Monte Carlo Simulation to relate primary and final fragments mass and kinetic energy distribution from low energy fission of ^{234}U

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Resumen

La distribución de la energía cinética como función de la masa de los fragmentos finales (m) de la fisión a baja energía del ^{234}U, medida por Belhafaf *et al*. con el espectrómetro Lohengrin, presenta un pico alrededor de $m = 109$ y otro alrededor de $m = 122$. Los autores atribuyen el primer pico a la evaporación de un gran número de neutrones alrededor del correspondiente número de masa; y el segundo pico a la distribución de la energía cinética de los fragmentos primarios. Sin embargo, un cálculo teórico relacionado a la distribución primaria hecho por H.R Faust y Z. Bao no presenta un pico alrededor de $m = 122$. Para esclarecer la aparente controversia, hemos realizado un experimento numérico en la cual las masas y las energías cinéticas de los fragmentos son calculadas asumiendo una distribución inicial de energía cinética sin picos en la desviación estándar como función de la masa de los fragmentos. Como resultado hemos obtenido un pico en la distribución estándar alrededor de $m = 109$, y una deflexión de $m = 121$ a $m = 129$, y un pequeño pico alrededor de $m = 122$, el cual no es tan grande como el medido por Belhafaf *et al.* Nuestra simulación también reproduce el resultado experimental en el rendimiento de masas finales, el número promedio de neutrones emitidos como función de la masa provisional (calculada a partir de de los valores de la energía cinética y los fragmentos complementarios finales) y el valor promedio de la energía cinética como función de la masa final.

Abstract

The kinetic energy distribution as a function of mass of final fragments (m) from low energy fission of ^{234}U, measured with the Lohengrin spectrometer by Belhafaf *et al.*, presents a peak around $m = 109$ and another around $m = 122$. The authors attribute the first peak to the evaporation of a large number of neutrons around the corresponding mass number; and the second peak to the distribution of the primary fragment kinetic energy. Nevertheless, the theoretical calculations related to primary distribution made by Faust *et al.* do not result in a peak around $m = 122$. In order to clarify this apparent controversy, we have made a numerical experiment in which the masses and the kinetic energy of final fragments are calculated, assuming an initial distribution of the kinetic energy without peaks on the standard deviation as function of fragment mass. As a result we obtain a pronounced peak on the standard deviation of the kinetic energy distribution around $m = 109$, a depletion from $m = 121$ to $m = 129$, and an small peak around $m = 122$, which is not as big as the measured by Belhafaf *et al.* Our simulation also reproduces the experimental results on the yield of the final mass, the average number of emitted neutrons as a function of the provisional mass (calculated from the values of the final kinetic energy of the complementary fragments) and the average value of fragment kinetic energy as a function of the final mass.

1. Introduction

One of the most studied quantities to understand the fission process is the fission fragment mass and kinetic energy distribution, which is very closely related to the topological features in the multi-dimensional potential energy surface of the fissioning system [1]. Structures on the distribution of mass and kinetic energy may be interpreted by shell effects on that potential energy, determined by the Strutinsky prescription and discussed by Dickmann *et al.* [2] and Wilkins *et al.* [3].

In order to investigate the dynamics of the fission process, the distribution of final fragment kinetic energy (e) as a function of final fragment mass (m), from thermal neutron induced fission of ^{233}U, was measured by Belhafaf *et al.* [4], using the Lohengrin spectrometer. This distribution

was represented by the mean value of kinetic energy (e) and the standard deviation (SD) σ_e as function of m. The results present a first peak on σ_e (m) around m = 109 and a second one around m = 122, see Fig. 1.

The authors attribute the first peak to a large number of evaporated neutrons (ν) around the corresponding primary mass (A). Based on the small number of emitted neutron measured around A = 122, the second peak is attributed to the distribution of the primary fragment kinetic energy (E). However, theoretical calculations made by Faust *et al.* [5] do not result in a peak in SD for the distribution of primary fragment kinetic energy σ_E around A = 122.

In order to clarify this apparent controversy, it is crucial to find the relation between the primary and the final kinetic energy distributions; the relation between the primary Y (A) and the final mass yield Y (m); as well as the relation between the average value of the number of emitted neutron $v = \bar{v}$ as a function of the primary fragment mass and the values corresponding to the experimental results. To address this question we present Monte-Carlo simulation results for thermal neutron induced fission of ^{233} U, i.e. low energy fission of ^{234} U.

