CALCULATIONS OF FISSION BARRIERS WITH DEFORMATION-DEPENDENT ATTENUATION OF SHELL CORRECTIONS*

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(Received December 28, 2001)

A macroscopic model for calculating fission barriers (saddle-point energies) in two versions: with and without accounting for shell effects, is presented. Results of calculations with shell effects switched off agree very well with previous purely macroscopic calculations done by A.J. Sierk. Complete calculations of fission barriers (including shell effects) are done for nuclei in the range $66 \leq Z \leq 100$, for all isotopes with experimentally determined barrier heights. With a value of the shell-energy-damping parameter that fits the ground-state masses of deformed nuclei, shell effects almost completely disappear at the saddle configuration, thus leading to a strong manifestation of the ground-state shell effects, in agreement with experimental data.

PACS numbers: 25.85.–w

1. Introduction

Precise knowledge of fission-barrier heights is essential for quantitative description of nuclear fission and fusion–fission reactions. In the present work we give account of our calculations of the saddle-point energies based on a macroscopic approach of Sierk [1], extended by inclusion of shell effects. We calculate the total potential energy of the fissioning nucleus as the sum of the Coulomb energy (assuming a diffuse charge distribution), and the nuclear energy taken as the Yukawa-plus-exponential potential [2] (replacing the surface energy in the liquid drop model). For shell-correction energies we take ground-state "shell effect" energies tabulated in the Thomas–Fermi model mass predictions of Myers and Swiatecki [3]. Attenuation of the shell energies with deformation is done according to a phenomenological formula of Myers and Swiatecki [4].

* Presented at the XXVII Mazurian Lakes School of Physics, Krzyże, Poland, September 2–9, 2001.

2. Parametrization of nuclear shapes

We consider potential energies of fissioning nuclei in configurational space parametrized the same way as it was done in Ref. [5]. The shapes are assumed to consist of two spheres connected smoothly by a portion of a quadratic surface of revolution. There are three variables defining the volume conserving shapes: distance $\rho = r/(R_1 + R_2)$, neck $\lambda = (l_1 + l_2)/(R_1 + R_2)$, and asymmetry $\Delta = (R_1 - R_2)/(R_1 + R_2)$.

In the above definitions, r is the distance between centers of the spheres of radii R_1 and R_2. Distances from the inner tips of two spheres to the respective junction points with the middle quadratic surface of revolution are denoted by l_1 and l_2. As a parameter determining the transition from mononuclear to dinuclear regime, we take the window opening parameter $\alpha = [1 - (1 - \lambda)\rho]/(1 - \Delta^2)$. A value of this parameter $\alpha = 1$ corresponds to the transition between concave and convex shapes. For $\alpha > 1$ we have convex mononuclear shapes, while for $\alpha < 1$ shapes become dinuclear. They approach scission line for $\alpha = 0$.

In our calculations we attempt to determine the fission barrier for a given nucleus that represents the height of the saddle point with respect to the equilibrium shape. The search of the saddle point is done in two-dimensional space (ρ, λ), assuming symmetric fission, *i.e.*, we assume $\Delta = 0$.

3. Potential energy

The potential energy is calculated as a sum of the nuclear potential taken in form of the Yukawa-plus-exponential potential of Krappe, Nix and Sierk [2] and the Coulomb potential taken for realistic charge distribution with surface diffuseness [6]. In addition to the macroscopic energy, shell corrections are also included in the total potential energy.

3.1. Nuclear energy

Following prescription of Ref. [2], the nuclear part of the potential energy is given as a double volume integral of the Yukawa-plus-exponential folding function

$$E_n = -\frac{C_s}{8\pi^2 r_0^2 a^3} \iint \left(\frac{\sigma}{a} - 2\right) \frac{\mathrm{e}^{-\sigma/a}}{\sigma} d^3\vec{r}\, d^3\vec{r}\,' \,, \tag{1}$$

where $\sigma = |\vec{r} - \vec{r}\,'|$, $C_s = a_s(1 - k_s I^2)$ and $I = (N - Z)/A$. For parameters r_0, a, a_s and k_s we have taken values obtained from the fit to nuclear masses [7]. After applying the Gauss divergence theorem, Eq. (1) can be transformed into the double surface integral. For axially symmetric shapes, Eq. (1) reduces to the following three-dimensional integral:

$$E_n = \frac{C_s}{4\pi r_0^2} \iiint \left(2 - \left[\left(\frac{\sigma}{a}\right)^2 + 2\frac{\sigma}{a} + 2 \right] \mathrm{e}^{-\frac{\sigma}{a}} \right) \frac{P_2(z,z')P_2(z',z)}{\sigma^4} dz\, dz'\, d\phi\,, \tag{2}$$

where

$$P_2(z,z') = P(z) \left[P(z) - P(z')\cos\phi - \frac{dP}{dz}(z-z') \right]. \tag{3}$$

Here $\rho = P(z)$ represents equation of nuclear surface in cylindrical coordinates ρ, z, ϕ. In these coordinates, the distance σ is given by $\sigma = [P^2(z) + P^2(z') - 2P(z)P(z')\cos\phi + (z-z')^2]^{1/2}$.

