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The Evaluation of Fission Barrier Height by Fission Toy Model Approach

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ABSTRACT

Fission yields are compulsory data on the development of nuclear technology. Therefore, it is necessary to provide complete data. However, the expected experimental data encompass only a tiny fraction of various nuclides; not even all nuclides have fission product data. JENDL and ENDF are databases that have completed the experimental data. These databases were obtained through the process of evaluating experimental data. The evaluation technique used includes the results of theoretical research that has been carried out. Fission Toy Model (FTM) is a fission model proposed to complement the preexisting ones. Each model has advantages and disadvantages. The advantage of the FTM model is that it uses stochastic principle in its calculations.This research aims to obtain a fission barrier through the FTM. The work is related to calculating the fission barrier using the random nature of nucleon position. The calculation technique is basically to take advantage of the random nature of the nucleon position to calculate the Coulomb energy. Then, by calculating several essential points, a data set was obtained that can be used to produce a curve that relates the Coulomb energy to the mass number and the atomic number of a nuclide.The success of this research is indicated by the calculation results that are close to the experimental value compared to other methods.

INTRODUCTION

Fission yield is a part of nuclear data needed to figure out the fission product from a nuclear fission reaction [1]. A theoretical approach is dispensable to obtain complete fission yield data. These methods are semi-empirical [2-4], microscopic [5], or macroscopic [6,7]. In addition to the methodology, there are two types of step to gain the fission yield, namely fission barrier [8] and direct calculation without going through the fission barrier [9]. Although the calculations of fission barrier have long been carried out [10-12], none of them were related to the utilization of the nucleon distribution when the fission process takes place. As an example of a recent study, Khuyagbaatar [13] has succeeded in calculating the fission barrier using semi-empirical predictions. Then, C. Ling [14] used density functional theory, while Z. Chai [15] applied multi-dimensional surface energy to get the triaxial effect on the fission barrier. Those three examples are sufficient to provide evidence that research on the calculation of the fission barrier from these various aspects has not touched the stochastic aspect of the position of nucleons in space.

To observe how far the development of research on fission using stochastic properties began 62 years ago, Whetstone [16] demonstrated the random nature of nuclear fission events. Referring to these results, various fission models that use random numbers appeared. For example, random neck rupture model was introduced by Brosa [17]. This model describes the nuclear rupture process as an arbitrary event. Later in 1965, Ramanna [18] demonstrated fission of nuclei as a Markov process. Ramanna describes the formation of fissionable nuclides as a probability matrix. Brosa and Ramannause random numbers in a macroscopic view of nuclear fission. As for the microscopic,

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it was shown by Marshalek [19] in 1969. F. Minato [20] assigned random properties to the Hamiltonian while the fission barrier still used the usual steps. Bland et al. in 2021 [21] put the stochastic aspect in determining thesurface energy through the random walk principle. This surface energy is then combined with coulomb energy into deformation energy. Finally, in 2021, a dissertation explicitly discussed the application of random walk in fission and fusion processes [22]. From these references, it can be concluded that there is still a gap in applying the random nature of the nucleon position to the calculation of the fission barrier.

Based on these references, there are three rationales for the formation of fission toy model. The first reason is that fission products cannot be determined with certainty but can be approximated with probability. Second, the expected value of the fission product can be developed from the probability value by the number of events that occur. Lastly, the random location of the nucleons causes the termination of the neck to be aimless as well. The position of these nucleons can represent both microscopic and macroscopic views simultaneously.

Fission toy model is a method that includes the distribution of nucleons as a major component in a fission event [23,24]. This model uses random numbers for all physical quantities that are owned by a fission process.

There is an open opportunity for research on nuclear mass fragments, that is replacing the Coulomb interactions between two candidate nuclides [25] with direct interactions between nucleons. The location of the nucleons is determined randomly through a horizontal distribution function.

The advantage of this technique is that the model can produce the peak of the fission barrier curve and can describe the nucleons distribution during fission process simultaneously. The word "toy" is taken from the parable of nucleons as marbles and random numbers as fission generators. A certain random number produces a fission event. In this model, the random number acts as the initiator of a corresponding quantity.

