MONTE-CARLO SIMULATION FOR FRAGMENT MASS AND KINETIC ENERGY DISTRIBUTIONS FROM NEUTRON - INDUCED FISSION OF $^{235}$U

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Abstract

The mass and kinetic energy distribution of nuclear fragments after neutron - induced fission of $^{235}$U have been studied using a Monte-Carlo simulation. Besides reproducing the pronounced peak in the standard deviation of the kinetic energy $\sigma_k(m)$ at the fragment mass number around $m = 109$, our simulation also produces a second peak at about $m = 126$. These results are in good agreement with experimental data obtained by Belhafa et al. We conclude that the obtained results are consequence of the characteristics of the fragments’ neutron evaporation and of the sharp variation on the primary mass yield curve.

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Keywords: $^{235}$U, mass yield, neutron emission, Monte - Carlo, energy distribution

Resumen

Mediante la simulación con el método Monte-Carlo se estudia la distribución de masas y sus respectivas energías cinéticas de los fragmentos de fisión nuclear del $^{235}$U inducida por neutrones. Además de reproducir un pico pronunciado en la desviación estándar de la energía cinética $\sigma_k(m)$ en las cercanías de los fragmentos de masa $m = 109$, nuestra simulación también produce un segundo pico alrededor de $m = 126$. Estos resultados se encuentran en buena concordancia con los datos experimentales obtenidos por Belhafa et al. Concluimos que los resultados obtenidos son consecuencia de las características de la evaporación neutónica de los fragmentos y de la variación brusca de la curva de rendimiento de masas primarias.

Palabras claves: $^{235}$U, rendimiento de masas, emisión de neutrones, Monte-Carlo, distribución de energía.

1. Introduction

Since the discovery of the neutron - induced fission of uranium by Hahn and Strassmann in 1938 1, much effort has been made to understand the process involved in it and to measure the relevant fission parameters. Nowadays several aspects of heavy nuclei fission seem to be clarified. Meitner and Frisch suggested a theoretical explanation based on a nuclear liquid-drop model2, and in a recent paper, Pomorsky and Dudek3 have revisited this model and included in it the nuclear surface-curvature terms and their effects. It is known that the de-excitation by fission of heavy nuclei depends on the quantum properties of the saddle point and the associated fission barrier.

The detection of fission isomers have been interpreted by the secondary well in the fission barrier4. The nascent fragments begin to be formed at the saddle point and the system falls down to the fission valley (energetically preferred paths to fission) and end at the scission configuration where fragments interact only by Coulomb force. Moreover, at scission, the fragments have acquired a pre-scission kinetic energy. Over the fission valley, the system could be described by collective variables (deformation, vibration, rotation, etc.) and intrinsic variables (quasi-particles excitations). Nevertheless, the dynamics of the fission process are not yet completely understood. In particular, it is neither known the nature of the coupling between the collective and intrinsic degrees of freedom during the

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descend from the saddle to scission, nor known how it does arise.

In the low-energy fission, several final fragment characteristics can be explained in terms of a static scission model of two coaxial juxtaposed deformed spheroidal fragments, provided shell effects, affecting the deformation energy of the fragments. These shell effects corrections, determined by Strutinsky prescription and discussed by Dickmann et al. and by Wilkins, subsequently generate secondary minima in the total potential energy surface of fragments having some particular neutron or proton shell configurations. If the final fragment characteristics were governed by the properties of the fragments themselves, a basic argument in any statistical theory, one would expect an increase in the width of the kinetic energy distribution curve for fragment masses, $A$, having the above mentioned special neutron or proton shell arrangements.

In order to answer this question, the fission parameters of the primary fragments (pre-neutron emission) that have been the most studied are the mass yield distribution, $Y(A)$, and the kinetic energy distribution, $E(A)$. Nevertheless, measurement can only be carried out only on the final fragments (post neutron emission) mass yield distribution, $Y(m)$, and the final kinetic energy distribution, $e(m)$. Therefore it is crucial to find out what is the relation between the final kinetic energy distribution $e(m)$ and the initial one, $E(A)$, as well as the relation between the $Y(A)$ and $Y(m)$ distributions.

For neutron-induced fission of $^{235}$U, the $e(m)$ distribution was measured by Brissoit et al. This distribution was represented by the mean value of the kinetic energy $e$ and the standard deviation (SD) of kinetic energy $\sigma_e$ as function of the final mass $m$.

As seen in Fig. 1, the plot of both the measured $\sigma_e$ and the Monte-Carlo simulation of $\sigma_e$ from a primary distribution $E(A)$ without peaks, shows the one pronounced of peak at $m = 109$. This Monte Carlo simulation result suggests that the peak does not exists on the $\sigma_e$ of the primary fragment kinetic energy expressed as a function of the primary fragment mass.

