the energy range from threshold to 20MeV. The calculation was done by using exciton model, the combination of multi-step direct and multi-step compound model (MSD/MSC) and all four level density models which are given in Table 1 and 2. Similarly, evaluation has been done with TALYS 1.8 code using ldmodel 1–6 and considering both exciton model and MSD/MSC model are shown in Table 3 and 4.

It can be observed in Tables 1–4, that the cross section is changed for different level density models. The contribution of pre-equilibrium emission in (n, p) and (n, 2n) reactions have been studied at neutron energy of 14.5 MeV and it is found that the effect of pre-equilibrium emission is larger for (n, p) as compared to (n, 2n) reaction as given in Table 6.

From the literature survey, it was found that the contribution from the pre-equilibrium emission is dominated when one particle is emitted whereas in the case of two particle emission the effect of pre-equilibrium on the second emitted particle is very less that's why in our calculations the contribution of pre-equilibrium of (n,2n) reaction is less than (n,p) reaction [6–7].

Calculations have also been done with different choices of OM potential and the cross section for different choices of OM potentials are observed to vary within 10% in all reactions except for ^{208}Pb (n,p) where the variation is as large as ~35% was observed.

The theoretical model calculations for ^{67}Zn(n,p)^{67}Cu, ^{92}Mo(n,p)^{92m}Nb, ^{96}Mo(n,p)^{96}Nb, ^{208}Pb(n,p)^{208}Tl and ^{70}Zn(n,2n)^{69m}Zn, ^{100}Mo(n,2n)^{99}Mo reactions are given in Table 1–5. However, Table 5 contains only those data that reproduces the experimental results.

For ^{67}Zn(n,p)^{67}Cu reaction

The graph between theoretical and experimental cross section data of ^{67}Zn(n,p)^{67}Cu reaction from threshold to 20 MeV has been plotted in Fig. 1. The theoretical cross section data for the above reaction have calculated by using different models of EMPIRE and TALYS, which are following as, for EMPIRE code: (i) Exciton model with HFB level density model and Koning OM potentials have been used and for TALYS code: (i) Exciton model with Back-shifted Fermi gas level density model and Koning local OM potential have opted.

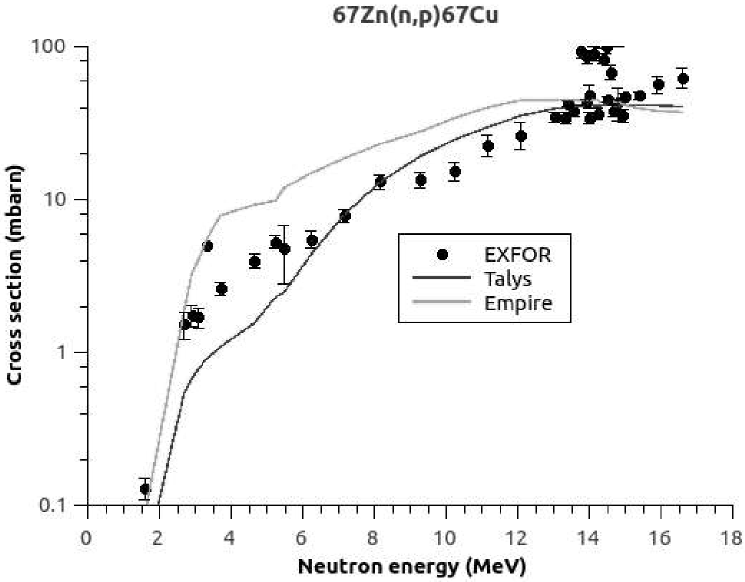

Fig. 1. Cross section of $^{67}Zn(n,p)^{67}Cu$ reaction at different neutron energies estimated in present work and experimental data taken from EXFOR database.

