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ORIGINAL RESEARCH

(p,α) Reaction Cross Sections Calculations of Fe and Ni Target Nuclei Using New Developed Semi-empirical Formula

E. Tel · S. Akca · A. Kara · M. Yiğit · A. Aydın

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Abstract Iron (Fe) and nickel (Ni) are important fusion structural materials in reactor technology. The gas production in the metallic structure arising from many different types of nuclear reactions has been a significant damage mechanism in structural components of fusion reactors. The hydrogen and its isotopes at high temperatures leave out of the metallic lattice but the alpha (α) particles that remain in the lattice generate helium (He) gas bubbles. In other words, the α particles can cause serious changes in the physical and mechanical properties of the fusion structural materials. In this study, the excitation functions of ^{54,57}Fe(p,α) and ^{58,60,61,64}Ni(p,α) reactions have been investigated in the incident proton energy range of 10–40 MeV to estimate the radiation damage effects on fusion structural materials used in the construction of the first walls and core of the reactor. The calculations of (p,α) reaction cross sections on ^{54,57}Fe and ^{58,60,61,64}Ni have been made by using PCROSS code and CEM95 code. The full exciton and cascade exciton model (CEM95) for pre-equilibrium calculations and Weisskopf-Ewing model for equilibrium calculations are used. Besides, the semi-empirical cross section formula with new coefficient obtained by Tel et al. (Pramana J Phys 74:931–943, 2010) has been applied for (p,α) reactions at 17.9 MeV proton incident energy.

Keywords Proton induced reaction · Iron and nickel isotopes · Cross section · Fusion structural material

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Introduction

When a charged particle produced in reactors or accelerators interacts with a target nucleus, a reaction takes place, resulting in a radioactive or stable product nucleus. The nuclear reaction studies play a key role for many nuclear physics applications as medical radionuclide production, accelerator driven subcritical systems, fusion and fission reactors. Especially, the theoretical model calculations and experiments via nuclear reactions induced by charged particles are very important for fusion technology and medical radionuclide production. The incoming charged particle can produce different types of reactions depending on its energy. Quantitative measurement of probability of occurrence of a specific nuclear reaction under certain conditions relates to cross section of the process. The cross section data of gas production created by particle (neutron, alpha, proton, etc.) induced reactions hold an important place in fusion reactor technology, especially in the calculation of nuclear conversion ratios, radiation damage and nuclear heating as a consequence of gas production [1–3].

In fusion reactor structures, gas production in structural materials as a result of various nuclear reactions, to a certain extent (p,p), (p,n), (p,α) reactions above a certain critical threshold energy, can be provided by the particle irradiation [4]. As the hydrogen and its isotopes at high temperatures leave out of the metallic lattice but the alpha (α) particles that remain in the lattice generate helium gas bubbles. Consequently, α particles cause swelling in the material. The alpha, neutron, proton, and also other particle irradiation makes up considerable changes in the physical and mechanical properties of fusion structural material [5, 6].

There are a lot of important structural materials in fusion reactor technologies [5, 7–10]. Fe and Ni have been used in medical applications for radioisotope production and in energy applications as structural material. In present study, the cross sections of (p,α) reactions on Fe and Ni isotopes have been investigated in the proton energy range of 10–40 MeV to estimate the radiation damage effects on fusion structural materials used in the construction of the first walls and core of the reactor. A number of proton accelerators built for various purposes has increased recently. Protons accelerated in the facilities has been used for investigation of nuclear reactions occurred in structural materials of fusion reactors. In the research centers and Institutes such as PSI, the studies are carried out to improve target material for proton accelerator driven systems and liquid metal target technology [11, 12].

Lately, several experimental studies have been carried out to determine the cross section of nuclear reactions induced by protons. The experimental cross sections of proton induced reactions are available in EXFOR/CSISRS [13] data files.

These values help to explain mechanisms of nuclear reaction, the properties of the excited nuclear states in different energy ranges and develop more theoretical calculation models [14]. In our calculations, equilibrium and pre-equilibrium reaction processes were used for excitation function of helium production. The pre-equilibrium processes were calculated by using cascade exciton model (CEM) and full exciton model. The equilibrium processes were calculated with a traditional compound nucleus model developed by Weisskopf-Ewing (WE) model [15]. Besides, (p,α) reaction cross sections were calculated using new semi empirical systematic formula developed by Tel et al. [16, 17] at 17.9 MeV proton energy.

