Fission barriers with the Weizsäcker-Skyrme mass model*

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Abstract: Based on the Weizsäcker-Skyrme (WS4) mass model, the fission barriers of nuclei are systematically studied. Considering the shell corrections, macroscopic deformation energy, and a phenomenological residual correction, the fission barrier heights for nuclei with $Z \geqslant 82$ can be well described, with an rms deviation of 0.481 MeV with respect to 71 empirical barrier heights. In addition to the shell correction at the ground state, the shell correction at the saddle point and its relative value are also important for both deformed and spherical nuclei. The fission barriers for nuclei far from the β-stability line and super-heavy nuclei are also predicted with the proposed approach.

Keywords: fission barrier, shell correction, saddle point, macroscopic-microscopic model

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I. INTRODUCTION

Studies on nuclear fission are of considerable research interest [1−6]. As one of the key and sensitive physical parameters, fission barriers of nuclei are frequently used in nuclear physics [7−12], reactor physics [13] and nuclear astrophysics [14, 15]. In the synthesis of super-heavy nuclei (SHN) through fusion reactions, the prediction of the evaporation-residue cross section for SHN strongly depends on the fission barrier height of the compound nuclei adopted in the calculations [16−20]. An 1-MeV shift of the barrier height may change the calculated cross section of 3n or 4n reactions by 2−3 orders of magnitude [21, 22]. Considering the complexity of a typical fission process, in which not only large-scale collective participation of nucleons is witnessed but also super-deformed shapes of nuclei are encountered, accurate description of the corresponding fission barrier is of great interest but at the same time remains challenging.

The fission barriers of nuclei can be described with some nuclear mass models, such as macroscopic-microscopic models [23−25] and microscopic models based on the Skyrme energy density functionals [26−28] or covariant density functionals [29−31], in which the model parameters are usually determined by the nuclear properties at the ground state. For unmeasured SHN, the uncertainty of the barrier heights predicted using these different models reaches a few MeV [22, 24]. Considering the strong influence of the barrier height on the prediction of cross section, as mentioned above, it becomes necessary to improve the model accuracy for describing the fission barriers of unstable nuclei.

Inspired by the Skyrme energy-density functional, the Weizsäcker-Skyrme (WS4) mass model was proposed [32], with which the known masses can be reproduced with an rms error of ~ 0.3 MeV [33] and the known α-decay energies of SHN can be reproduced with deviations smaller than 0.5 MeV [34−36]. Therefore, it would be interesting to apply the WS4 model for describing the fission barrier. In this work, we attempt to systematically calculate the fission barrier height based on the WS4 model, considering the shell correction at the ground state and that at the saddle point.

II. THEORETICAL FRAMEWORK

In the macroscopic-microscopic model, the fission barrier height of a nucleus at zero temperature is expressed as the difference between the energy of the nucleus at saddle point $E_{\rm sad}$ and that at its ground state $E_{\rm gs}$,

$$B_{\rm f} = E_{\rm sad} - E_{\rm gs} = (E^{\rm mac}_{\rm sad} - E^{\rm mac}_{\rm gs}) + (U_{\rm sad} - U_{\rm gs}) + \Delta B. \quad (1)$$

Here, $E^{\rm mac}_{\rm sad}$ and $E^{\rm mac}_{\rm gs}$ denote the macroscopic energy at the saddle point and that at the ground state, respectively. $U_{\rm sad}$ and $U_{\rm gs}$ denote the corresponding shell corrections. ΔB denotes the residual correction. With the macroscopic fission barrier height $B^{\rm mac}_{\rm f} = E^{\rm mac}_{\rm sad} - E^{\rm mac}_{0}$ and the macroscopic deformation energy $B_{\rm def} = E^{\rm mac}_{\rm gs} - E^{\rm mac}_{0}$, the fission

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barrier height can be re-written as

$$B_{\rm f} = B_{\rm f}^{\rm mac} - U_{\rm gs} + (U_{\rm sad} - B_{\rm def}) + \Delta B. \quad (2)$$

For spherical nuclei, the barrier height can be estimated as $B_{\rm f}^{(0)} = B_{\rm f}^{\rm mac} - U_{\rm gs}$ if neglecting the saddle point shell correction and the residual correction.