3.2. Coulomb energy

The Coulomb energy is calculated for a diffuse charge distribution simulated by folding the Yukawa function with a range a_c over sharp charge distribution. We can write the Coulomb energy as $E_c = E_c^{\rm sharp} + \Delta E_c$. Using a similar procedure as for nuclear part of the potential energy, the sharp cut-off component of the Coulomb energy takes the following expression:

$$E_c^{\rm sharp} = \frac{\pi}{6}\rho_0^2 \iiint \frac{P_2(z,z')P_2(z',z)}{\sigma} dz\, dz'\, d\phi, \tag{4}$$

where ρ_0 is the charge density.

Similarly, the correction of the Coulomb energy for the diffuseness can be expressed as:

$$\Delta E_c = -\frac{\pi}{a_c}\rho_0^2 \iiint \frac{P_2(z,z')P_2(z',z)}{\sigma_c^4} \times \left[2\sigma_c - 5 + \left(5 + 3\sigma_c + \frac{1}{2}\sigma_c^2 \right) \mathrm{e}^{-\sigma_c} \right] dz\, dz'\, d\phi, \tag{5}$$

where $\sigma_c = \sigma / a_c$.

All contributions to the potential energy given by Eqs. (2), (4) and (5) are three-dimensional integrals which have to be calculated numerically.

3.3. Shell corrections

As it was mentioned previously, we correct the potential energies at the equilibrium shape by shell corrections taken from the Thomas–Fermi ground-state mass tables of Myers and Swiatecki [3]. We assume that the shell-correction energies S are attenuated by deformation according to a phenomenological formula [4]:

$$\tilde{S}(\text{shape}) = S(1 - 2\Theta^2)\mathrm{e}^{-\Theta^2}, \tag{6}$$

where

$$\Theta^2 = \frac{1}{4\pi a^2} \int [r(\theta, \phi) - R_0]^2 \, d\Omega \tag{7}$$

is a measure of departure from spherical shape. The constant $a^2 = 0.265$ fm^2 has been determined in Ref. [4] by fitting ground-state masses of deformed nuclei.

An effective shell correction at the saddle configuration is intermediate between mononuclear and dinuclear regimes, dominated by the shell structure of the compound nucleus and fission fragments, respectively. To make a smooth transition between both regimes we calculate the shell correction for a given shape as

$$\tilde{S}(\text{shape}) = \tilde{S}_{\text{c.s.}} \sin\alpha + (\tilde{S}_1 + \tilde{S}_2)(1 - \sin\alpha) \ , \tag{8}$$

where α is defined in Sec. 2, $\tilde{S}_{\text{c.s.}}$ is the shell energy of the deformed composite system treated as a mononucleus, while $\tilde{S}_1$ and $\tilde{S}_2$ are shell energies of the two fragments viewed as components of a dinuclear system. All three shell energies, $\tilde{S}_{\text{c.s.}}$, $\tilde{S}_1$ and $\tilde{S}_2$, are calculated according to Eqs. (6) and (7).

4. Results

We calculate fission barriers for different nuclei by determining the extremum (saddle point) of two-dimensional potential-energy function $E_{\text{pot}}(\rho, \lambda)$, taken relative to the ground-state energy.

In Fig. 1 we show the fission-barrier heights calculated with our model in two versions: with and without shell effects. It is seen that the calculations without shell effects agree very well with purely macroscopic predictions of Sierk [1]. This result shows that heights of the "macroscopic" fission barriers are not sensitive to particular choice of shape parametrization, the only factor the two schemes of calculations differ.

Very different predictions of the fission barriers are obtained, however, in calculations with inclusion of shell corrections (see triangles in Fig. 1). Obviously, the most spectacular increase of the fission barrier is predicted for a closed-shell nucleus ^{208}Pb. As a consequence of the inclusion of shell effects, a kind of stabilization of the fission barriers for the heaviest nuclei at a level of 5–6 MeV is observed, whereas results of the calculations without shell corrections show steady decrease, and finally disappearance of fission barriers for the heaviest nuclei.

