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Examination of the Effects of Level Density Models in Cross-Section Calculations of Some (p,x) Reactions on Natural Palladium

Özlem Y. TOYKAN CIFTLIKLI[*1], Abdullah KAPLAN[1]

[1]Department of Physics, Faculty of Engineering and Natural Sciences, Süleyman Demirel University, 32260, Isparta, Turkey
https://orcid.org/0000-0002-2339-9822
ozlemtoykan@gmail.com
[1]Department of Physics, Faculty of Engineering and Natural Sciences, Süleyman Demirel University, 32260, Isparta, Turkey
https://orcid.org/0000-0003-2990-0187
abdullahkaplan@sdu.edu.tr

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Abstract:

In this study, reaction cross-section calculations of some proton-induced reactions on ^{nat}Pd have been investigated under the effects of level density models. All calculations involving level density models have been done employing the TALYS code's 1.95 version. TALYS is an open-source software. It gives foresight to the researchers about many parameters of a desired nuclear reaction, one of which is known as cross-section, when it is not possible to perform it due to specific reasons. The TALYS 1.95 code consists of six different level density models, which have all been included in this study. All obtained cross-section results gathered from the utilization of level density models have been compared with available experimental data. The mentioned available experimental data used in this study have been obtained from the International Experimental Nuclear Reaction Data Library (EXFOR) database. A graphical representation of generated calculation results, and available experimental data have been displayed for these comparisons. These graphical representations are also used to point out the most consistent level density model with respect to the experimental data for each reaction investigated in this study. The use of level density models was found to affect the results of cross-sectional calculations.

Keywords: Palladium, Cross-section, Level density, EXFOR

1. Introduction

Palladium (Pd), a platinum group metal element, is widely used in many industrial fields such as many industries of electronics and petroleum, manufacturing of electrode and ceramic capacitors, surgical instruments, jewelries, composite dental alloys, and wastewater treatment. This widespread use makes palladium one of the most valuable members of the platinum group metals. The importance of platinum group metals, and their isotopes has increased in recent years as the industrial, and technological needs have increased. From a different perspective, the fact that many precious metals, including platinum group elements, are waiting as nuclear waste has led researchers to study these materials. Ongoing studies on the recovery of nuclear waste, and alternative production techniques for valuable isotopes are of universal importance [1-3].

Natural palladium consists of six stable isotopes, which are; ^{102}Pd, ^{104}Pd, ^{105}Pd, ^{106}Pd, ^{108}Pd, and ^{110}Pd. The relative abundances of these palladium isotopes are; 1.02 %, 11.1 %, 22.3 %, 27.3 %, 26.5 %, and 11.7 %, respectively. The half-lives ($t_{1/2}$) of some unstable isotopes of palladium are 6.5 million years for ^{107}Pd, 17 days for ^{103}Pd, 3.63 days for ^{100}Pd, 8.47 for hours ^{101}Pd, 13.7 hours for ^{109}Pd, and 21 hours for ^{112}Pd [4].

In this study, natural isotope of palladium has been used as target, and the effects of level density models on the cross-section calculations for (p,x) reactions on ^{nat}Pd-targeted reactions have been investigated. The term cross-section can be defined simply, and succinctly as the probability of a nuclear reaction taking place. It is very important in determining the atomic structure in atomic, and molecular physics in addition to the understanding of the mechanisms of a nuclear reaction in nuclear physics. There are many parameters that is known to affect the theoretical cross-section calculations where one of them is the level density models. The term level density can be defined as the number of excited energy levels in an infinite energy range [5].

In many cases, the cross-section values can be obtained by performing specific reactions. However, there may be cases where many reasons create obstructions to achieving the desired typical reaction. In these circumstances, theoretically obtained cross-section values may give researchers a foresight. To avoid from any mistake, fault, error or any other human origin negative outcome, that may arise while performing the hand-made calculations, computer aided software have been used to obtain the cross-section results for a specific reaction. For this purpose, many codes have been developed such as CEM95 [6], EMPIRE [7], GEANT [8], ALICE/ASH [9], PCROSS [10], and TALYS [11]. In this study, the code TALYS with the version of 1.95 has been utilized to perform the level density model included calculations. The motivation for selecting the TALYS code in this study is directly related to the existing literature in which the performance, reliability, compatibility, and wide usage possibilities are shown in many studies [12-21].

As of gathering the calculation results obtained via utilizing the level density models of the TALYS code, the need of their comparison has arisen. To perform a logic, and equitable comparison of the obtained cross-section results, experimental data for each investigated reaction have been used. These mentioned experimental are taken from a database, known as the EXFOR [22, 23], which is a freely accessible online platform. All calculation results, and experimental data have been graphed together for each reaction to perform a visual representation, and comparison. As a result of these graphical representations, the level density model that gives the most consistent outcomes with the experimental data have been able to point out.