Methods of Calculation

The PCROSS code [18], CEM95 code [19] and semi-empirical systematic formula by Tel et al. [17] were applied to calculate the excitation functions of the proton induced reactions on ^{54,57}Fe and ^{58,60,61,64}Ni isotopes for the production of ^{51,54}Mn and ^{55,57,58,61}Co radioisotopes. EXFOR/CSISRS data files were used for the experimental cross sections at proton induced reactions.

The compound nucleus reactions, 'the equilibrium process' in the other expression, occur on a very much longer time about between 10^{-16} and 10^{-18} s. This process is described in detail by the WE. Excitation function of the equilibrium process is calculated by using WE model [15] by disregarding the angular momentum. In the Griffin's exciton model [20], the states of the independent-particle are classified according to the number of particles and holes (referred to as *excitons*). The exciton number is described as $n = p + h$ where p and h denote the numbers of excited particles above the Fermi energy and below it, respectively. Excitons are assumed to be excited pairs from the ground state of an even-even nuclei. In even-even nuclei, all nucleons are paired, and a stronger interaction takes place between the nucleons. The total angular momentum of the even-even nucleus is always zero in the ground state and nucleons are more bounded. The detailed knowledge of the exciton model can be found in Ref. [20, 21].

The full exciton model is used a unified model based on the solution of the master equation. The formalizations of the full exciton model with PCROSS code [18] take cognizance of the direct gamma emission and use the initial exciton number as n_o =1. Then, *Kalbach* proposed some parameterizations which are used in the calculations of internal transitions ratios and it is shown that the calculated emission spectra strongly depend on the parameter of matrix element [22, 23]. In the other hand, PCROSS code uses the parameterization of transition radios suggested by Blann and Mignerey [24]. The CEM [19] assumes that the nuclear reactions consist of three phases: intra nuclear cascade (INC), equilibrium (or compound nucleus) and pre-equilibrium. In general, these three phases may contribute to any experimentally measured components [25–27]. Particularly, for the inclusive particle spectrum;

$$\sigma(p)\mathrm{d}p = \sigma_{in}[N^{cas}(p) + N^{prq}(p) + N^{eq}(p)]\mathrm{d}p, \qquad (1)$$

here p denotes linear momentum. The values σ_{in}, N^{cas}, N^{prq} and N^{eq} define the inelastic cross section, the total particle number of the cascade, the pre-equilibrium and the equilibrium phases, respectively. The detailed knowledge of the CEM95 (cascade exciton model) can be found in Ref. [19].

(p,α) Empirical Cross Section Formula at 17.9 MeV

The first systematics for (p,n) reaction cross sections was discussed by Broeders and Konobeyev [28, 29]. For (p,α), (p,np) and (p,nα) cross sections, the semi-empirical formulas were derived by using analytical expressions defining the equilibrium and non-equilibrium particle emission by Broeders and Konobeyev [28]. The semi-empirical systematics for (p,α) and (p,np) reaction cross sections were achieved at 17.9 and 22.3 MeV incident energies [28]. Finally, Tel et al. [17] obtained empirical and semi-empirical systematics of (p,α) nuclear reaction cross sections at the incident proton energy 17.9 MeV [16, 17].

The empirical cross sections of reactions induced by proton can be approximately expressed as follows [16, 17]

$$\sigma(p,x) = C\sigma_{pinel}\exp[as], \qquad \sigma_{pinel} = \pi r_0^2\left(A^{1/3}+1\right)^2, \tag{2}$$

here σ_{pinel} represents the proton inelastic cross section, and C and a are the fitting parameters and $s = (N-Z)/A$ is asymmetry parameter.

The systematics used in the calculations are based on analytical formulas with the evaporation model, the pre-equilibrium exciton model and semi-empirical mass formula. A new empirical formula, including Coulomb effects of the cross sections of the (p,α) reactions at 17.9 MeV proton incident energy using recent experimental data, was offered.