2. Monte Carlo simulation model

2.1 Fragment kinetic energy and neutron multiplicity

In the process of thermal neutron induced fission of ^{233} U, the excited composed nucleus ^{234} U* is formed first. Then, this nucleus splits in two complementary primary fragments having A_1 and A_2 as mass numbers, and E_1 and E_2 as kinetic energies, respectively. Using relations based on momentum and energy conservation, the total kinetic energy of complementary fragments is,

$$TKE = E_1 + E_2 = \frac{A_1 + A_2}{A_1} E_2 \qquad (1)$$

The total excitation energy is given by

$$TXE = Q + \varepsilon_n - TKE \qquad (2)$$

where Q is the difference between fissioning nucleus mass and the sum of two complementary fragments masses, and ε_n is the separation neutron energy of ^{234} U.
From Eq. (1) and (2), taking into account that $A_1 + A_2 = 234$, results

$$TXE = Q + \varepsilon_n - \frac{234}{234 - A} E \qquad (3)$$

where A and E are the primary mass number and kinetic energy, respectively, of one of the two complementary fragments. It is reasonable to assume that the excitation energy of one complementary fragment (E^*) is proportional to the total excitation energy, thus,

$$E^* \propto TXE = Q + \varepsilon_n - \frac{234}{234 - A} E \qquad (4)$$

It is also reasonable to assume that the number (ν) of neutrons emitted by a fragment is proportional to its excitation energy, i.e.

$$\nu \propto E^* \qquad (5)$$

From relations (4) and (5) we obtain a linear relation between ν and E:

$$\nu = a + b \; E \qquad (6)$$

Taking into account that there is no neutron emission (ν = 0) for fragments having the maximal kinetic energy ($E = E_{max}$) and assuming that $\bar{v} = v$ for the average value of fragment kinetic energy, the relation (6) results:

$$\nu = \bar{v}\left(\frac{E_{max} - E}{E_{max} - \overline{E}}\right) \qquad (7)$$

Let the parameter β define the maximal value of kinetic energy by the relation

$$E_{max} = \overline{E} + \frac{\sigma_E}{\beta} \qquad (8)$$

Then, the relation (7) may be expressed as

$$\nu = \bar{v}\left(1 - \beta\left(\frac{E - \overline{E}}{\sigma_E}\right)\right). \qquad (9)$$

Because the neutron number N is an integer, it will be defined as the integer part of (9),

$$N = Integer\ part\ of\ (\alpha + \overline{v}(1 - \beta(\frac{E - \overline{E}}{\sigma_E})))\quad(10)$$

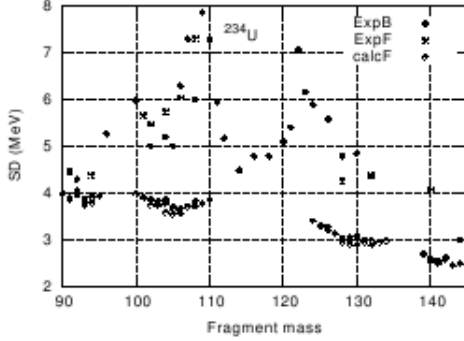where α is used to compensate the effect of the change from a real number ν to an integer number N.

Figure 1: SD of the final fragment kinetic energy distribution as a function of the final mass *m* as measured by Belhafaf *et al*. [4](•), and Faust *et al*. [5] (*), respectively; and SD as a function of primary mass (⊗) as calculated by Faust *et al*. [5]

2.2 Simulation process

In our Monte Carlo simulation the input quantities are the primary fragment yield (Y), the average kinetic energy ($\overline{E}$), the SD of the kinetic energy distribution (σ_E) and the average number of emitted neutron ($\overline{V}$) as a function of primary fragment mass (*A*). The output of the simulation for the final fragments are the yield (*Y*), the SD of the kinetic energy distribution (σ_e) and the average number of emitted neutron ($\overline{V}$) as a function of final fragment mass *m*.

For the first simulation, we take *Y* and $\overline{E}$ from Ref. [4]. The first SD σ_E curve is an extrapolation of calculation results obtained by Faust *et al*. [5]. Then, we adjust *Y*(*A*), *v*(*A*), $\overline{E}(A)$ and σ_E (*A*) in order to get *Y*(*m*), *v*(*m*), e(*m*), σ_e(*m*) in agreement to experimental data.

In the simulation, for each primary mass *A*, the kinetic energy of the fission fragments is chosen randomly from a Gaussian distribution.

$$P(E) = \frac{1}{\sqrt{2\pi}\sigma_E}\exp\left[\frac{-(E - \overline{E})^2}{2\sigma_E^2}\right]\quad(11)$$

where *P*(*E*) is the probability density of energy with mean value $\overline{E}$ and SD σ_E.