2. Material and Method

As mentioned earlier this paper aims to investigate the effects of level density models on the cross-section calculations of (p,x) reactions on ^{nat}Pd. To this end, six different level density models which are available in the version 1.95 of the TALYS code have been employed. TALYS is a computer software, which is developed to provide various calculations in accordance with the users' wishes, and directions given in an input file. This input file must contains four fundamental, and mandatory parameters, such as the name of the projectile, the energy range of the incident particle, symbol or name of the target, and the atomic mass number of the target. In addition to all these, users may change other parameters which allows them to manipulate various models, and parameters. The power of the TALYS code and one of its common preferring reasons lies along in its strong ability to change models, and their parameters. Each model and/or parameter is defined by a keyword in TALYS, and there are more than 600 keywords. Some examples

of these parameters are related to masses, and deformations, discrete levels, level densities, gamma emissions, optical models, astrophysics, medical isotope production, and etc. [11]. Many studies in the literature can be shown where some of these parameters' effects on different calculations have been examined [13-16].

In simple terms, level density can be defined as the number of excited energy levels in an infinite energy range, or the function used to determine these energy ranges. This model neglects the interaction of nucleons with each other and assumes that the particles in the single-particle system are placed in equal energy levels, and do not contain collective levels [5]. The code TALYS includes six level density models, of which the default one is based on the Fermi Gas Model (FGM) [24]. The TALYS code contains six different six-level density models. Three of these models can be grouped as phenomenological models hypothetically based on the FGM [24]. Among the phenomenological models, the so-called Constant Temperature Fermi Gas Model (CT+FGM) was developed to correct the failure of the FGM in the high energy region by assuming that constant temperature laws are valid in the zero-match energy range, and the FGM is valid in the higher energy region [25, 26]. In addition to this model, many modifications, and developments have been done over the years with respect to the improvements in the theoretical models. Herewith, TALYS contains two more phenomenological level density models, which are named as Back Shifted Fermi Gas Model (BSFGM) [27, 28], and Generalized Superfluid Model (GSM) [29, 30].

In addition to these phenomenological level density models, TALYS offers three microscopic level density models to the users. These models are named after the scientists who came up with the idea of the development of these models and provide indisputable contributions to the literature. The microscopic level density models are implemented into the TALYS code from the study of Goriely et al., [31], Hilaire, and Goriely [32], Hilaire et al., [33]. In the rest of this study, all level density models are shown with abbreviations. In this direction, abbreviations for phenomenological level density models are used as given above. On the other hand, for microscopic level density models, names of the models, and abbreviations are used as given below; Skyrme Force-Goriely level densities from numerical tables (SFG) [31], Skyrme Force-Hilaire level densities from numerical tables (SFH) [32], and Temperature-dependent Gogny-Hartree-Fock-Bogoluybov level densities from numerical tables (GFD) [33]. In this study, ^{nat}Pd(p,x)^{97}Ru, ^{nat}Pd(p,x)^{100}Pd, ^{nat}Pd(p,x)^{101}Pd, ^{nat}Pd(p,x)^{103}Ag, ^{nat}Pd(p,x)^{103}Ru, ^{nat}Pd(p,x)^{105}Ag reactions have been selected where all include ^{nat}Pd as target, and proton as incident particle. In each reaction, all mentioned level density models have been utilized, and reaction cross-section calculations have been done with the TALYS code's 1.95 version. Obtained results have been compared with each other, and available experimental data for each reaction, and the findings are given as graphical representations.

3. Results

In this study, seven proton-induced reactions for the ^{nat}Pd isotope have been investigated. The reactions investigated in this study are ^{nat}Pd(p,x)^{97}Ru, ^{nat}Pd(p,x)^{100}Pd, ^{nat}Pd(p,x)^{101}Pd, ^{nat}Pd(p,x)^{103}Ag, ^{nat}Pd(p,x)^{103}Ru, ^{nat}Pd(p,x)^{105}Ag, and ^{nat}Pd(p,x)^{105}Rh. Figures 1-7 show the comparisons between the computational results, and available experimental data of six different level density models for each reaction.

The cross-section values of the ^{nat}Pd(p,x)^{97}Ru reaction, which takes place around the energy range of 30-80 MeV. The experimental data for this reaction are taken from the studies of Tarkanyi et al. [34], and Ditrio et al. [35]. The compatibility of these data with the calculation results have been shown in Figure 1. As can be clearly seen from this

figure, between the energy range of around 30 MeV to 55 MeV almost all theoretical calculation results are obtained below the experimental data. Other than this energy region, which falls between the energy range of around 55 MeV to 80 MeV, the model results became closer to each other, and some of them approached the experimental data more than the others. It is seen that the closest fit with the experimental results is achieved with the GFD model, while the GSM is lower than the data obtained with other models, and the experimental results.