Table 1: Cross section estimated through exciton model by using different level density options of EMPIRE 3.2.2 code at neutron energy 14.5 MeV

Reactions	LEVDEN 0 (mb)	LEVDEN 1 (mb)	LEVDEN 2 (mb)	LEVDEN 3 (mb)
$^{67}Zn(n,p)^{67}Cu$	110.97	74.62	25.982	43.13
$^{92}Mo(n,p)^{92m}Nb$	121.18	79.411	258.36	100.36
$^{96}Mo(n,p)^{96}Nb$	28.332	14.374	288.19	19.081
$^{208}Pb(n,p)^{208}Tl$	0.1943	0.1079	5.3704	0.2148
$^{70}Zn(n,2n)^{69m}Zn$	610.56	737.79	25.846	730.46
$^{100}Mo(n,2n)^{99}Mo$	1641.3	1680	182.54	1670.5

Table 2: Cross section estimated through MSD/MSC model by using different level density options of EMPIRE 3.2.2 code at neutron energy 14.5 MeV

Reactions	LEVDEN 0 (mb)	LEVDEN 1 (mb)	LEVDEN 2 (mb)	LEVDEN 3 (mb)
$^{67}Zn(n,p)^{67}Cu$	94.91	59.62	12.53	29.42
$^{92}Mo(n,p)^{92m}Nb$	104.32	63.13	239.41	84.01
$^{96}Mo(n,p)^{96}Nb$	21.39	8.12	268.60	12.58
$^{208}Pb(n,p)^{208}Tl$	0.1011	0.0171	5.1307	0.1211
$^{70}Zn(n,2n)^{69m}Zn$	583.85	692.17	71.88	687.18
$^{100}Mo(n,2n)^{99}Mo$	1524.9	1559.8	193.9	1551.3

For $^{92}Mo(n,p)^{92m}Nb$ reaction

The graph between theoretical and experimental cross section data of $^{92}Mo(n,p)^{92m}Nb$ reaction from threshold to 20 MeV has been plotted in Fig. 2. The theoretical cross section data for the above reactions have calculated by using different models of EMPIRE and

TALYS. For EMPIRE code (i) MSD/MSD model with Generalized Super fluid level density Model and Koning OM potentials have been used and for TALYS (i) exciton model with back-shifted Fermi gas level density model and Koning local OM potential have opted.

Table 3: Cross section estimated through exciton model by using different level density options of TALYS 1.8 code at neutron energy 14.5 MeV

Reactions	ldmodel 1 (mb)	ldmodel 2 (mb)	ldmodel 3 (mb)	ldmodel 4 (mb)	ldmodel 5 (mb)	ldmodel 6 (mb)
^{67}Zn(n,p)^{67}Cu	33.36	41.83	22.14	72.11	51.44	65.73
^{92}Mo(n,p)^{92m}Nb	84.84	62.20	36.07	65.66	87.49	166.85
^{96}Mo(n,p)^{96}Nb	30.66	21.14	22.38	30.41	33.84	35.02
^{208}Pb(n,p)^{208}Tl	0.7687	0.5836	159.30	0.8936	1.068	0.9120
^{70}Zn(n,2n)^{69m}Zn	686.53	667.44	512.49	512.49	667.44	686.53
^{100}Mo(n,2n)^{99}Mo	1536.3	1524.6	1323.04	1518.8	1537.2	1309.1

Table 4: Cross section estimated through MSD/MSC model by using different level density options of TALYS code at neutron energy 14.5 MeV

Reactions	ldmodel 1 (mb)	ldmodel 2 (mb)	ldmodel 3 (mb)	ldmodel 4 (mb)	ldmodel 5 (mb)	ldmodel 6 (mb)
^{67}Zn(n,p)^{67}Cu	63.38	68.76	61.82	102.34	81.53	96.25
^{92}Mo(n,p)^{92m}Nb	85.29	65.56	38.55	64.61	89.78	180.09
^{96}Mo(n,p)^{96}Nb	46.51	39.10	36.80	45.86	50.26	51.62
^{208}Pb(n,p)^{208}Tl	9.77	9.86	201.7	9.86	10.47	10.52
^{70}Zn(n,2n)^{69m}Zn	700.70	687.36	561.85	681.62	747.35	593.62
^{100}Mo(n,2n)^{99}Mo	1588.2	1582.0	1486.2	1568.5	1587.3	1332.2

For ^{96}Mo(n,p)^{96}Nb reaction

The graph between theoretical and experimental cross section data of ^{96}Mo(n,p)^{96}Nb reaction from threshold to 20 MeV have been plotted and shown in Fig. 3. The theoretical cross section data for the above reactions have calculated by using different models of EMPIRE and TALYS. For EMPIRE code (i) MSD/MSD model with EGSM level density Model and Koning OM potential have been used and for TALYS (i) exciton model with back-shifted Fermi gas level density model and Koning local OM potential have opted.

