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Theoretical Calculations of the Cross-Sections for (n, α) and (n, xα) Reactions on the Structural Material for Fusion Reactor $^{46\text{-}50}$Ti

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Abstract

The biggest problem of structural materials for fusion reactor is the damage caused by the fusion product neutrons to the structural material. If this problem is overcomed, an important milestone will be left behind in fusion energy. One of the important problems of the structural material is that nuclei forming the structural material interacting with fusion neutrons are transmuted to stable or radioactive nuclei via (n, x) (x; alpha, proton, gamma etc.) reactions. In particular, the concentration of helium gas in the structural material increases through deuteron- tritium (D-T) and (n, α) reactions, and this increase significantly changes the microstructure and the properties of the structural materials. Therefore, in this study, the effects of the different nuclear level density models on the excitation functions of the (n, α) reactions on $^{46\text{-}50}$Ti isotopes, an attractive candidate for the structural material for fusion reactors, have been investigated for the first time. Also, the differential cross-sections with respect to alpha energy for the emission of alpha particles of the $^{46\text{-}50}$Ti (n, xα) reactions have been investigated at 14.1 MeV incident neutron energy. The calculations are performed using the two-component exciton model in the TALYS 1.9 code, and the results are compared with available experimental data. The results of this study will contribute to nuclear database as required for improving, design and operations of the important facilities as ITER (International Thermonuclear Experimental Reactor), DEMO (The demonstration power plant) and ENS (European Nuclear Society).

Article Info.

Keywords
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1. Introduction

Thanks to the serious developments for fusion energy in the past years, unlimited energy is approached step by step. Despite these significant developments for reaching unlimited energy, there is still a long path for a safe and commercial fusion reactor. One of the issues that should be handled on this path is the selection of appropriate structural material. Because the high energy neutrons of fusion reactions create a very severe environment for the structural materials of fusion reactor components such as the first wall, divertor, limiters and breeding blanket, etc. [1]. One of the considered candidate elements as the structural material is titanium (Ti) because of some of its properties such as the high electrical resistivity, heat capacity, low long term residual radioactivity, high corrosion resistance together with a good compatibility with coolants, etc. [1].

The 80% of the energy released from a D-T fusion reaction is carried with the product neutron (14.1 MeV) and the remaining part of the energy is carried with alpha particles (the helium). The ~10% of the neutron energy is accumulated in the first wall and the remaining neutron energy is mostly transferred to the breeding blanket [1]. The neutrons with 14.1 MeV can induce nuclear reactions with nuclei of atoms of the structural material, since the neutrons for the reactions lead to open the reaction channels by surpassing threshold energies [2]. This situation does not cause only (n, x) reactions, but also induces charged particles (alpha, proton, deuteron and tritons) reactions [2, 3]. Consequently, these reactions bring about nuclear transmutations of the structural material and these transmutations change the alloy composition of the structural material[4]. Moreover, the helium, which is derived from D-T and (n, α) reactions, has particular importance, because even at low concentrations, the helium is not soluble in the metal lattice of the structural material and can severely change the microstructure and properties of the structural materials [4, 5].

Therefore, the predictions of the behavior of the structural material facing the aforementioned nuclear events are crucial and the predictions can be made via the obtained nuclear data using the nuclear models. Nuclear data forms the basis of the fusion technology and with increasing numbers of the data, the requested on data quality are evenly increasing[6]. The nuclear cross-section data are important for radiation damaging and for nuclear transmutation calculations in the structural materials [7]. They are obtained through various nuclear reaction models and one of the appropriate models is the two-component exciton model, which is a pre-equilibrium reaction process between direct and compound reaction process. Furthermore, nuclear level density which is one of the characteristic properties of all nuclei plays an important role in the cross section calculations [8].