For each *E* value, the simulated number of neutrons N is calculated with the relation (10). The final mass of the fragment will be, *m* = *A* − N. Furthermore, assuming that the fragments loose kinetic energy only by neutron evaporation and not by gamma emission or any other process, and neglecting the recoil effect due to neutron emission, the kinetic energy e(*m*) of the final fragment will be given by,
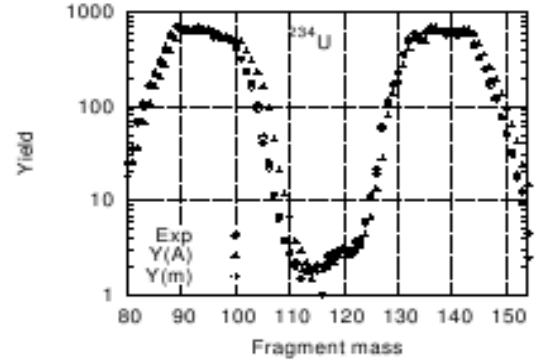
$$e(m) = \left(1 - \frac{N}{A}\right)E\quad(12)$$

Figure 2: Simulation results for the primary (Δ) and final (⊗) mass yields are presented together with experimental data (•), taken from Ref. [4]

With the ensemble of values corresponding to *m*, e and N, we calculate *Y*(*m*), $e\ m$, σ_e(*m*) and *v*(*m*).

To obtain an acceptable statistics during the simulation, we have considered a total number of fission events of ^{234}U of the order of 10^8, and we have computed the SD of all the relevant quantities by means of the following expression:

$$\sigma^2(m) = \frac{\sum_{j=1}^{N_j(m)} e_j^2(m)}{N_j(m)} - \overline{e}^2(m)\quad(13)$$

where $\overline{e}(m)$ is the mean value of the kinetic energy of final fragments with a given mass *m*, and $N_j(m)$ is the number of fission events corresponding to that mass.

3. Results and interpretation

The simulated final mass yield curve Y(*m*) and the primary one Y(*A*) are illustrated in Fig. 2. As expected due to neutron emission, the Y(*m*) curve is shifted from Y(*A*) towards smaller fragment masses.
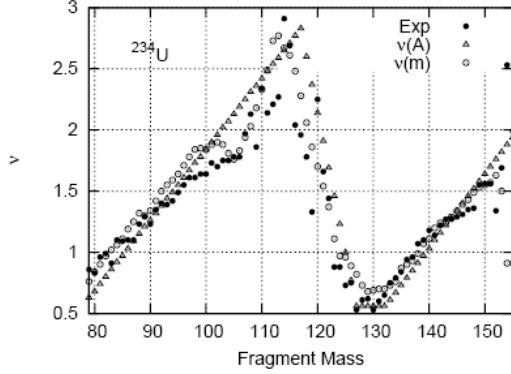

Figure 3: The average number of emitted neutrons from fission of ^{234}U: as a function of the primary fragment mass A(Δ), as function of finalfragment mass ($\otimes$) both as result of simulation and experimental data ($\bullet$), taken Ref. [6].
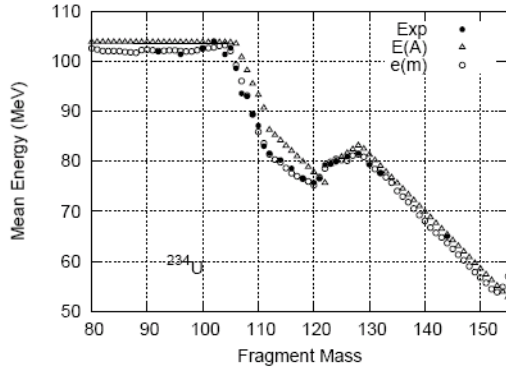

Figure 4: Mean kinetic energy of the primary fragments (Δ) and mean kinetic of the final fragment ($\otimes$), as a result of simulation in this work, to be compared to experimental data ($\bullet$ and *) as measured by Belhafaf *et al*. [4] and Faust et al. [5], respectively.

The simulated average number of emitted neutron $\overline{\nu}(m)$ curve is shifted from $\overline{\nu}(A)$ in a similar way as Y(*m*) relative to Y(A)(see Fig. 3). As stated in sect. II, the primary kinetic energy E(*A*) is generated from a gaussian distribution, while the final kinetic energy e(*m*) is calculated through Eq. (12).