Following Cohen-Swiatecki's formula [1], the macroscopic fission barrier height is expressed as

$$B_{\rm f}^{\rm mac} = \begin{cases} 0.38(3/4 - x)E_s & : \quad 1/3 < x \leqslant 2/3 \\ 0.88(1-x)^3 E_s & : \quad 2/3 < x \leqslant 1 \end{cases} \quad (3)$$

with the ratio $x = \frac{E_c}{2E_s}$. $E_c = a_c Z^2/A^{1/3}$ denotes the Coulomb energy and $E_s = a_s A^{2/3}(1-\kappa I^2)$ denotes the surface energy with isospin asymmetry $I = (N-Z)/A$. The coefficients $a_c = 0.7092$ MeV, $a_s = 17.4090$ MeV and $\kappa =$ 1.5189 are taken from the WS4 model [32]. Together with the shell corrections $U_{\rm gs}$, $U_{\rm sad}$ and the macroscopic deformation energy $B_{\rm def}$ also from the WS4 model predictions, the fission barrier heights for all bound heavy nuclei can be calculated as follows:

$$B_{\rm f}^{\rm WS4} = B_{\rm f}^{\rm mac} - U_{\rm gs} + U_{\rm sad} - B_{\rm def}, \quad (4)$$

neglecting the residual correction ΔB. The influence of ΔB will be discussed later.

In this work, the saddle point of a nucleus is determined from the surface of the shell correction $U(\beta_2,\beta_4)$ based on the WS4 calculations in which the Strutinsky shell correction is obtained from single-particle levels of an axially deformed Woods-Saxon potential. As two examples, we show in Fig. 1 the contour plot of the shell correction surface for nuclei ^{208}Pb and ^{238}U. Here, other deformations such as β_3 and β_6 are neglected in the calculations. The contour plot reveals that the shell correction $U_{\rm sad}$ at the saddle point is approximately 2.2 MeV for ^{208}Pb and 1.0 MeV for ^{238}U. In our calculations, we introduced a truncation for the macroscopic deformation energy, *i.e.* $B_{\rm def} \leqslant B_{\rm f}^{\rm mac}$, and we neglected the influence of $U_{\rm sad}$ for nuclei with $U_{\rm sad} < 0$.

III. RESULTS AND ANALYSIS

In Fig. 2(a), we show the discrepancies between the empirical fission barrier heights $B_{\rm f}^{\rm emp}$ [3] and the model predictions for 71 nuclei with $Z \geqslant 82$. For actinides, we take the mean value of the inner and the outer barrier height as the value of $B_{\rm f}^{\rm emp}$ in the comparisons. Evidently, with the saddle point shell correction $U_{\rm sad}$ and the macroscopic deformation energy $B_{\rm def}$ taken into account, the root-mean-square (rms) deviation with respect to the fission barrier heights is significantly reduced, from 2.410 MeV to 0.873 MeV. We note that, for both spherical and deformed nuclei, the fission barrier heights are generally better described by $B_{\rm f}^{\rm WS4}$. For doubly-magic nucleus ^{208}Pb, the calculated $B_{\rm f}^{(0)} = 25.1$ MeV, which is smaller than the empirical barrier height by 2.3 MeV. Considering $U_{\rm sad} = 2.2$ MeV for ^{208}Pb, we obtain $B_{\rm f}^{\rm WS4} = 27.3$ MeV, which is very close to the empirical value. For deformed nucleus ^{238}U, the calculated $B_{\rm f}^{(0)} = 9.2$ MeV, which is higher than the empirical barrier by 2.9 MeV. With the macroscopic deformation energy of $B_{\rm def} = 3.4$ MeV and $U_{\rm sad} = 1.0$ MeV, we obtain $B_{\rm f}^{\rm WS4} = 6.8$ MeV for ^{238}U, which is comparable to the empirical value. From Fig. 2(a), it is evident that the values of $B_{\rm f}^{\rm emp} - B_{\rm f}^{(0)}$ can be categorized into two groups: approximately 2 MeV for nuclei with $A \sim 210$ and approximately -3 MeV for