In this study, the calculations of the (n, α) reaction cross-sections on the natural isotopes of Ti element are presented. The reason for selecting natural Ti element is that, it is an attractive candidate for the structural material of fusion reactors. Another reason, is that the ^{48}Ti (n, α) reaction is the only reaction in the literature that is studied on. The study was performed by Dzysiuk et al. [6], the cross-sections of the (n,x) reactions on some nuclei which are regarded as the structural material in the range of 0-30 MeV incident neutron energy were calculated through the TALYS 1.8 code[9]. Apart from this study, there isno other study on $^{46\text{-}50}$Ti (n, α) reactions in literature. Therefore, the effects of different nuclear level density models on the excitation functions of ^{46}Ti (n, α) ^{43}Ca, ^{47}Ti (n, α) ^{44}Ca, ^{48}Ti (n, α) ^{45}Ca, ^{49}Ti (n, α) ^{46}Ca, ^{50}Ti (n, α) ^{47}Ca reactions are investigated for the first in the present study. The calculations have been performed by the two-component exciton model in the TALYS 1.9 code [10]. In addition, the differential cross-section with respect to alpha energy for the emission of alpha particles of the $^{46\text{-}50}$Ti (n, xα) reactions at 14.1 MeV incident neutron energy have been calculated by the two-component exciton model in the same code. The main goal of this study is to analyze and improve the cross-section data of the$^{46\text{-}50}$Ti (n, α) for fusion reactor technology and to provide theoretical data sets for the reactions of which experimental data are not available or limited.

2. Calculations

All calculations of (n, α) and (n, xα) reactions were performed by the two-component exciton model with TALYS 1.9 code in the range of 0 to 30 MeV neutron incident energy. The two-component exciton model, which is an exclusive version of the exciton model, is based on the pre-equilibrium reaction mechanism [10-13]. The neutron or proton types of particles and holes are followed throughout a nuclear reaction in this model [10]. In this model, the temporal development of the system is described by the master equation that is defined by the gain and loss terms for a particular class of exciton states [10]. However, the pre-equilibrium differential cross section for the emission of a particle k with emission energy (E_k) is obtained by integrating the master equation over time up to the equilibration time yields the mean lifetime of the exciton state (τ) [13]. The expression for the differential cross section in terms of the composite nucleus formation cross-section (σ^{CF}) and the emission rate (W_k) is given as following:

$$\frac{d\sigma_k^{PE}}{dE_k} = \sigma^{CF} \sum_{p_\pi=p_\pi^0}^{p_\pi^{max}} \sum_{p_\upsilon=p_\upsilon^0}^{p_\upsilon^{max}} W_k(p_\pi, h_\pi, |p_\upsilon, h_\upsilon, E_k)\tau(p_\pi, h_\pi, p_\upsilon, h_\upsilon)P(p_\pi, h_\pi, p_\upsilon, h_\upsilon) \quad \mathbf{(1)}$$

where the P is the part of the pre-equilibrium population that has survived emission from the previous states and now passes through the (p_π, h_π, p_υ, h_υ) configurations, averaged over time [10]. The p_π^0 and p_υ^0 are the initial proton and neutron particle numbers, respectively. In the reaction process, any exciton state is $h_\pi = p_\pi - p_\pi^0$ and $h_\upsilon = p_\upsilon - p_\upsilon^0$, the initial proton and neutron hole numbers for primary pre-equilibrium emission are zero ($h_\pi^0 = h_\upsilon^0 = 0$) [13].

TALYS is a simulation tools for nuclear reactions. The modern nuclear models include all main nuclear reaction mechanisms for incident particles such as protons, neutrons, photons, deuterons, tritons, ^{3}He, and alpha particles [10]. The simulation of nuclear reactions in this code can be performed for target mass numbers from 12 to 339 in the range of 1 KeV - 200 MeV incident energy range [10]. Moreover, the users can change many parameters related to a nuclear reaction. One of the alterable parameters is nuclear level density models which are one of the important characteristic properties of nuclei.