The Plots of the simulated mean kinetic energy for the primary and final fragments as

function of their corresponding masses are shown in Fig. 4. In general, the simulated average final kinetic energy curve as a function of final mass $\overline{e}(m)$ have roughly a shift similar to that of Y(*m*) curve, and a diminishing given by relation (12) with $N = \overline{\nu}$.

Furthermore, Fig. 5 displays the standard deviation of the kinetic energy distribution of the primary fragments and the SD of the kinetic energy of the final fragments $\sigma_e(m)$. The simulated initial distribution of the kinetic energy have not structures on the SD. The plots of $\sigma_e(m)$ reveal the presence of a pronounced peak around *m* = 109 in agreement with the experimental results obtained by Belhafaf *et al.*[4], and Faust *et al.* [5], respectively. The peak on the SD around *m* = 122 resulting from simulation is not as big as the obtained by Belhafaf. Moreover a depletion on the SD in the mass region from *m* = 121 to *m* = 129 is obtained as a result of simulation. These results were obtained with a simulated primary fragment kinetic energy distribution (see Fig. 5, Δ) without peaks in the range of fragment masses *A* from 90 to 145. If one simulates an additional source of energy dispersion in σ_E, without any peak, no peak will be observed on σ_e.
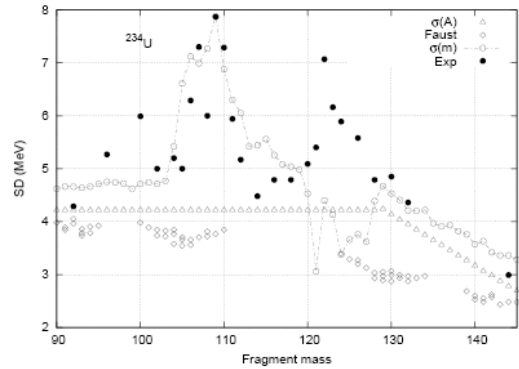

Figure 5: SD of primary fragments kinetic energy distribution (Δ), as simulated in this work, to be compared to results of calculations ($\Diamond$) made by Faust et al. [5]; and SD of final fragment kinetic energy distribution ($\otimes$) to be compared to experimental data ($\bullet$ and *) as measured by Belhafaf *et al.* [4] and Faust et al. [5].

Both the shape and height of the peaks of $\sigma_e(m)$ are sensitive to the value of parameter α and β appearing in Eq. (10). The effect of β on peak depends much on mass region. For the region $m = 109$, a higher value of β will produce a larger peak of σ_e.
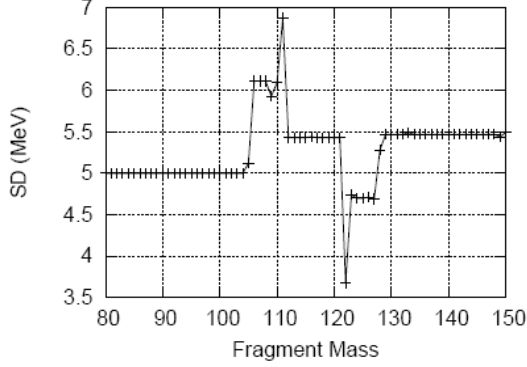

Figure 6: SD of final fragments kinetic energy distribution calculated assuming that i) Y(A) is constant, ii) $\sigma_E(A)$ is constant, iii) fragments with $E > \overline{E}$ do not emit neutrons and fragments with $E < \overline{E}$ emit one neutron and iv) neutron emission have no recoil effect on fragment kinetic energy. $\overline{E}(A)$ values are taken from data.
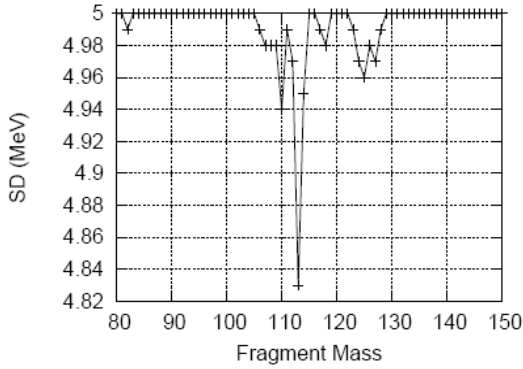

Figure 7: SD of final fragments kinetic energy distribution calculated under the assumption that i) $\sigma_E(A) = 5Mev$, ii) $\overline{E}(m+1) = \overline{E}(m)$ and iii) neutron emission have no recoil effect on fragment kinetic energy. Y (A) values are taken from data.