The empirical cross sections including Coulomb effects of reactions induced by proton can be expressed as follows [16],

$$\sigma_{Coul} \approx b\frac{Z^2}{A^{1/3}+1}, \tag{3}$$

where σ_{Coul} and b are the proton Coulomb effect cross section and constant coefficient, respectively. The empirical cross sections with proton inelastic cross section and Coulomb effects of proton induced reactions were expressed in the following form [16],

$$\sigma(p,x) = C\sigma_{pinel}\sigma_{Coul}\exp[as], \qquad \sigma_{pinel}\sigma_{Coul} \approx \pi r_0^2 Z^2(A^{1/3}+1) \tag{4}$$

$$\sigma(p,x) = C'Z^2\left(A^{1/3}+1\right)\exp[as] \tag{5}$$

here $\sigma_{pinel}\sigma_{Coul}$ is the proton inelastic and Coulomb effect cross section, and C' and a are new coefficients.

Tel formula with new coefficient for (p,α) reactions at 17.9 MeV [16];

even−Z, even−N

$$\sigma(p,\alpha) = 0.067Z^2\left(A^{1/3}+1\right)\exp[-29.32s]$$

even−Z, odd−N

$$\sigma(p,\alpha) = 1.83Z^2\left(A^{1/3}+1\right)\exp[-54.62s] \tag{6}$$

Results and Discussions

In the present study, the excitation functions for proton induced reactions on Fe and Ni isotopes with the emission of the alpha particle were calculated using PCROSS and CEM95 code. The equilibrium effects were performed with WE model. The pre-equilibrium calculations were calculated according to the full exciton model and CEM. The full exciton model and CEM calculations were made by using PCROSS computer code and CEM95 computer code, respectively. Also, Tel et al. empirical cross section formula with new coefficient was applied for (p,α) reactions at 17.9 MeV. The (p,α) reaction cross section results of ^{54,57}Fe and ^{58,60,61,64}Ni as some structural fusion materials were calculated with the equilibrium and pre-equilibrium in the proton energy range of 10–40 MeV in Figs. 1, 2, 3, 4, 5, 6.

Excitation functions of (p,α) reaction for ^{54}Fe target nucleus are shown in Fig. 1. The model calculations with PCROSS code and Tel Model for ^{54}Fe(p,α) reaction are in good agreement with experimental measurements in energy range between 15 and 18 MeV. In Fig. 2, PCROSS code and Tel Model for ^{57}Fe(p,α) reaction show good agreement with experimental data around 20 MeV. The curve for CEM95 code shows similar behavior for energies up to 25 MeV but systematically lower than experimental data. Cross section results of ^{58}Ni(p,α) reaction are given in Fig. 3 and it is seen that calculated (p,α) reaction cross section values by using the new semi-empirical cross section formula [16] show the best agreement with WE model calculations. Moreover, experimental data and the full exciton model calculations give nearly same results in the range from 10 to 20 MeV. Information on the cross section values of ^{60}Ni(p,α) nuclear reaction is presented in Fig. 4. Experimental data and PCROSS is consistent for the

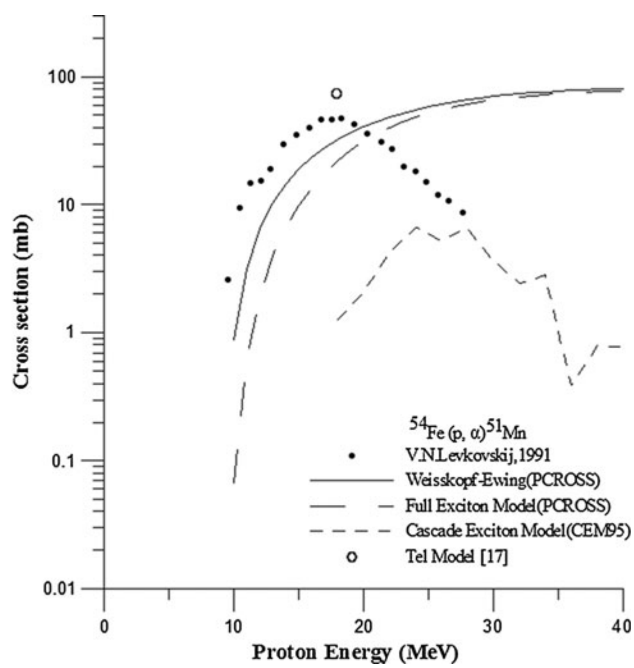

Fig. 1 The model calculations for ^{54}Fe(p,α)^{51}Mn nuclear reaction and comparison with available experimental measurement