Nuclear level density is defined as the total number of energy levels per unit energy at some excitation energy of nucleus. There are six level density model options in the TALYS code, and these options are three phenomenological level density models and three microscopic level density options. The phenomenological level density models are the constant temperature plus Fermi gas model (CT+FGM), the back-shifted Fermi gas model (BSFGM) and the generalized superfluid model (GSM). The calculations of level density in the CT+FGM are used as a constant temperature formula for the first energy levels up to~10 MeV and at the higher energies the conventional shifted Fermi gas formula is used [14-16]. Another phenomenological level density model is the BSFGM and the level densities in this model are obtained by the calculated excitation energies using Fermi gas formula at all way down to 0 MeV, and the pairing energy in this model is an adjustable parameter [10,15,16]. The GSM, which is based on the pairing correlations of the Bardeen-Cooper-Schrieffer (BCS) theory, is defined by a phase transition from superfluid behavior at low energy to the Fermi gas model at high energies [10, 17, 18]. The CT+FGM, the BSFGM and the GSM are represented by “ldmodel 1”, “ldmodel 2” and “ldmodel 3” keywords, respectively, in TALYS code [10]. The extensive reviews for phenomenological level density models was reported by Koning et al. [10] and Zelevinsky and Horoi [19]. Besides all these, the microscopic level density approaches are the microscopic level densities (Skyrme force) from Goriely’s tables (MLD-1), the microscopic level densities (Skyrme force) from Hilaire’s combinatorial tables (MLD-2) and the microscopic level densities (temperature dependent Hartree-Fock-Bogolyubov, Gogny force) from Hilaire’s combinatorial tables (MLD -3). The MLD-1 stands for the level densities based on the Hartree-Fock calculations for excitation energies up to 150 MeV and for spin values up to I = 30 as were calculated by S. Goriely for RIPL database [10, 20]. Another microscopic level density approach, the level densities in the MLD-2 are based on the deformed Skyrme-Hartree-Fock-Bogolyubov calculations for more than 8500 nuclei, excitation energies up to 200 MeV and spin values up to J = 49 [10, 21]. The MLD-3, last microscopic level density approach, which relies on temperature-dependent HartreeFock-Bogolyubov calculations using the D1M Gogny Force [10, 22]. The MLD-1, the MLD-

2 and the MLD-3 approaches are represented by "ldmodel 4", "ldmodel 5" and "ldmodel 6" keywords, respectively, in TALYS code [10].

3. Results and discussion

Investigation of the effects of the level density models on (n, α) reactions of $^{46-50}$Ti isotopes is objected in this study. For this aim, the excitation functions for $^{46-50}$Ti (n, α) reactions in the 0-30 MeV incident neutron energy range are calculated by the two-component exciton model and presented in Figs. 1-5. In addition, the results were compared with the available experimental data[23-39]. The obtained excitation functions for $^{46-50}$Ti (n, α) reactions using different level density models were very close to each other up to ~7 MeV, ~5 MeV, ~7 MeV, ~6 MeV and ~9 MeV incident neutron energies, and after this energy, different level densities indicate its influence on the cross-sections for these reactions (Figs.1-5).

For ^{46}Ti (n, α) reaction, the values of cross-section for phenomenological and microscopic level density models at some incident neutron energies have the same values, as seen in Fig.1. The results of the GSM and the CT+FGM tend to converge on each other at more than 21 MeV incident neutron energy. Nevertheless, while the highest excitation function corresponding to incident neutron energies is obtained using the MLD-2 for this reaction, the lowest excitation function is obtained using the MLD-3.

The results of the CT+FGM and the MLD-2 models for ^{47}Ti (n, α) reaction (Fig. 2) have very close values at all incident neutron energies and the calculated cross-sections using the MLD-3 for this reaction are also close to those of the two models at ~19 MeV neutron energy. Theoretical cross-sections of the BSFGM and the MLD-1 have the same value as that at ~17 MeV neutron energy. The obtained excitation function using the GSM for this reaction has larger values than those of other level density models (as seen in Fig.2).This excitation function is close to the experimental data reported by Khromyleva et al. (2018) [24]. Also, the obtained cross-section using the GSM for this reaction at the 16 MeV incident neutron energy is 154.628 mb and this cross-section value is the maximum probability among the handled reactions in this study (Table 1).