For ^{208}Pb(n,p)^{208}Tl reaction

The graph of theoretical and experimental cross section data of ^{208}Pb(n,p)^{208}Tl from the reaction threshold to 20 MeV has been plotted and shown in Fig. 4.The theoretical cross section data for the above reactions have calculated by using different models of TALYS. For EMPIRE code (i) exciton model with microscopic level densities (temperature dependent HFB, Gogny force) from Hilaire's and Koning local OM potential.

During calculations with EMPIRE, it was found that for ^{208}Pb(n,p) case the EMPIRE 3.2.2 was not suitable to calculate fission cross section due to the absence of fission barrier parameters in EMPIRE data library for reaction product ^{209}Pb and since EMPIRE considers ^{209}Pb to be fissile and due to missing of parameters, it shows error in the output file without calculating any cross section. So, to calculate the ^{208}Pb(n,p) cross section we edit the input file with optional input keyword FISSHI 2.0 which is used to ignore the fission channel.

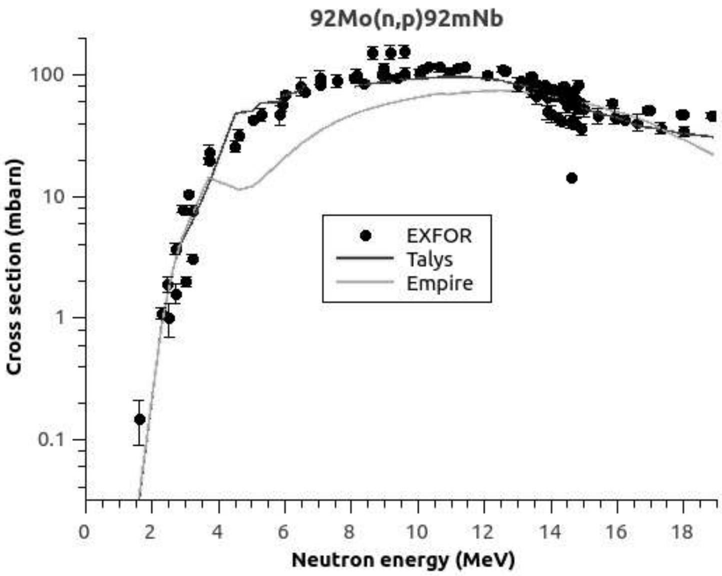

Fig. 2. Cross section of $^{92}Mo(n,p)^{92m}Nb$ reaction at different neutron energies estimated in present work and experimental data taken from EXFOR database.

For $^{70}Zn(n,2n)^{69m}Zn$ reaction

Fig. 5 shows the graph of theoretical and experimental cross section data of $^{70}Zn(n,2n)^{69m}Zn$ reaction from threshold to 20 MeV. The theoretical cross section data for the above reaction has been calculated by using different models of EMPIRE and TALYS. For EMPIRE code (i) MSD/MSD model with EGSM level density Model and Koning OM potentials and for TALYS (i) exciton model with Generalised super fluid level density model and Koning local OM potential.