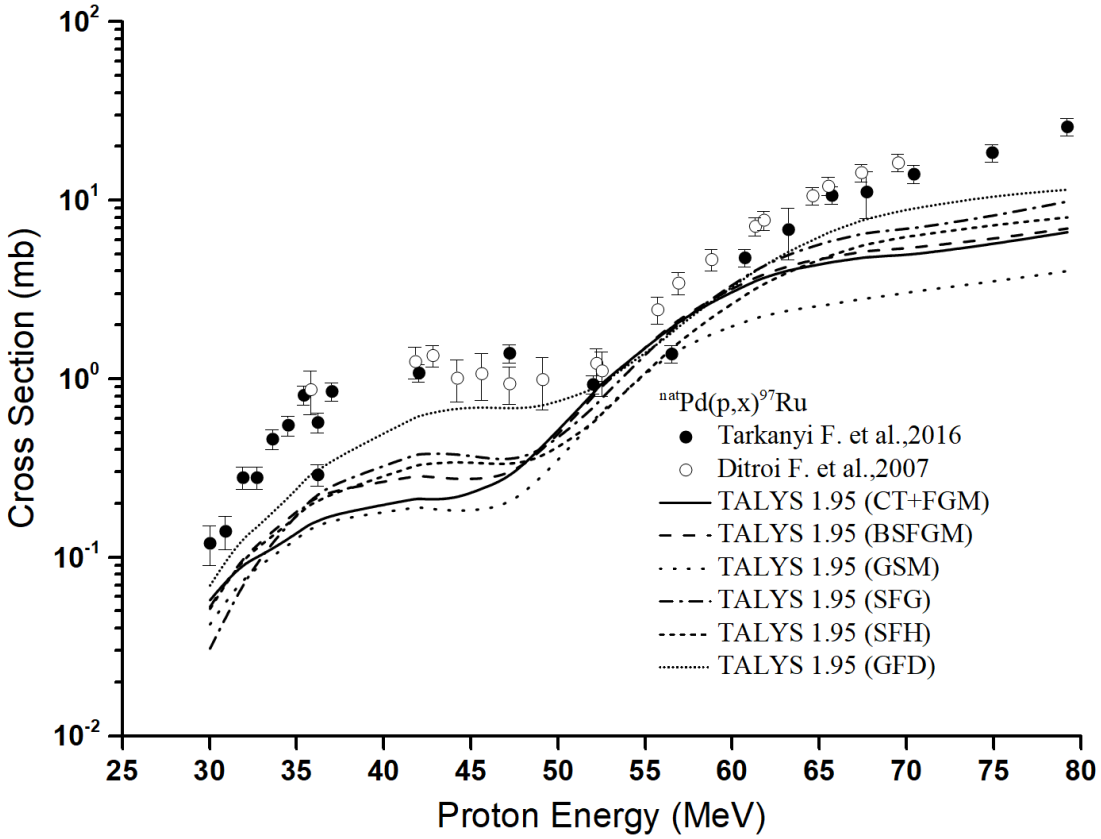

Figure 1. Graphical representation comparing level density model calculations with the Ref [34,35] for the ^{nat}Pd(p,x)^{97}Ru reaction

For the ^{nat}Pd(p,x)^{100}Pd reaction in almost 25-80 MeV proton incident energy range all computation results, and available experimental data [34-37] have been shown together in Figure 2. Among the experimental data given in Figure 2, the data of Tarkanyi et al. [34] are seen as clustered between the energy range of almost 25-40 MeV. Also, it is observable that data taken from both Nguyen et al. [36], and Khandaker et al. [37] are located below the other experimental data in adding to the calculation results. After this energy range, available experimental data of Tarkanyi et al. [34], and Ditrio et al. [35] are shown as in agreement with each other. In all the energy ranges examined for this reaction, all level density model calculations are obtained to show general geometrically compatibility with the experimental values. After 60 MeV energy reaction cross-section data from GSM, GFD, and SFG models are obtained lower than the experimental values.