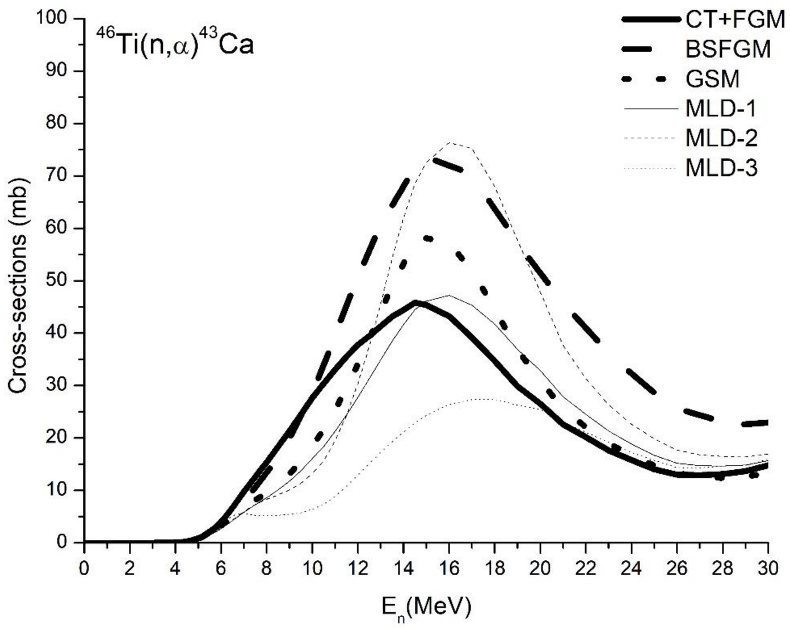

Figure 1: The theoretically calculated excitation functions for ^{46}Ti (n, α) ^{43}Ca reaction.

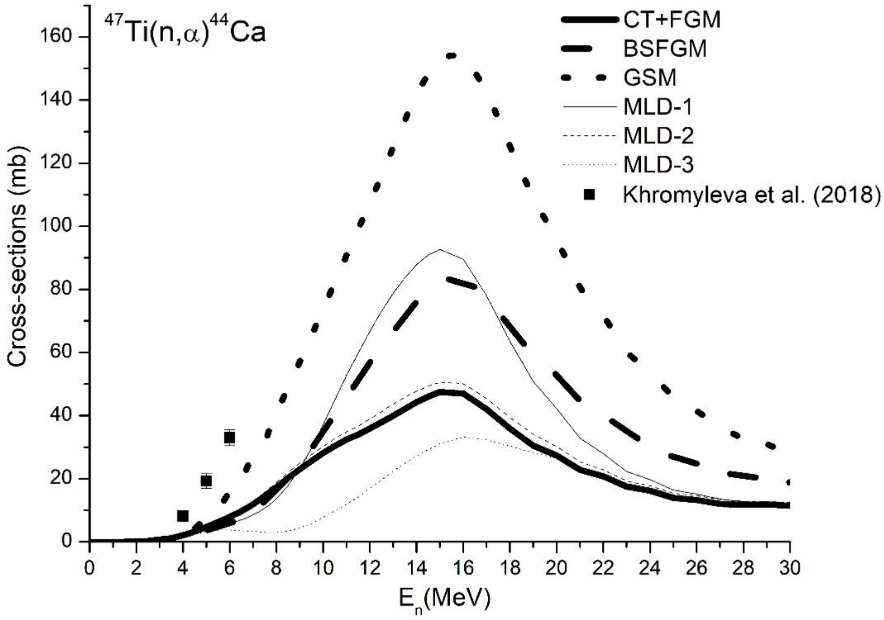

Figure 2: The comparison of the theoretically calculated excitation functions with experimental data [24] for ^{47}Ti (n, α) ^{44}Ca reaction.

In the case of ^{48}Ti (n, α) reaction, the MLD-2 and the MLD-3 results have higher values than those of other level density models (Fig. 3). Nevertheless, the obtained cross-sections using the MLD-2 and the MLD-3 at 13-15 MeV incident neutron energy range are more consistent with the experimental data of Qaim et al.(1992) [35], Yu and Gardner (1967) [26] and Cross and Pai (1963) [25]. At energy larger than 15MeV, the BSFGM is the best level density model for this reaction up to ~19.5 MeV incident neutron energy. The larger than 24 MeV energy, all the density level models are close to each other. On the other hand, the calculated cross-section using the MLD-2 at the 14.1 MeV incident neutron energy is very close to the experimental results of Yu and Gardner (1967) [26], as presented in Fig. 3. However, the obtained cross-sections using the MLD-3 and the BSFGM models at 14.1 MeV incident neutron energy are in the range of the experimental error of the results obtained by Yu and Gardner (1967) [26]. Finally for this reaction, the maximum cross-section values were obtained using the MLD-3 at 17 MeV neutron induced energy. Also, the product nucleus of ^{48}Ti (n, α) reaction is a radioactive one (^{45}Ca; $T_{1/2}$=162.61 d and 100% β^- emitter). The radioactive product ^{45}Ca of this reaction transforms to the stable nucleus (^{45}Sc) after 162.61 d.