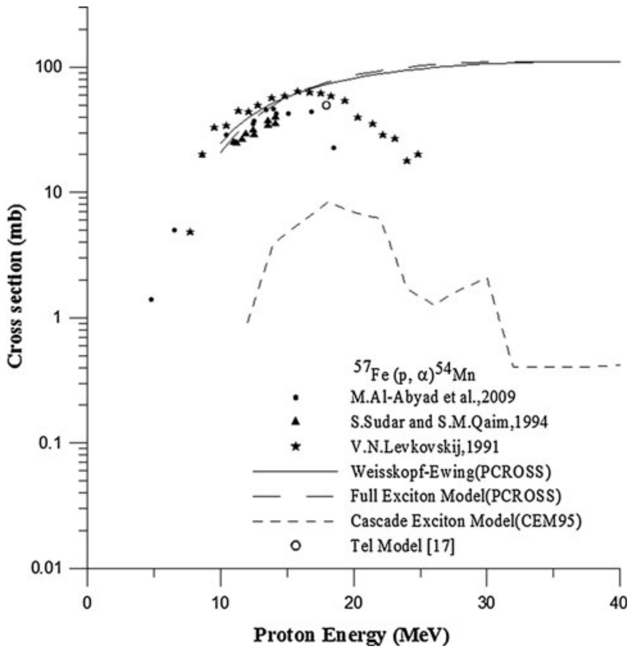

Fig. 2 The model calculations for $^{57}Fe(p,\alpha)^{54}Mn$ nuclear reaction and comparison with available experimental measurement

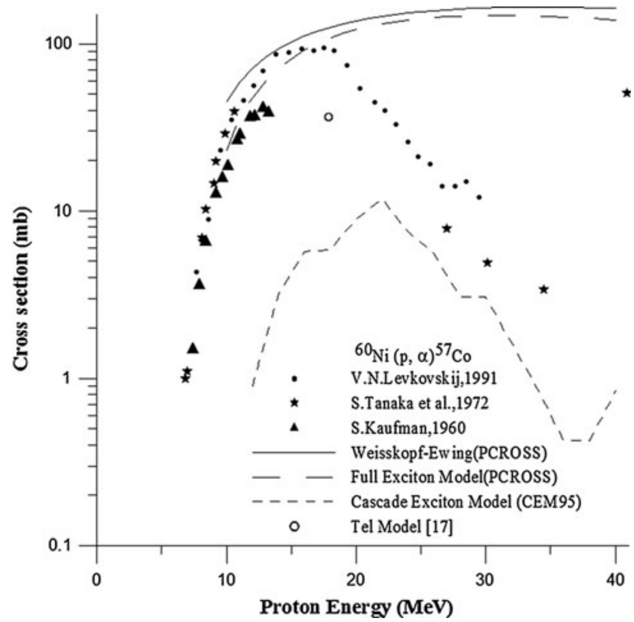

Fig. 4 The model calculations for $^{60}Ni(p,\alpha)^{57}Co$ nuclear reaction and comparison with available experimental measurement

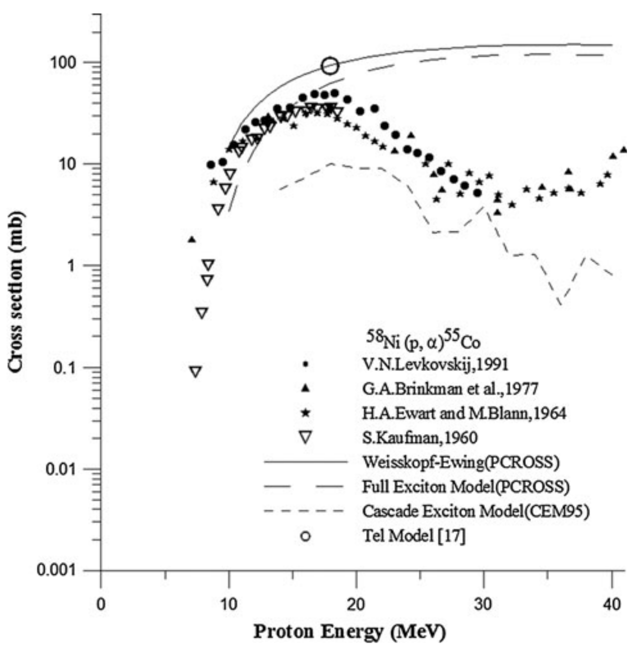

Fig. 3 The model calculations for $^{58}Ni(p,\alpha)^{55}Co$ nuclear reaction and comparison with available experimental measurement