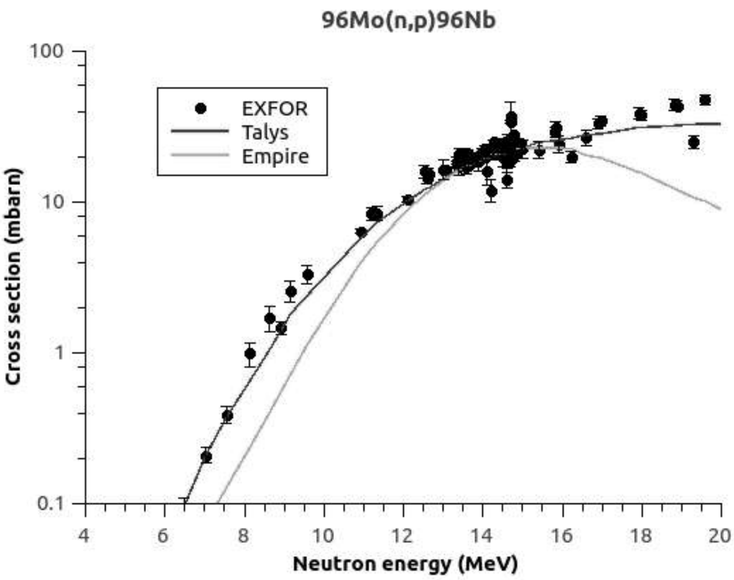

Fig. 3. Cross section of $^{96}Mo(n,p)^{96}Nb$ reaction at different neutron energies estimated in present work and experimental data taken from EXFOR database.

Table 5: Comparison of all reactions cross section data at neutron energy 14.5 MeV

Reactions	Experimental data (mb)	EMPIRE 3.2.2 (mb)	TALYS 1.8 (mb)
^{67}Zn(n,p)^{67}Cu	44.9±2.1	43.13	41.83
^{92}Mo(n,p)^{92m}Nb	56.3±8	63.13	62.20
^{96}Mo(n,p)^{96}Nb	20±2.7	21.39	21.14
^{208}Pb(n,p)^{208}Tl	0.94±0.18	0.2148	0.9120
^{70}Zn(n,2n)^{69m}Zn	547±22	583.85	512.49
^{100}Mo(n,2n)^{99}Mo	1377±86	1524.9	1323.04

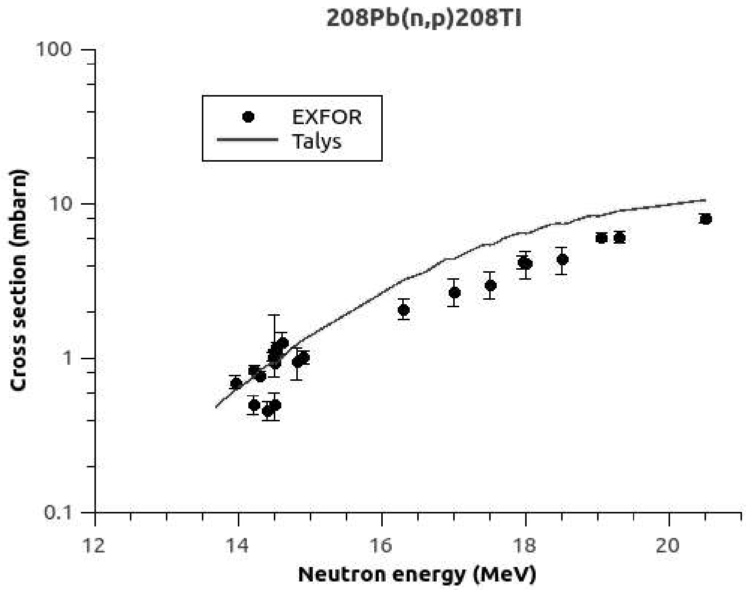

Fig. 4. Cross section of ^{208}Pb(n,p)^{208}Tl reaction at different neutron energies estimated in present work and experimental data taken from EXFOR database.

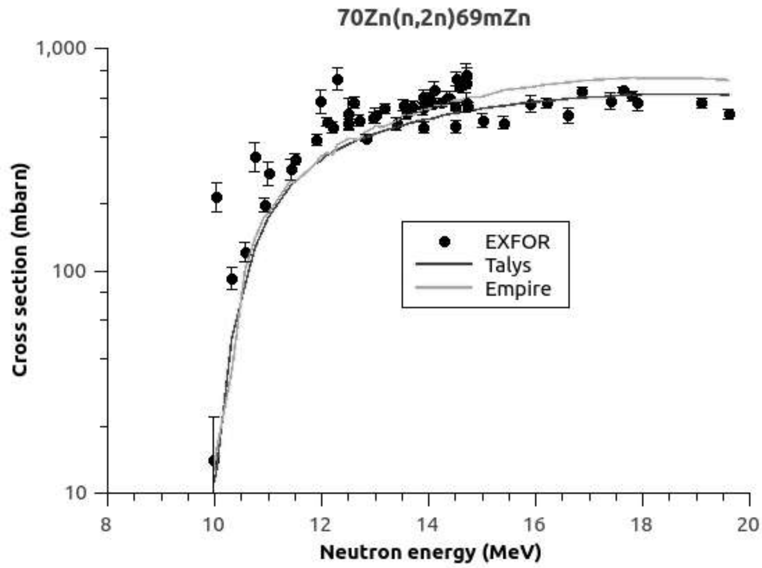

Fig. 5. Cross section of ^{70}Zn(n,2n)^{69m}Zn reaction at different neutron energies estimated in present work and experimental data taken from EXFOR database.