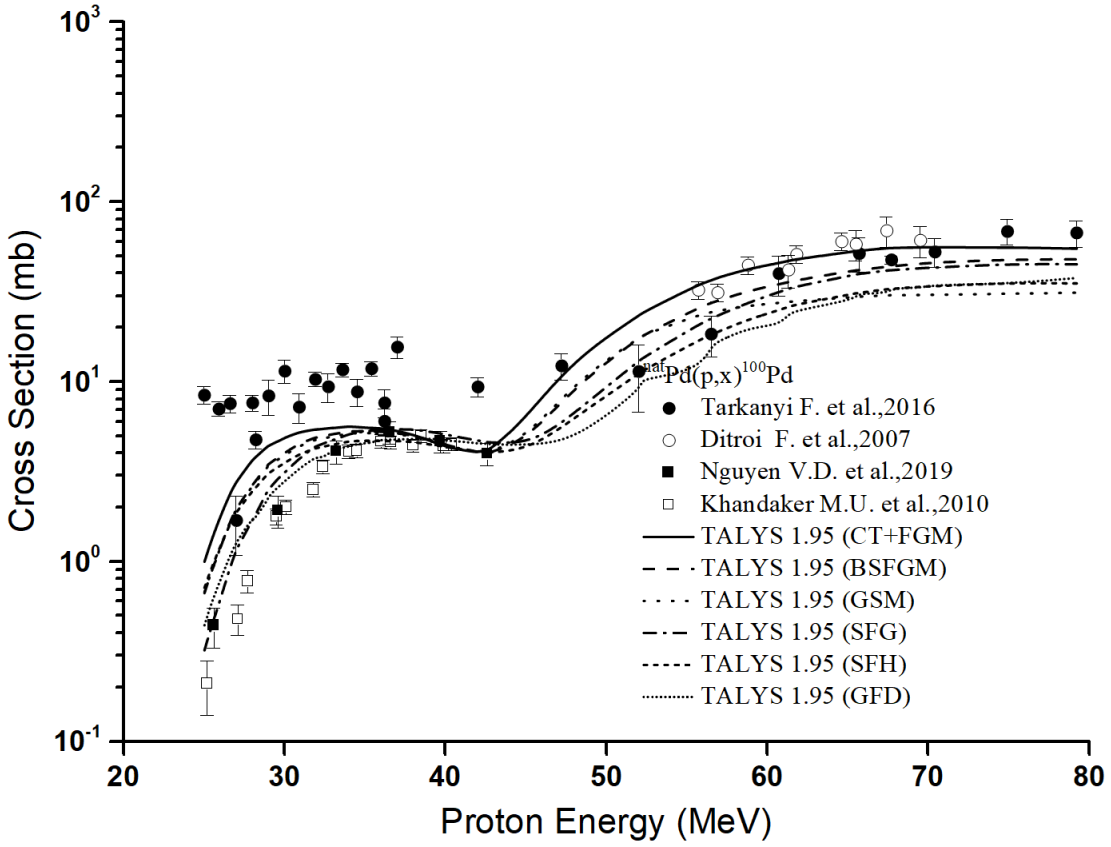

Figure 2. Graphical representation comparing level density model calculations with the Ref [34-37] for the $^{nat}Pd(p,x)^{100}Pd$ reaction