The obtained excitation functions using microscopic level density models and the CT+FGM model for ^{49}Ti (n, α) reaction are similar at the incident neutron energies, as seen in Fig.4. While the highest excitation function is obtained for the GSM, the lowest one is obtained for the MLD-3, like ^{47}Ti (n, α) reaction. The obtained excitation functions for ^{50}Ti (n, α) reaction using different level density models were compared to experimental data [25–39], as shown in Fig.5. The results of the BSFGM are the closest to the experimental data among the obtained findings for this reaction, especially after 12 MeV incident neutron energy. The calculated cross section values using the BSFGM model at incident neutron energy of 14.1 MeV are the closest to the experimental data of Yu and Gardner (1967) [26] and Subasi et al.(1996) [32] than the results of the other models. The obtained cross-section using the BSFGM for this reaction at the 19 MeV incident neutron energy was 13.059 mb it is the minimum value among the cross-section values of the reactions handled in this study (Table 1). This result is important in terms of radiotoxicity of the structural material for fusion reactor, because, the ^{50}Ti (n, α) reaction is the second reaction after ^{48}Ti (n, α) reaction having radioisotope product among the (n, α) reactions of natural titanium isotopes. According to the results of this study, the probability of ^{47}Ca radioisotope accumulation into the structural material is low, if the structural material contains titanium. However, the product of this reaction is ^{47}Ca radioisotope ($T_{1/2}$ = 4.536 d) that decays via β^- emission (100%) [40]. This radioisotope decays to ^{47}Sc radioisotope ($T_{1/2}$=3.349 d and 100% β^- emitter) which decays to the stable nucleus (^{47}Ti) after 3.349 d.

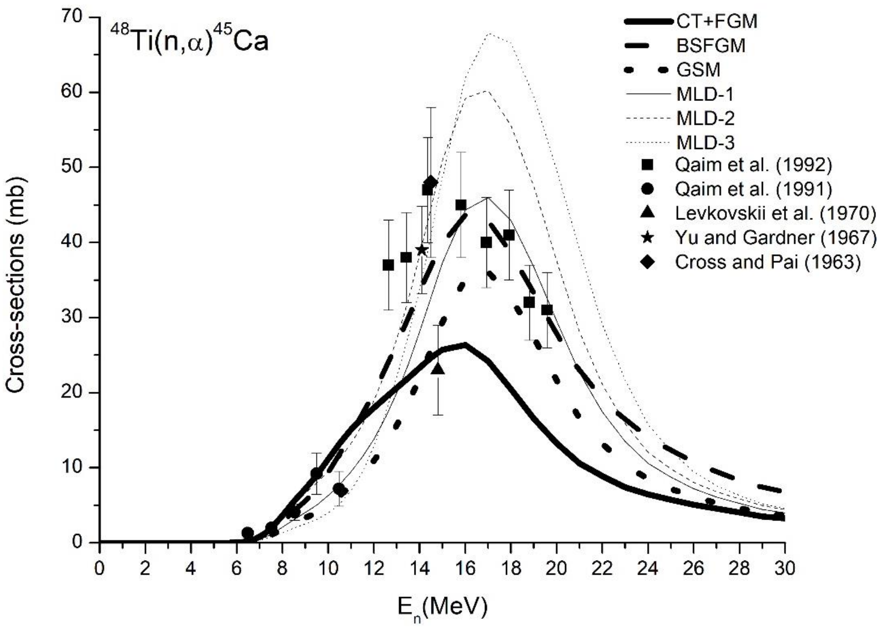

Figure 3: Comparison of the theoretically calculated excitation functions with the experimental data[25–27, 35, 37] for ^{48}Ti (n, α) ^{45}Ca reaction.