For ^{100}Mo (n, 2n) ^{99}Mo reaction

The graph of theoretical and experimental cross section data of ^{100}Mo(n,2n)^{99}Mo reaction from threshold to 20 MeV has been shown in Fig. 6. The theoretical cross section data for the above reactions have calculated by using different models of EMPIRE and TALYS. For EMPIRE code (i) MSD/MSD model with EGSM level density Model and Koning OM potentials and for TALYS (i) exciton model with Generalised super fluid level density model and Koning local OM potential.

Table 6: Contribution of pre-equilibrium in (n, p) and (n, 2n) reactions which is calculated through TALYS code at neutron energy 14.5 MeV

Reactions	TALYS 1.8 (with PE) (mb)	TALYS 1.8 (without PE) (mb)
^{67}Zn(n,p)^{67}Cu	41.83	13.58
^{92}Mo(n,p)^{92m}Nb	62.20	49.63
^{96}Mo(n,p)^{96}Nb	21.14	4.55
^{208}Pb(n,p)^{208}Tl	0.9120	0.2125
^{70}Zn(n,2n)^{69m}Zn	512.49	641.834
^{100}Mo(n,2n)^{99}Mo	1323.04	1652.5

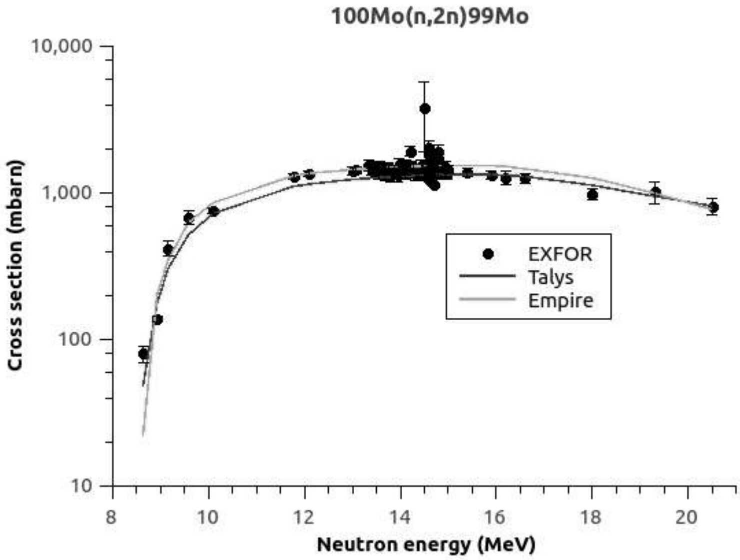

Fig. 6. Cross section of ^{100}Mo(n,2n)^{99}Mo reaction at different neutron energies estimated in present work and experimental data taken from EXFOR database.

Summary and Conclusions

1. We have calculated the neutron induced reaction cross section for the reactions ^{67}Zn(n,p)^{67}Cu, ^{92}Mo(n,p)^{92m}Nb, ^{96}Mo(n,p)^{96}Nb, ^{208}Pb(n,p)^{208}Tl and ^{70}Zn(n,2n)^{69m}Zn, ^{100}Mo(n,2n)^{99}Mo over the neutron energy range from threshold to 20 MeV.
2. In this model calculation, it was observed that the cross section is very sensitive to the optical model potential, level density model, and nuclear reaction models.
3. The result of calculations by TALYS 1.8 and EMPIRE 3.2.2 codes with allowance for pre-equilibrium processes are in best agreement with experimental data.

4. This comparison of theoretical data and experimental data is important in fusion/fission reactors and medical application technologies.

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