In summary, this work includes generating random numbers for many existing nucleons; then, these numbers were used to determine the position of the nucleons in calculating the Coulomb energy. After obtaining the Coulomb energy, it was proceeded with the calculation of the surface energy. This surface energy was obtained through the surface curve of the shape of the nucleus droplets. The main droplet surface parameter is the parameter related to the droplet neck. This situation happens because the neck-breaking event occurs when the droplet neck shrinks to a specific size. The shrinking of the neck is due to the enlargement of the earlier parameters. One time the evolution of droplet shape is a period of the parameter change from small to large. Because this one evolution is quite time-consuming, to simplify computations, calculations have been carried out for several nuclides and several deformation points. These points were used to perform curve-fitting to obtain a function that relates the Coulomb energy and surface energy to the atomic number and mass number. In the end, a curve will be obtained that corresponds to the deformation energy to the atomic number and mass number of a nuclide. As for the microscopic aspects, it was ignored in this study. Therefore, the shell correction [26] was not included in the calculation of the deformation energy. The consequence of neglecting shell correction is that nuclear interactions were not involved.

Through the explanation above, it can be concluded that this research aims to obtain a new method that can reduce computational time and observe what happens when a fission event takes place. Reduced computational time means speeding up calculations, while knowing in detail what happened means gathering a more complete information to make predictions when another nuclear reaction event occurs.

METHODOLOGY

The methodology was divided into three stages: particle treatment in the fission toy model, droplet selection, and calculation of Coulomb energy.

The first step was to treat the nucleons as particles in the fission toy model. Basically, it is a model that treats nucleons as if they were very hard ball-shaped marbles so that collisions between nucleons do not reduce their kinetic energy. In addition, there is no interaction between these nucleons, and the random nucleon positions follow the given pattern. In addition to applying the fission toy model to the nucleon position, it should also be applied to the shape of the nucleus' surface undergoing fission. However, this was ignored to see the contribution of the fission toy model to the determination of Coulomb energy. As a result, the use of surface evolution only made use of the long-known forms of droplet evolution.

The next step in this calculation began with determining the shape of the droplet. For the droplet shape evolution, the existing evolutionary model was still used, namely using the parameters that were first proposed by Jr Nix and other references [27-31].

The form was then re-expressed in the form of a Legendre polynomial expansion [32]. In this work, improvisation of the nuclear radius has been carried out. The improvisation was done to explicitly place the first term of the polynomial Legendre (n = 0) and limit the expansion to only order n = 2. The limitation was intended so that the nucleus is maintained in a quadrupole condition. Meanwhile, adding n = 0 was done so that the parameterization for quadrupole is more than one. Thus, the nuclear radius is expressed in Eqs. (1-3).

$$R(\theta) = R_0(\sum_{i=0}^{2} \beta_i \cos^i(\theta)) \quad (1)$$

$$\beta_0 = 1 + \frac{a_0}{2}\sqrt{\frac{1}{\pi}} - \frac{a_2}{4}\sqrt{\frac{5}{\pi}}$$

$$\beta_1 = \frac{a_1}{2}\sqrt{\frac{3}{\pi}} \quad (2)$$

$$\beta_2 = \frac{3a_2}{4}\sqrt{\frac{5}{\pi}}$$

$$R_0 = \frac{1}{\eta} 35 A^{1/3} r_0$$

$$\eta = 35\beta_0^3 + 35\beta_0^2\beta_2 + 35\beta_0\beta_1^2 \quad (3)$$

$$21\beta_0\beta_2^2 + 21\beta_1^2\beta_2 + 5\beta_2^3$$

where the above equations are the main equations used to calculate surface energy, E_{surf} in Eq. (4).