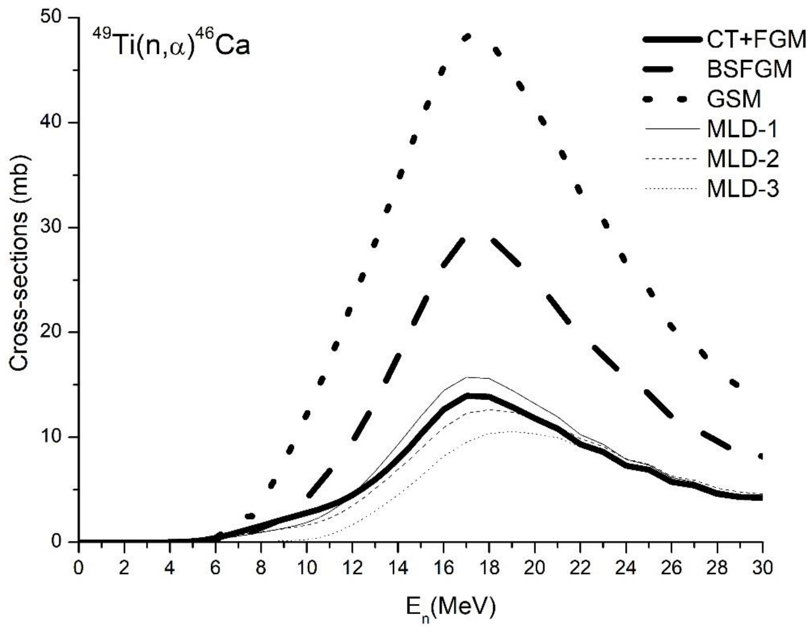

Figure 4: The theoretically calculated excitation functions for ^{49}Ti (n, α) ^{46}Ca reaction.

Threshold energy, Q-value and incident neutron energy corresponding to the highest cross-sections for the reactions of this study are presented in Table 1. According to the results in Table 1, two reactions having Q > 0, which are $^{47,49}Ti$ (n, α) reactions. The cross-section values of ^{47}Ti (n, α) reaction has higher than those of the handled reactions, and also its Q value has a positive value. In terms of these two results, ^{47}Ti (n, α) reaction is the most likely reaction to occur between these reactions in this study. This is an important result in view of using titanium as the structural material due to being the stable (^{44}Ca) of product nucleus of ^{47}Ti (n, α) reaction. On the other hand, Q values of the ^{46,48,50}Ti (n, α) reactions are negative and the threshold energies for these reactions are 0.074 MeV, 2.077 MeV and 3.510 MeV, respectively. The incident neutron energies that correspond to the highest cross-section values of ^{46,48,50}Ti (n, α) reactions are respectively 216, 8.8 and 5.4 times higher than the threshold energies for these reactions.

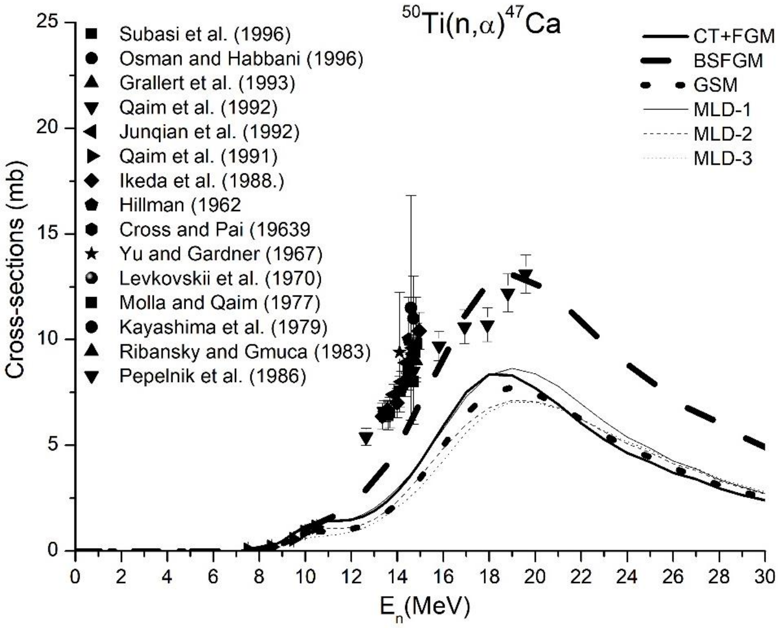

Figure 5: Comparison of the theoretically calculated excitation functions with experimental data for ^{50}Ti (n, α) ^{47}Ca reaction.