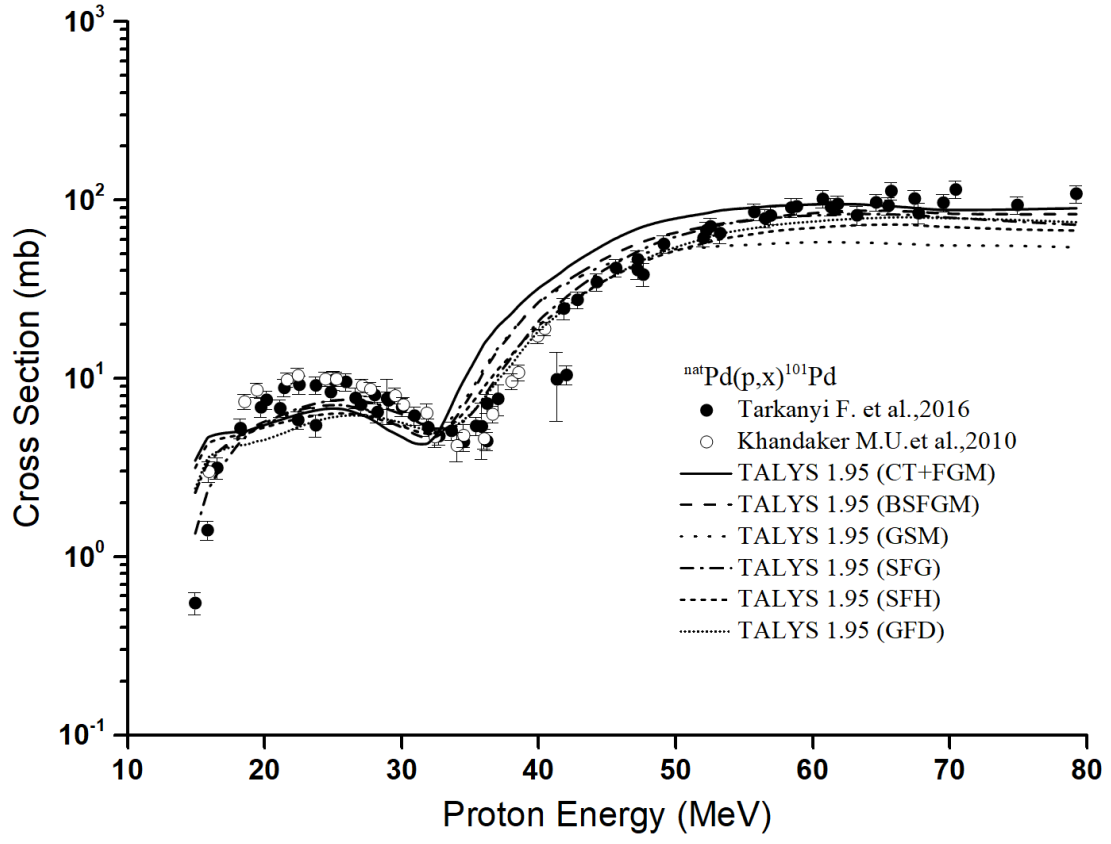

Figure 3. Graphical representation comparing level density model calculations with the Ref [34,37] for the $^{nat}Pd(p,x)^{101}Pd$ reaction

In Figure 3, available experimental data [34,37], and calculation results for $^{nat}Pd(p,x)^{101}Pd$ reaction are plotted together. The representation of the experimental data, and calculation results exhibit a similar geometrical distribution to the $^{nat}Pd(p,x)^{100}Pd$ reaction, which is given in Figure 2. However, for the $^{nat}Pd(p,x)^{101}Pd$ calculation, cross-section results obtained the use of utilizing level density models have been obtained close to each other with respect to the outputs given in Figure 2. On the other hand, if closer attention is given to the energy region greater than 50 MeV, it is seen that the results form GSM are obtained as slightly lower than the experimental values. Apart from all these, after around 35 MeV to around 55 MeV energy region, it is also seen that the results from CT+FGM, and FGM are obtained slightly higher than the experimental values.

$^{nat}Pd(p,x)^{103}Ag$ reaction is one other investigated reaction in this study. The graphical representation comparing level density model calculations with the experimental measurements [34, 37-38] for these reactions are given in Figure 4. Unlike the previously given three reaction results shown in Figures 1-3, outcomes for $^{nat}Pd(p,x)^{103}Ag$ reaction do not exhibit a similar manner to provide an increase in the cross-section data as the energy of the incident particle increases. Even this, in all examined energy ranges for this reaction, all model results, except for GSM, show similar, and compatible distribution with the general trend of the experimental data. In GSM detail, it can be interpreted that, the outcomes via utilizing this model have achieved lower than both the experimental data, and the results of other models.