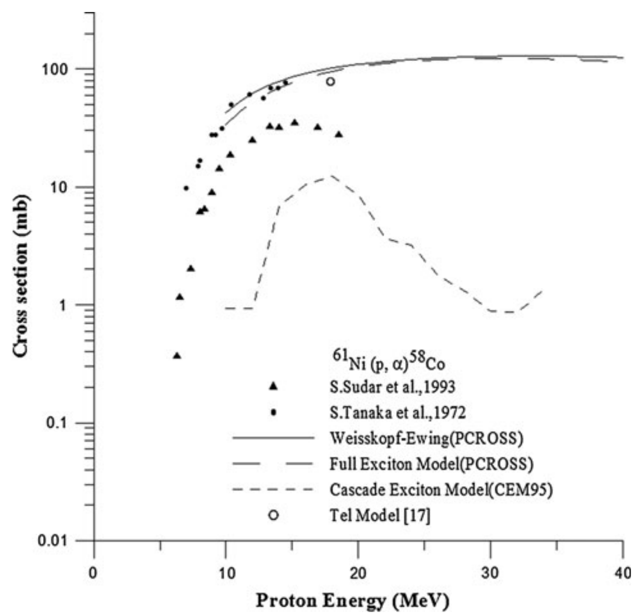

Fig. 5 The model calculations for $^{61}Ni(p,\alpha)^{58}Co$ nuclear reaction and comparison with available experimental measurement

energies between 10–15 MeV whereas the large discrepancies in the excitation functions of $^{60}Ni(p,\alpha)$ are determined between PCROSS code and CEM95 code calculations. The cross section results of $^{61}Ni(p,\alpha)$ nuclear reaction are shown in Fig. 5. And calculated cross sections by using PCROSS code are almost constant above 20 MeV. The cross sections of $^{64}Ni(p,\alpha)$ reaction are shown in Fig. 6. The calculated cross sections with the PCROSS code for $^{64}Ni(p,\alpha)$ reaction show good agreement with experimental results for incident proton particle up to 20 MeV. Moreover, the cross section results calculations of the CEM95 code at the all excitation functions of (p,α) reaction in Figs. 1, 2, 3, 4, 5, 6 give the lowest results for all investigated nuclei.

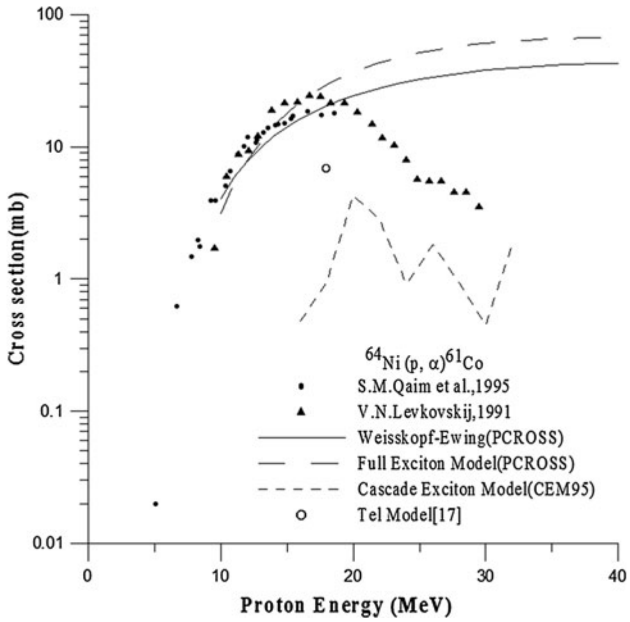

Fig. 6 The model calculations for ^{64}Ni(p,α)^{61}Co nuclear reaction and comparison with available experimental measurement