Table1: Threshold energy, Q-values, and the incident neutron energies that correspond to the highest cross-section values of (n, α) nuclear reactions on $^{46-50}$Ti isotopes.

Reaction	Threshold Energy (MeV)	Q-Value (MeV)	Incident Neutron Energy (MeV)	Highest cross-section (mb)			
				BSFGM	GSM	MLD-2	MLD-3
^{46}Ti (n, α)	0.074	-0.073	16	-	-	76.361	-
^{47}Ti (n, α)	-	2.178	16	-	154.628	-	-
^{48}Ti (n, α)	2.077	-2.034	17	-	-	-	67.881
^{49}Ti (n, α)	-	0.222	17	-	48.252	-	-
^{50}Ti (n, α)	3.510	-3.441	19	13.059	-	-	-

The quality of the calculated cross-sections using different level density models of the reactions of this study were also estimated on basis of statistical analysis (Table 2). For this aim, the mean weighted deviation (F) and the relative variance (D) were calculated using the theoretical and the experimental data [41]. F and D quantities are:

$$\boldsymbol{F} = \left\{ \frac{\mathbf{1}}{\boldsymbol{N}} \sum_{\boldsymbol{i}=\mathbf{1}}^{\boldsymbol{N}} \left[\left(\boldsymbol{\sigma}_{\boldsymbol{i}}^{\boldsymbol{calc}} - \boldsymbol{\sigma}_{\boldsymbol{i}}^{\boldsymbol{exp}} \right) / \Delta\, \boldsymbol{\sigma}_{\boldsymbol{i}}^{\boldsymbol{exp}} \right]^{\mathbf{2}} \right\}^{\mathbf{1/2}} \tag{2}$$

and

$$\boldsymbol{D} = \left\{ \frac{\boldsymbol{1}}{\boldsymbol{N}} \sum_{\boldsymbol{i}=\boldsymbol{1}}^{\boldsymbol{N}} \left| \boldsymbol{\sigma}_i^{calc} - \boldsymbol{\sigma}_i^{exp} \right| / \boldsymbol{\sigma}_i^{exp} \right\} \qquad (\mathbf{3})$$

where σ_i^{calc} and σ_i^{exp} are the theoretical and experimental cross-section, respectively. $\Delta\sigma_i^{exp}$is the experimental uncertainty and N is the number of cross-section data points. If the values of F and D quantities are low, the obtained theoretical results are coherent. The statistical analyze was solely made for ^{47,48,50}Ti (n, α) reactions, because the experimental data for these reactions are available in literature. According to the results of the analysis, it can be said that the best level density models among the models employed in this study for the calculations of the cross-section are the GSM for the ^{47}Ti (n, α) reaction and the BSFGM for the ^{48,50}Ti (n, α) reactions. Meanwhile, the numbers of experimental cross-section in the literature for statistical analysis are 3 for ^{47}Ti (n, α) reaction, 16 for ^{48}Ti (n, α) reaction and 32 for ^{50}Ti (n, α) reaction. Certainly, the numbers are small for statistical analysis, but at least they give an idea for testing the reliability of theoretical data.

Table 2: Statistical analysis of ^{47,48,50}Ti (n, α) reaction cross-sections.

The weighted deviation (F)						
Reaction	**CT+FGM**	**BSFGM**	**GSM**	**MLD-1**	**MLD-2**	**MLD-3**
^{47}Ti (n, α)	8.486	9.025	**7.144**	9.053	8.339	9.493
^{48}Ti (n, α)	2.559	**1.566**	2.198	1.859	2.311	3.269
^{50}Ti (n, α)	7.059	**4.002**	7.941	6.898	7.862	8.369
The relative variance (D)						
Reaction	**CT+FGM**	**BSFGM**	**GSM**	**MLD-1**	**MLD-2**	**MLD-3**
^{47}Ti (n, α)	0.752	0.800	**0.635**	0.801	0.835	0.835
^{48}Ti (n, α)	0.420	**0.255**	0.373	0.307	0.355	0.531
^{50}Ti (n, α)	0.533	**0.294**	0.582	0.513	0.574	0.637