In a latter experiment, Belhafaif et al. repeated the experiment of Brissoit et al. for neutron induced fission of $^{235}$U, obtaining a second peak around $m = 126$ (see Fig. 2). A Monte-Carlo simulation made by these authors, from a distribution $E(A)$ without a peak, reproduced the experimental peak on $\sigma_e$ at $m = 109$, but failed to reproduce the peak at $m = 126$. They suggested that this peak must exist in the primary fragment kinetic energy distribution $E(A)$, and accordingly they fitted their experimental data from a distribution with a peak at $m = 126$.

Fig. 1. Experimental (full circles) and simulated by Monte-Carlo (open circles) standard deviation of final fragment kinetic energy as function of the final mass.

In this paper, we present new Monte-Carlo simulation results for low energy fission of $^{235}$U. We compute both the mass and kinetic energy distributions of the primary and final fission fragments, and show that the peaks on the $\sigma_e$ curve at the final fragment masses at $m = 109$ and at $m = 126$ can be reproduced without assuming an adhoc initial structure on $E(A)$.

Fig. 2. Experimental (full circles) and simulated by Monte-Carlo (open circles) standard deviation of final fragment kinetic energy as a function of the final mass.

2. Monte-Carlo Simulation Model

In what follows, we shall assume that the total kinetic energy distribution of the fission fragments can be approximated by a Gaussian distribution

$$P(E_T) = \frac{1}{\sqrt{2\pi}\sigma_{ET}} \exp \left[ -\frac{(E_T - \bar{E}_T)^2}{2\sigma_{ET}^2} \right]$$

with mean $\bar{E}_T$ and standard deviation $\sigma_{ET}$. 

Moreover, we shall denote by $E(A)$ and $\sigma_k(A)$ the mean and standard deviation, respectively, of the initial kinetic energy distribution expressed as functions of the primary fragment mass $A$; and, by $\bar{N}(A)$ the average number of neutrons emitted by the fragments, also expressed as function of the fragment mass $A$.

The total number of emitted neutrons will be a function of the excitation energy $U$.

$$U = Q - E_f,$$  \hspace{1cm} (2)

where $Q$ is the available energy for fission and $E_f$ is the initial total fragments kinetic energy.

In order to simulate the mass and kinetic energy distribution of the fragments for each fission event, the kinetic energy $E(A)$ is chosen randomly from a Gaussian distribution with mean value $\bar{E}(A)$ and standard deviation $\sigma_k(A)$.

If we consider that the neutron emission by the fragments takes place according to the expression,

$$n(A) = \left[\frac{E(A) - \bar{E}(A)}{3\sigma_k(A)}\right]$$ \hspace{1cm} (3)

with the square bracket meaning the integer part of the argument, then the final mass $m$ of the fragment will be just,

$$m = A - n(A)$$ \hspace{1cm} (4)

Furthermore, assuming that the fragment loose energy only by neutron evaporation and not by gamma radiation or any other processes, and neglecting the recoil effect due to neutron emission, then the kinetic energy $e(m)$ of the final fragment will be given by

$$e(m) = \left(1 - \frac{n(A)}{A}\right)E(A)$$ \hspace{1cm} (5)

On the other hand, to obtain an acceptable statistic during the simulation, we have considered a total number of fission events of $10^8$ of the order of $10^8$. At the same time, we have used the Box-Muller method to generate the random numbers with the required normal distribution, and have computed the standard deviation of all the relevant quantities by means of the following expression which for $e(m)$, say, read as

$$\sigma_e^2(m) = \frac{1}{N_f(m)} \sum_{i=1}^{N_f(m)} e_i^2(m) - (e(m))^2$$ \hspace{1cm} (6)

where $\langle e(m) \rangle$ is the mean value of the kinetic energy of the final fragments with a given mass $m$, and $N_f(m)$ is the number of fission events corresponding to that mass.

3. Results of Simulation and Discussion

The simulated final mass yield curve $\gamma(m)$ and the primary mass yield curve $\gamma(A)$ are illustrated in Fig. 3. As expected, the $\gamma(m)$ curve is shifted from $\gamma(A)$ towards smaller fragment mass due to neutron emission.

As stated in sect. 2, the primary kinetic energy $E(A)$ is generated from a Gaussian distribution while the final kinetic energy distribution $e(m)$, is generated through Eq. (5). The plots of the simulated mean kinetic energy for the primary and final fragments are shown in Fig. 4 as function of their corresponding masses. For the symmetrical fission fragments ($A = 118$) the kinetic energy presents a minimum of approximately 81 MeV.

Furthermore, Fig. 5 displays the standard deviation $\sigma_k(A)$ of the kinetic energy of the primary fragments and the standard deviation $\sigma_e(m)$ of the kinetic energy of the final fragments as function of their corresponding masses. The plots of $\sigma_k(A)$ reveals the presence of two peaks: one pronounced peak at $m=109$ and the other small at around $m=126$. In contrast, the simulation of the primary fragment kinetic energy distribution (see Fig. 5, open circles), shows no peaks in the range of fragment mass $A$ from 80 to 150.