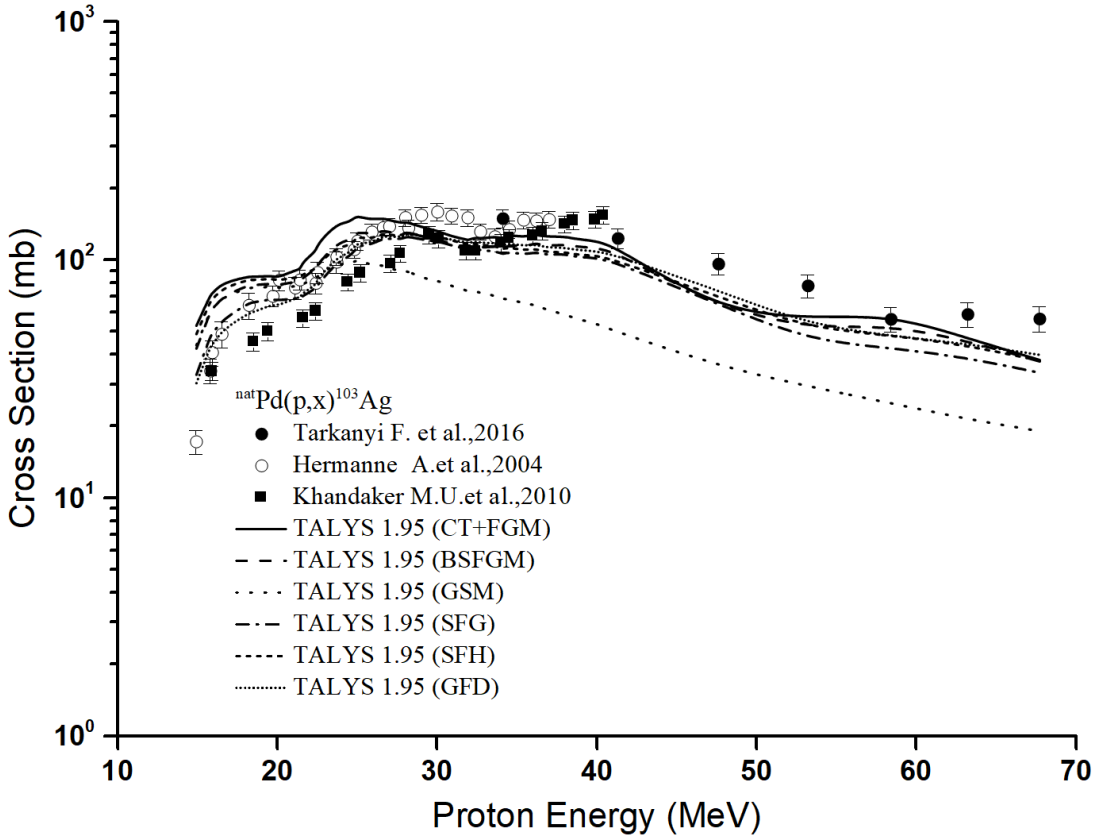

Figure 4. Graphical representation comparing level density model calculations with the Ref [34, 37-38] for the $^{nat}Pd(p,x)^{103}Ag$ reaction

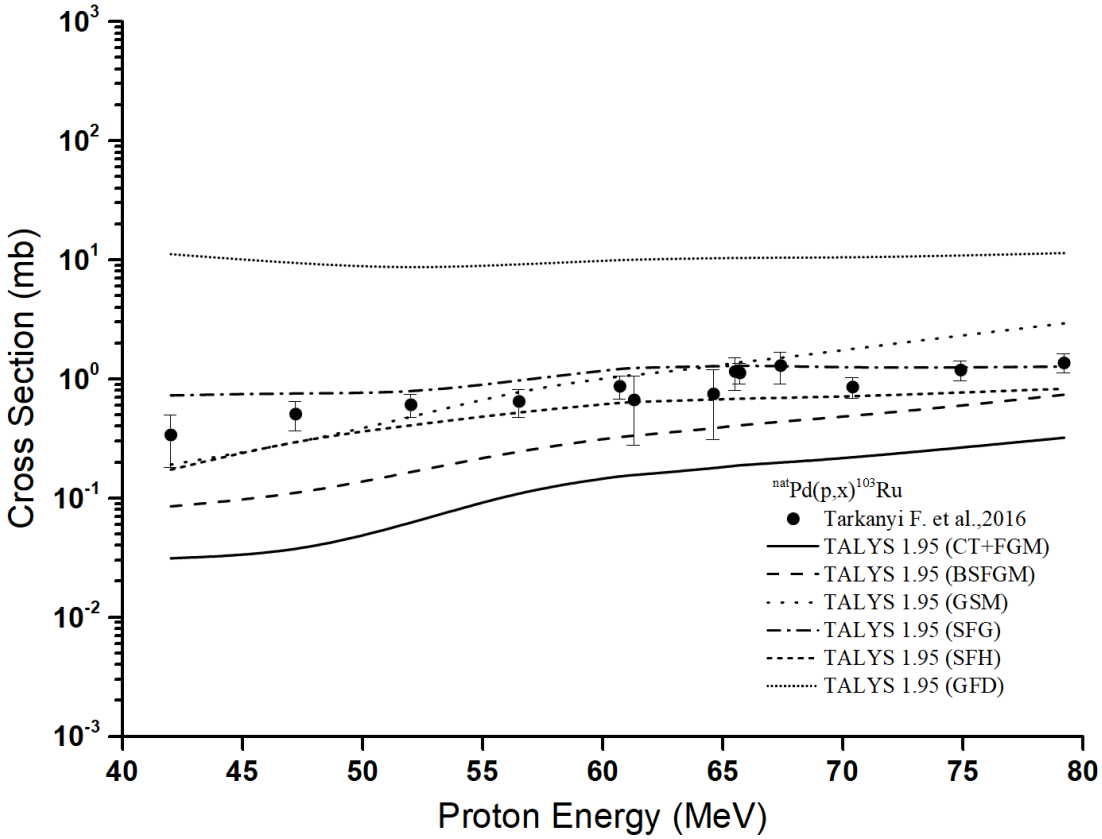

Figure 5. Graphical representation comparing level density model calculations with the Ref [34] for the $^{nat}Pd(p,x)^{103}Ru$ reaction