The simulated results for $\sigma_e(m)$ presented in Fig. 5 were obtained with $\alpha = 0.62$ y $\beta = 0.35$. The presence of peaks about $m = 109$ could be associated with neutron emission characteristics (approximately $\overline{v} = 2$) and a very sharp fall kinetic energy from E = 96 Mev to E = 90 Mev,

corresponding to A = 109 and A = 111, respectively. A similar result was obtained for low energy fission of ^{236}U in [7].

In order to interpret easily the influence of variation of $\overline{E}(A)$ on $\sigma_e(m)$, we derive an analytical relation assuming that: i) Y(A) is constant, ii) $\sigma_E(m)$ is constant and iii) fragments with $E > \overline{E}$ do not emit neutrons and fragments with $E < \overline{E}$ emit one neutron. Then for each final mass there is a contribution from fragments with primary mass m that do not emit any neutron and from fragments with primary mass m + 1 that emit one neutron. With these conditions we can show that,

$$\sigma_e(m) = \left[\sigma_E^2 - \sqrt{\frac{2}{\pi}} \sigma_E \Delta E + \left(\frac{\Delta E}{2} \right)^2 \right]^{\frac{1}{2}}$$
(14)

where $\Delta \overline{E} = \overline{E}(m+1) - \overline{E}(m)$

The equation (14) corresponds to a parabola with a minimum value

$$\sigma_{e_{min}} = \sqrt{1 - \frac{2}{\pi}} \sigma_E = 0.6\sigma_E$$
(15)

which occurs when

$$\Delta \overline{E} = 2\sqrt{\frac{2}{\pi}} \sigma_E = 1.6\sigma_E$$
(16)

As we can see on Fig. 6, the $\sigma_e(m)$ curve, calculated with relation (14), presents a peak around $m = 109$ in agreement with the experimental data. In that region $\Delta\overline{E} < 0$, then from relation (14) $\sigma_e(m) > \sigma_E(A)$. The depletion on the simulated $\sigma_e(m)$ on the mass region between $m = 121$ and $m = 129$ is explained by the fact that $\Delta\overline{E} > 0$. Using the relation (14), we obtain that $\sigma_e(m) < \sigma_E(A)$.

In order to more easily evaluate the influence of variation of Y on $\sigma_e(m)$, we derive an analytical relation assuming that (i) $Y(m+1) = rY(m)$, (ii) $\sigma_E(A)$ constant, (iii) $\overline{E}(m+1) = \overline{E}(m)$ and (iv) neutron emission have no recoil effect on fragment kinetic energy. Then we can show that

$$\sigma_e(m) = \sigma_E \left[1 - \frac{2}{\pi} \left(\frac{1-r}{1+r} \right)^2 \right]^{\frac{1}{2}}$$
(17)

The $\sigma_e(m)$ values calculated with relation (17) are lower than $\sigma_E(A)$ and higher than

$$\sigma_e(m) = \sqrt{1 - \frac{2}{\pi}} \sigma_E = 0.6\sigma_E \qquad (18)$$

The SD curve calculated with this relation is presented on Fig. 7. Using the relation (18) we can estimate a peak at *m = 122* assuming that around this mass *Y* increase very rapidly with A except that $Y(123) = Y(122)$. However, we can not reproduce the pronounced peak obtained by Belhafaf *et al.* [4].

4. Conclusions

Using a simple model for the neutron emission by fragments, we have carried out a Monte Carlo simulation fragments from thermal neutron induced fission of [233]U. In comparison with the primary fragments, the final fission fragments have eroded kinetic energy and mass values, as much as to give rise to the appearance of peaks in the SD of the final fragments kinetic energy as a function of mass $\sigma_e(m)$ around *m = 109*. This peak, which agrees with experimental results obtained by Belhafaf *et al.* [4] and Faust *et al.* [5], respectively is a consequence of neutron emission and variations of primary fragments yield *Y(A)* and mean kinetic energy $\overline{E}(A)$ curves. As a results of the simulation one obtains a depletion on the SD in the mass region from *m = 121* to *m = 129*, and an small peak on the SD around *m = 122* which is not as big as the measured by Belhafaf *et al.* Our simulation reproduces also the experimental results on the yield of the final mass, the average number of emitted neutrons as a function of the provisional mass (calculated from the values of the final kinetic energy of the complementary fragments) and the average value of fragment kinetic energy as a function of the final mass.

5. Bibliography

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