$$E_{surf} = \gamma \int 2\pi R(\theta)\sqrt{dz^2 + d\xi^2} \quad (4)$$

where,

$$dz = R_0(-\beta_0 sin(\theta) - \beta_1 sin(2\theta) - 3\beta_2 sin(\theta)cos^2(\theta))d\theta$$

$$d\xi = R_0(\beta_0 cos(\theta) + \beta_1 cos(2\theta) - \beta_2 sin(2\theta)sin(\theta) + \beta_2 cos^3(\theta))d\theta$$

$$\gamma = 0.9517(1 - 1.7826\left(1 - \frac{2Z}{A}\right)^2)MeV fm^{-2}$$

a_0, a_1 and a_2 are all Legendre polynomial expansion coefficients. a_0 and a_1 are parameters that give the shape of a droplet, while a_2 is a parameter that affects the thickness of the neck when fission occurs. Increasing the value of a_2 causes the droplet neck thickness to decrease. If a_1 anda_2 are zero, then the nucleus will be spherical. Through the numerical fitting method, the values ofa_0 and $a_1$were found to be 0.97777 and 0.4886, respectively.

θ is polar angle in spherical coordinate and R_0 is the normalization factor for the nucleus radius. This normalization factor serves as a limiter so that the nucleus density is always constant. The r_0 parameter is the radius parameter which has a value of 1.5 fm. A acts as the mass number of the nucleus which undergoes the fission process.

The last step, after the surface energy was obtained, it is only necessary to calculate the Coulomb energy to obtain deformation energy. Thereby, at the stage of calculating the Coulomb energy, lies the novelty of this research, that is a technique that utilizes the fission toy model especially the stochastic properties of the position of the nucleon space. The distribution of random numbers is shown in Eqs. (5a-5b).

$$\theta = \Gamma_{random}; \; F = F_{random} \quad (5a)$$

$$\begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} (2F-1)R(\theta).cos(\theta) \\ (2F-1)R(\theta).sin(\theta) \\ R(\theta).cos(\theta) \end{bmatrix} \quad (5b)$$

The gamma distribution function generator is symbolized by Γ_{random}, while the flat distribution functions by F_{random}.Through this distribution, we have succeeded in obtaining the distribution of nucleons during the fission process, which is isotropic in the X-Y plane direction and converges on the candidate nuclides at a central mass point to become fission products. This result is the success of this research that previous studies have not already shown.

Based on these coordinates, the value of the Coulomb energy E_{Coul}ws calculated, as shown in Eq. (6).

$$E_{Coul} = \sum_i \sum_{j \neq i} \frac{1}{l_{ij}} \quad (6)$$

with,

$$l_{ij}^2 = (X_i - X_j)^2 + (Y_i - Y_j)^2 + (Z_i - Z_j)^2$$

All the steps outlined above were repeated for the next a_2 value.

To reduce the computing time, the long-time calculation can be solved by curve-fitting from the previous 106 iteration data.

RESULTS AND DISCUSSION

Equations (7-8) are the results of the curve-fitting for Coulomb energy and surface energy respectively.

$$E_C(A,Z,a_2) = (0.0152Z + 0.00555A - 0.6426)a_2^4 - (0.2712Z + 0.1003A - 14.627)a_2^3 + (1.8007Z + 0.67205A - 113.62)a_2^2 - (5.2355Z + 1.96295A - 360.295)a_2 + (16.088Z + 6.035A - 2306.7) \quad (7)$$

.

$$E_S(A,a_2) = (0.038A + 0.4052)a_2^3 - (0.0546A + 6.3325)a_2^2 + (0.2329A + 26.945)a_2 - (1.2996A + 153.95) \quad (8)$$

The two equations above can be said formally as equations that connect between A,Z and a_2, with Coulomb energy and surface energy through fission toy model.

To see the reliability of these two equations, fission toy model was used to perform fission barrier height calculations for nine nuclides. The reason for the selection of the nine nuclides is simply due to the data availability [33].

Fission barrier heights for nine nuclides obtained through experiments and other calculations are compared with this work. In Fig. 1, it is shown that for seven nuclides (Ra, Ac, Th, Pa, U, Np, and Pu), the fission toy model calculations results are still within the range of the experimental results and other model calculations. However, for Am and Cm, there is a significant difference. The results of fission toy model calculations for these nuclides are beyond the range of the other results. The values of fission barrier heights Am and Cm tend to be smaller than the other data.