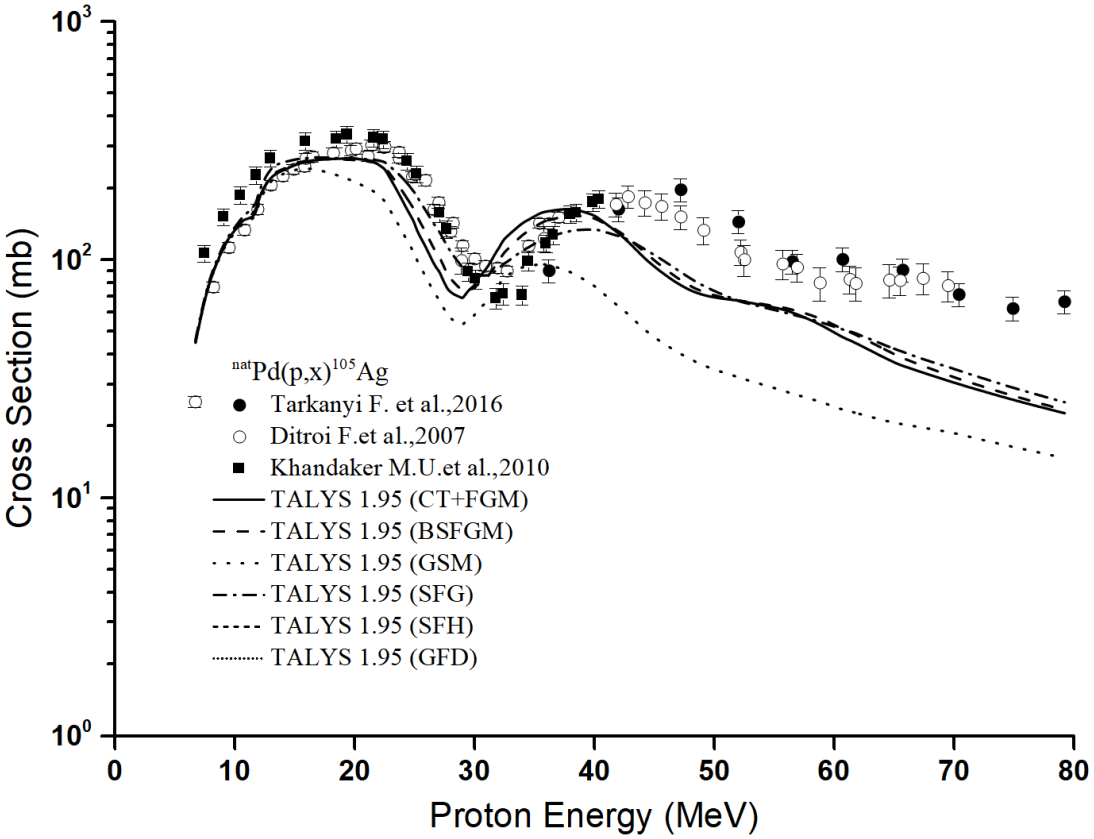

Figure 6. Graphical representation comparing level density model calculations with the Ref [34-35,37] for the $^{nat}Pd(p,x)^{105}Ag$ reaction

For the $^{nat}Pd(p,x)^{103}Pd$ reaction, in which the available experimental data [34] are in the range of almost 40-80 MeV, Figure 5 is given to compare the calculation results, and experimental data. Among all examined reactions in this study, $^{nat}Pd(p,x)^{100}Pd$ reaction is the one where the difference between the model calculation results, in addition to the experimental data, can be seen effortlessly. Between the calculation results obtained, values higher than the experimental data are obtained via utilizing GSM, while values lower than the experimental data are obtained using CT+FGM.

In Figure 6, the cross-section data of the $^{nat}Pd(p,x)^{105}Ag$ reaction in the energy range of almost 5-80 MeV incident proton particle are compared with the experimental data of Tarkanyi et al. [34], Ditrio et al. [35], and Khandaker et al. [37]. When the graphical representation is examined it is seen that all models, except for the GSM, are compatible with the experimental values up to 40 MeV. After 40 MeV, the results obtained with the models are compatible with each other but lower than the experimental values.