Summary and Conclusions

In the present study, (p,α) reaction cross section data for some fusion structural materials as ^{54,57}Fe and ^{58,60,61,64}Ni have been investigated in the bombarding proton energy range of 10–40 MeV . The theoretical and the semi-empirical cross sections have been compared with the existing experimental measurements and the obtained results can be summarized as follows:

- The Tel model and the PCROSS calculations for ^{54,57}Fe(p,α) nuclear reactions are in good agreement with experimental measurements in energy range between 15 and 18 MeV.
- The available experimental measurements and the Tel model result with new empirical formula including Coulomb effects of the cross section values of the ^{57}Fe(p,α) nuclear reaction have nearly the similar magnitude.
- The full exciton model and WE model computed with PCROSS code are almost constant between 30 and 40 MeV proton energy for the investigated reactions.
- The cross section values of the CEM95 code are lower than experimental and the other theoretical values for all nuclei in the present investigation.
- The present investigation contributes to the new researches on reaction cross section values for fusion reactor technology and helps to guide the experimental studies.

References

1. S. Şahin, M. Übeyli, Energ. Convers. Manag. **45**, 1497–1512 (2004)
2. E. Tel, A. Kara, J. Fusion Energ. **31**, 257–261 (2012)
3. A. Aydın et al., J Fusion Energ. **27**, 314–320 (2008)
4. E. Tel, J. Fusion Energ. **29**, 332–336 (2010)
5. E. Tel et al., J. Fusion Energ. **29**, 290–294 (2010)
6. E.E. Bloom, J. Nucl. Mater. **7**, 258 (1998)
7. S. Tarik, J. Reshid, Fusion Energ. **32**, 164–170 (2013)
8. H. Aytekin et al., J. Fusion Energ. **30**, 21–25 (2011)
9. C.M. Buczko et al., Phys. Rev. C **52**, 1940 (1995)
10. A. Kaplan et al., J. Fusion Energ. **32**, 97–102 (2013)
11. PSI (Paul Scherer Institute), Switzerland. (http://www.psi.ch/)
12. W. Wagner et al., J. Nucl. Mater. **361**, 274–281 (2007)
13. EXFOR/CSISRS (Experimental Nuclear Reaction Data). Database Version of February 26, 2013, Brookhaven National Laboratory, National Nuclear Data Center. http://www.nndc.bnl.gov/exfor/exfor00.htm; 2013
14. M.H. Bolukdemir et al., J. Fusion Energ. **29**, 13–18 (2010)
15. F. Weisskopf, D.H. Ewing, Phys. Rev. **57**, 472 (1940)
16. E. Tel et al., Phys. At. Nucl. **73**, 412–419 (2010)
17. E. Tel et al., Pramana J. Phys. **74**, 931–943 (2010)
18. Capote R, Osorio V, Lopez R, et al. Final Report on Research Contract 5472/RB, INDC(CUB)-004. Higher Institute of Nuclear Science and Technology, Cuba. Translated by the IAEA on March 1991 (PCROSS program code)
19. S.G. Mashnik, *User manual for the code CEM95* (Joint Institute for Nuclear Research, Dubna, 1995)
20. J. Griffin, Phys. Rev. Lett. **17**, 478 (1966)
21. E. Tel et al., J. Fusion Energ. **30**, 26–33 (2011)
22. C. Kalbach, C. Cline, Nucl. Phys. A **210**, 590–604 (1973)
23. C. Kalbach, Z. Phys. A **287**, 319–322 (1978)
24. M. Blann, A. Mignerey, Nucl. Phys. A **186**, 245–256 (1972)
25. K.K. Gudima et al., Nucl. Phys. A **401**, 329–361 (1983)
26. V.S. Barashenkov, V.D. Toneev, *Interaction of high energy particle and nuclei with atomic nuclei* (Atomizdat, Moscow, 1972)
27. V.S. Barashenkov et al., JINR report no. P2–4065; 1968 JINR report no. P2–4066, (1968). Acta Phys. Pol. **36**, 415 (1969)
28. C.H.M. Broeders, A.Y. Konobeyev, Appl. Radiat. Isot. **65**, 1249 (2007)
29. Brooders CHM, Konobeyev AY, Mertacali L. JEF/DOC-1154 (2006)