We now compare our simulated results for $\sigma_e(m)$ with the corresponding experimental data of Belhasaf et al. The comparison is shown in Fig. 6.
Fig. 4. Average kinetic energy of initial (o) and final (▲) fragments for neutron induced fission of $^{235}$U.

Fig. 5. Simulation results of the standard deviation of kinetic energy for final (▲) and primary (o) fragment mass for neutron induced fission of $^{235}$U.

Like the experimental data, the Monte Carlo results also exhibit two well defined peaks: one large, which corresponds well in location, height and full width at half maximum (FWHM) with the larger of the two experimental peaks; and one small, which is rather smaller and narrower than the smaller of the experimental peaks, and which is also slightly shifted from the latter by approximately 1 unit mass towards heavier nuclei.

The initial total kinetic energy distribution used and the simulated primary fragments kinetic energy (see Fig. 4) have no peaks. Thus, the behavior of the standard deviation of the final kinetic energy distribution is could not be caused by the structure on the primary kinetic energy distribution. Rather, the presence of the peaks could be associated with neutron emission characteristics. To see this more clearly, we plot in Fig. 7 the average number of neutrons emitted by the fragments both as a function of the primary fragment mass $A$ and as a function of the final fragment mass $m$. One can see that neutron emission has produced on $\mu(m)$ a valley at $m = 105$ and a small peak at $m = 127$ which were not present in the $\sigma(A)$.

Fig. 6 Standard deviation of fragment kinetic energy distribution as function of the fragment mass: (▲) - present MC results, (o) experimental data.

Fig. 7. The average number of emitted neutrons from neutron induced fission of $^{235}$U: (o) as function of primary fragment mass $m$, (▲) as function of final fragment mass $A$.

3.1 Interpretation of the Neutron Emission Effects on the Final Mass and Kinetic Energy Distributions

In our Monte Carlo simulation of an experiment at low energy fission, we have assumed that no fragment recoil occurs as a result of neutron emission; and that in consequence fragments can only loose kinetic energy through loosing mass.

For light fragments the shift of kinetic energy is significant, because the width of the final fragment
kinetic energy distribution may be enlarged by approximately 1 MeV. To understand this effect better, let us assume that in the neighborhood of \( A = 100 \) the average \( \bar{E} \) is 100 MeV and the standard deviation \( \sigma_E \) is 6 MeV. Let us also assume that the fragments with kinetic energy higher than \( \bar{E} \) (\( E > 100 \) MeV) emit no neutrons, and the fragments with energy less than \( \bar{E} \) (\( E < 100 \) MeV) emit just 1 neutron. If the mass yield and \( \bar{E} \) curves are flat, then, for each value of \( m \), half of the fragments will correspond to \( A = m + 1 \), and the width of the final kinetic energy distribution will be approximately 1 MeV larger than that of the primary fragment kinetic energy distribution (\( E(A) \)).

The standard deviation of the kinetic energy distribution is very dependent of the mass yield curve. In the above case, if there is a sharp increase in the mass yield on going from \( m \) to \( m \pm 1 \), the standard deviation of the distribution at \( m \) will be reduced approximately by half. For \( m = 100 \), only the higher half of the primary kinetic energy distribution (\( E > 100 \) MeV) will be taken into account because for this half there is no neutron emission. If the mass yield curve continues to increase, the standard deviation will be also depleted. When the \( Y \) curve flattens again, the \( \sigma_E \) will again become similar to \( \sigma_E \) around the inflection point of the mass yield. If the \( Y \) curve falls down as \( A \) diminishes, \( \sigma_E \) will drop again leaving a peak on this curve.

4. Conclusion

Using a simple model for the neutron emission by fragments, we have carried out a Monte-Carlo simulation for the mass and kinetic energy distribution of fission fragments. The final fission fragments (i.e. after the emission of neutrons) have eroded kinetic energy and mass values in comparison with initial fragments (i.e. before neutron emission). This fact together with the sharp variations observed in the yield curve of the primary fragment masses, give rise to the appearance of peaks in the standard deviation of the kinetic energy of the final fragments \( \sigma_E(m) \) when the latter is plotted as function of the final fragment mass \( m \). In the case of neutron-induced fission of \(^{235}\text{U}\), the peaks in the \( \sigma_E \) curve at \( m = 109 \) and \( m = 126 \) arise as a result of the neutron emission by fission fragments.

Since experimental investigations do not provide any information on the initial energy distribution of single fission fragments and due to crucial effect of neutron emission on final fragments mass and kinetic energy distribution, Monte-Carlo simulation is useful in order to relate primary and final fragments distributions.

References