This lower calculation result is possible due to several factors, such as protons accumulating in the neck area during deformation, skin correction is not involved, and the surface energy being too small. From the first factor, with the tendency of protons to gather in the neck, the Coulomb energy becomes very large; as a result, the deformation energy decreases. Therefore, the Coulomb energy should be corrected for a small distance to overcome decreasing energy problem. Thus, the potential barrier peak value may be higher if the Coulomb energy is corrected lower. In the fission toy model, this correction can be done by changing the proton distribution function; the function is separated from the neutron distribution function. In other words, there need to be a correction of the random number distribution function, which is the coordinates of the proton positions.

After that, a shell correction is needed. This correction is essential considering that the fission toy model considers fission events as a classical system, which is a system that has continuous energy. The last factor is to improve the droplet model. The droplet shape must be changed from the Legendre polynomial to a fourth-order polynomial around the neck. With this fourth-order polynomial, the neck becomes more sloping. According to the fission toy model, the sloping shape will reduce the chances of the nucleons being in the neck.Further analysis is needed to be able to correctly answer the problem of the low peak height of the curves for these two nuclides.

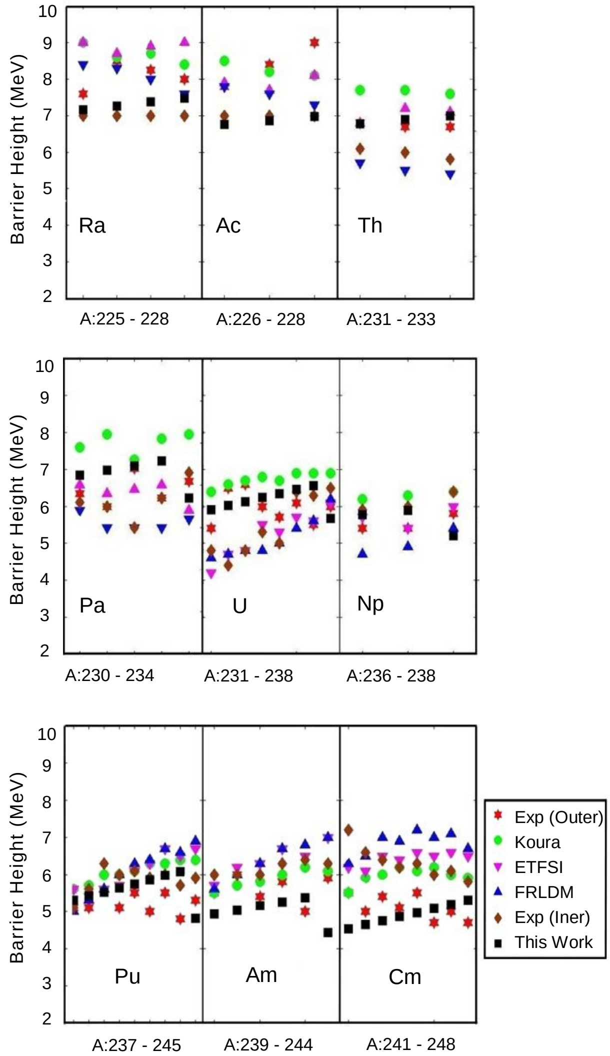

Fig. 1. Fission Barrier height for nine isotopes obtained through experiments and other calculations as a comparison, namely EFTSI [34], FRLDM [35] and Koura.

CONCLUSION

Based on the obtained results and the analysis that has been carried out, two important conclusions can be drawn. First, the fission toy model can be a technique that can generate heights from potential barrier peaks through the application of the stochastic principle to the position of nucleons in the space. Second, although it still looks rough, the fission toy model manages to provide a glimpse of how the nucleons spread during the fission process. This second conclusion can make a significant contribution to the previous models.

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AUTHOR CONTRIBUTION

R. Kurniadi contributed to the design of the calculation model, while the author Z. Suud contributed to the model validation and Y. S. Perkasa was responsible for the computational process. All authors read and approved the final version of the paper.

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