Also, the differential cross-sections with respect to the alpha emission energy (ε_α) of $^{46\text{-}50}$Ti (n, xα) reactions, is also called the alpha emission spectra, at the 14.1 MeV incident neutron energy are calculated using the different nuclear level density models. But the experimental alpha emission spectra for these reactions are not available in the literature. Therefore, the calculated alpha emission spectra for these reactions are not graphically presented here. The highest spectrum for the obtained alpha emission spectra using the different level density models for each reaction was chosen (as presented in Table 3). At the same time, the maximum differential cross-section of the alpha emission spectrum for each reaction is separately given in Table 3. According to results in Table 3, the differential cross-section for^{50}Ti (n, xα) reaction have the smallest value among $^{46\text{-}50}$Ti (n, xα) reactions. Also, when all differential cross-sections in Table 3 are generally evaluated, they are relatively small (in other words, the alpha emission probabilities of these reactions are low).

Table 3: The calculated differential cross-sections ($d\sigma/d\varepsilon_\alpha$) using the different nuclear models and the emission alpha energy (ε_α) for $^{46\text{-}50}$Ti (n, xα) reactions at the 14.1 incident neutron energy.

Reaction	**ε_α (MeV)**	**$d\sigma/d\varepsilon_\alpha$ (mb/MeV)**	**Used Level Density Model**
^{46}Ti (n, xα)	7	22.161	MLD-2
^{47}Ti (n, xα)	7.5	23.739	GSM
^{48}Ti (n, xα)	7.5	12.139	MLD-2
^{49}Ti (n, xα)	10.1	6.333	GSM
^{50}Ti (n, xα)	8.4	2.285	BSFGM

4. Summary and conclusion

In this study, the different nuclear level density model effects on the excitation functions of $^{46-50}$Ti (n, α) reactions and differential cross-sections with respect to alpha emission energy of $^{46-50}$Ti (n, xα) reactions was investigated using the two-component exciton model in the TALYS 1.9code. The obtained results can be summarized as follows:

1. The different nuclear level density model significantly affects the excitation functions of $^{46-50}$Ti (n, α) reactions. Nevertheless, according to the statistical analysis of the calculations in this study, it has been shown that the results of the GSM for ^{47}Ti (n, α) reaction and the BSFGM for ^{48,50}Ti (n, α) reactions can be chosen as the best level density models for the handled reactions. However, the best level density model for ^{46,49}Ti (n, α) reactions have not been decided, since the experimental data are not available for this reaction.
2. The product nuclei of ^{48,50}Ti (n, α) reactions are radioactive. The radioactive product nuclei of ^{48}Ti (n, α) ^{45}Ca and ^{50}Ti (n, α) ^{47}Ca reactions decays to stable nuclei (^{45}Sc and ^{47}Ti, respectively) after 162.61 d and 7.885 d, respectively. This situation can cause the accumulation of ^{45}Sc and ^{47}Ti nuclei into the structural material. Also, as the product nuclei of ^{46,47,50}Ti (n, α) reactions are ^{43,44,46}Ca (stable), calcium may accumulate in the fusion structure material. Besides, the interactions of the accumulated product nuclei in the structural material with neutrons of D-T fusion reactions are possible and as a results new radioisotope can be formed in the structural materials. Therefore, the radiotoxicity for the reactions in this study should be investigated in detail for future studies.
3. The differential cross-sections with respect to energy for the emission of alpha particles of $^{46-50}$Ti (n, xα) reactions at the 14.1 MeV incident neutron energy are calculated using different level density models in TALYS 1.9. As experimental data of the differential cross-sections of these reactions are not available in the literature, no comparison was possible. The obtained differential cross-sections were relatively small. This is a favorable result for the use of titanium as the structural material for fusion reactor, because the probability formation of helium gas bubbles on the structural material due to the alpha emission of $^{46-50}$Ti (n, xa) reactions is low.
4. The obtained data in this study can be helpful in a better evaluation of the cross sections of $^{46-50}$Ti (n, α) and $^{46-50}$Ti (n, xα) reactions in the future. Moreover, the findings of this and similar studies can contribute to nuclear database as required for improving design and operations of the important facilities as ITER (International Thermonuclear Experimental Reactor), DEMO (The demonstration power plant) and ENS (European Nuclear Society).

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Conflict of interest

Authors declare that they have no conflict of interest.

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