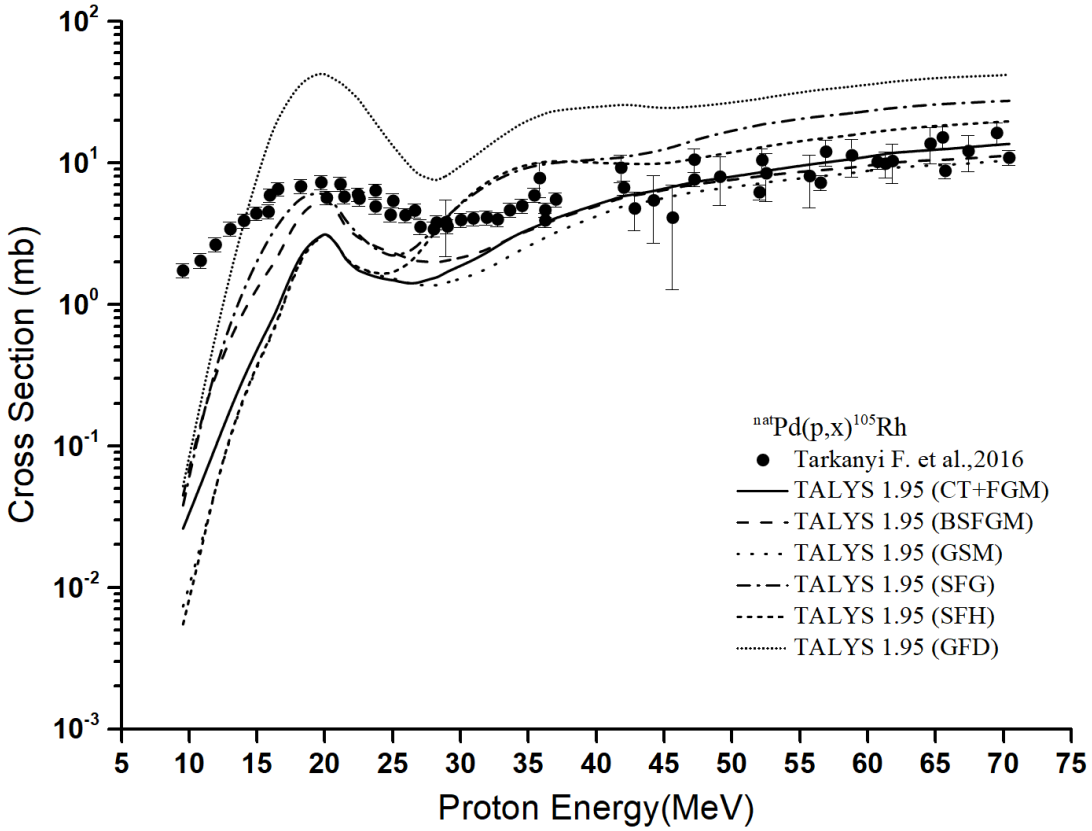

Figure 7. Graphical representation comparing level density model calculations with the Ref [34] for the $^{nat}Pd(p,x)^{105}Rh$ reaction

The comparison of the cross-sectional data for the $^{nat}Pd(p,x)^{105}Rh$ reaction with the experimental data of Tarkanyi et al. [34] are shown in Figure 7. Up to almost18 MeV incident particle energy, it is observed that the models deliver lower calculation results than the experimental data. After almost 40 MeV energy, it is observed that GFD, and SFG models give results that are higher than the experimental data, while the other model results are in agree with the experimental measurements taken for this reaction.

4. Conclusion

In this study, cross-section calculations for $^{nat}Pd(p,x)^{97}Ru$, $^{nat}Pd(p,x)^{100}Pd$, $^{nat}Pd(p,x)^{101}Pd$, $^{nat}Pd(p,x)^{103}Ag$, $^{nat}Pd(p,x)^{103}Ru$, $^{nat}Pd(p,x)^{105}Ag$, and $^{nat}Pd(p,x)^{105}Rh$ reactions have been calculated using macroscopic, and microscopic level density models which are available in the TALYS 1.95 code. Upon the completing of the cross-section calculations, obtained results are compared with the available experimental data taken from the literature, and all output are summarized below.

For some of the investigated reactions in this study, calculation results obtained by using some particular level density models have been given higher values than the experimental measurements while some particular level density models generate lower values than the experimental data. Accordingly, it is possible to interpret the outcomes of all investigated reactions in this study by taking them into account as a whole. The utilization of level density models clearly affects the results of cross-section calculations.

In cases where it may be impossible to perform a desired experimental measurement, obtaining the cross-section values for a specific reaction under specific conditions, and using the desired theoretical parameter set by using confirmed computer-aided calculation tools, like TALYS, which is the one employed in this study, could be more beneficial, and lead researchers to perform further studies concerning the model, and parameter development in addition to the more detailed comprehension of the nature of a nuclear reaction mechanism.

Authorship contribution statement

Ö. Y. TOYKAN CIFTLIKLI: Conceptualization, Methodology, Software, Investigation, Data Curation, Original Draft Writing, Review and Editing, Visualization; A. KAPLAN: Supervision/Observation/Advice

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

There is no acknowledgment.

Ethics Committee Approval and/or Informed Consent Information

As the authors of this study, we declare that we do not have any ethics committee approval and/or informed consent statement.

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