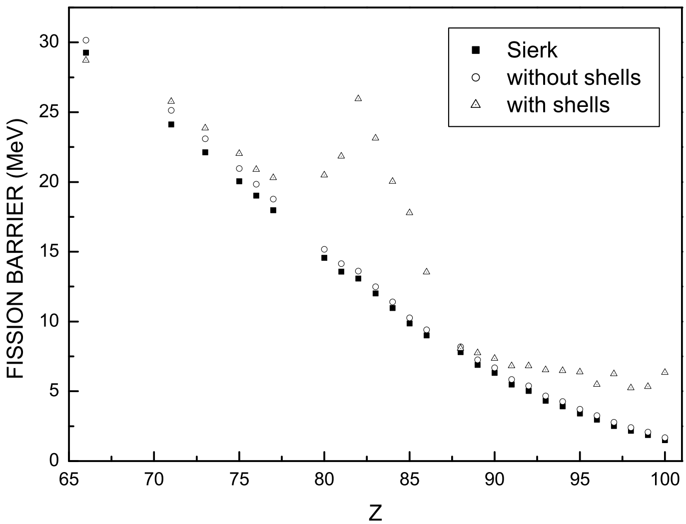

Fig. 1. Fission barriers for different atomic numbers of fissioning nuclei calculated in the present model, and compared with predictions of the macroscopic model of Sierk [1]. Calculations have been done for one isotope of each element.

It should be noted that the observed distinct dependence of fission barriers on shell effects is a consequence of a strong damping of shell effects with deformation, as prescribed by Eqs. (6)–(8). Our calculations show that attenuation of shell effects due to deformation of the fissioning nucleus is quite strong. With a value of the damping parameter $a^2 = 0.265$ fm^2 that fits [4] ground-state masses of deformed nuclei, shell effects get almost completely washed out at the saddle configuration. Myers and Świątecki comparing in Ref. [8] their predicted Thomas–Fermi fission barriers with experimental data also pointed out that shell effects almost completely vanish at deformations corresponding to the saddle point. Consequently, the fission barriers, calculated as the energy at the saddle point (with damped shell effects) relative to the ground-state energy, directly depend on the magnitude of the shell-correction energy at the ground state.

In Fig. 2 we present complete set of fission barriers calculated with inclusion of shell effects. These results are compared with experimental fission-barrier heights compiled in Refs. [9, 10]. One can see a very good agreement between theoretical and experimental results throughout the entire range of nuclei with known barriers, for elements from Dysprosium to Fermium. Very irregular behaviour in the vicinity of closed-shell nuclei is satisfactorily reproduced. Especially good agreement is observed for heavy nuclei. The overall average discrepancy between theoretical and experimental fission barriers is about 1 MeV.

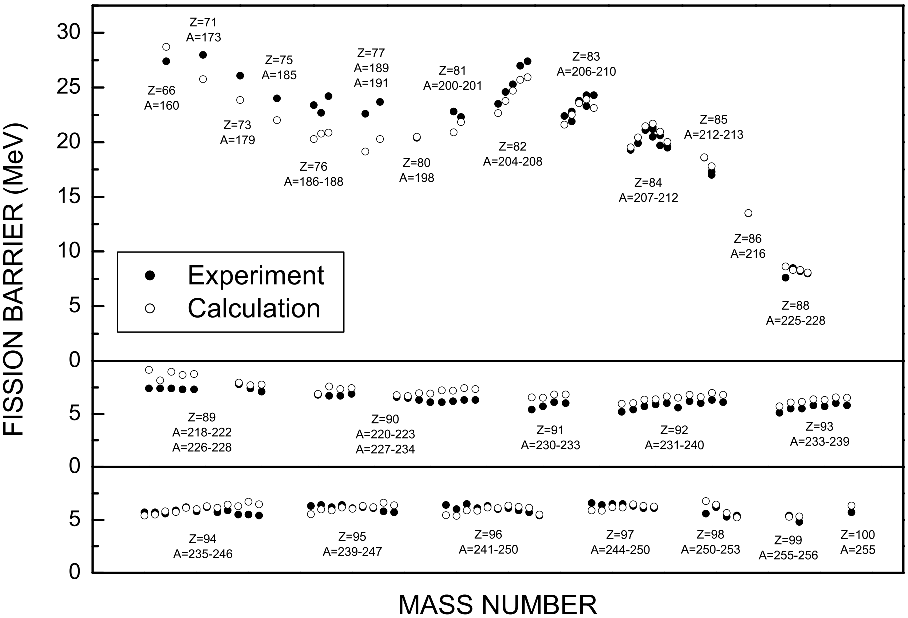

Fig. 2. Fission barriers deduced from experimental data [10,11] for over 120 isotopes of different elements of $66 \leq Z \leq 100$, compared with predictions of the present model.

This work was supported by the Poland–USA Maria Skłodowska-Curie Joint Fund II, under Project no. PAA/DOE-98-34, and by the Polish State Committee of Scientific Research (KBN), Grant no. 2P03B05419.

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