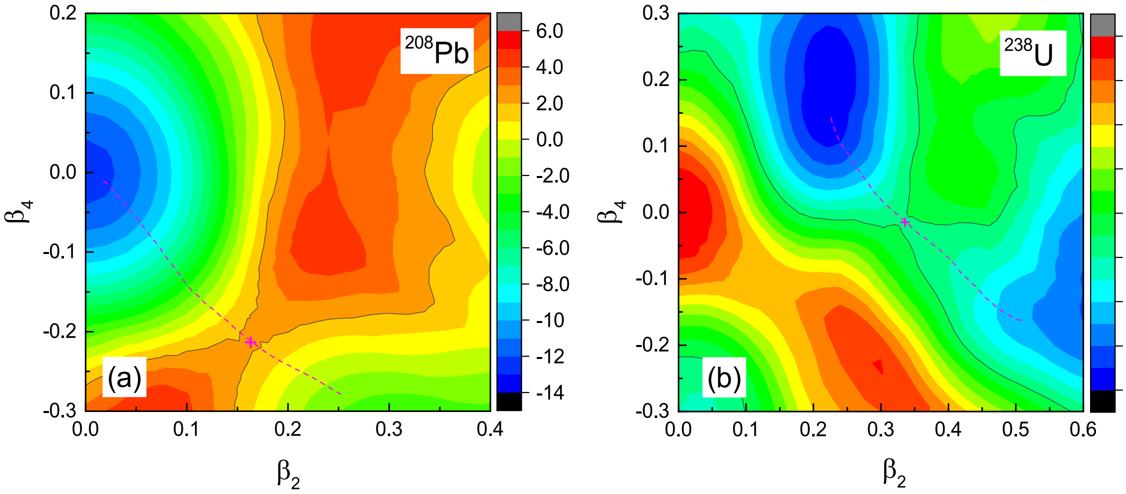

Fig. 1. (color online) Contour plot of the shell corrections for ^{208}Pb and ^{238}U. The dashed curves denote the possible fission paths. The crosses denote the positions of the saddle points.

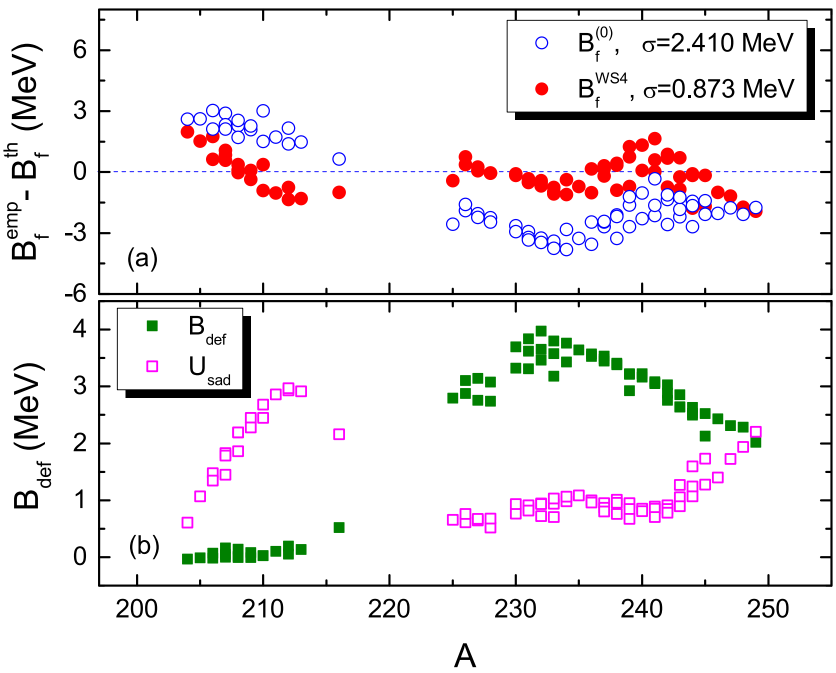

Fig. 2. (color online) (a) Discrepancies between the empirical fission barrier heights B_f^{emp} [3] and the model predictions. The open circles denote the results obtained using $B_f^{(0)} = B_f^{mac} - U_{gs}$ and the solid circles denote the results obtained from Eq. (4). (b) Macroscopic deformation energies B_{def} (solid squares) and shell corrections at the saddle points U_{sad} (open squares) for these nuclei.

$A > 225$. To understand the underlying physics, the macroscopic deformation energies B_{def} and the saddle point shell corrections U_{sad} for these nuclei are shown in Fig. 2(b). Evidently, for nuclei with $A \sim 210$, the values of U_{sad} are obviously higher than B_{def}, whereas for $A > 225$, $B_{def} > U_{sad}$ in general. The values of $U_{sad} - B_{def}$, therefore, can be categorized into two groups.

To further analyze the influence of the saddle point shell correction, we introduce $\delta U = (U_{sad} - U_{gs})/U_{gs}$ to describe the relative value of the shell correction. In Fig. 3, we show the values of $B_f^{emp} - B_f^{WS4}$ as a function of δU^2. Evidently, the difference between the empirical barrier heights and the model predictions systematically decreases with increasing δU^2. Comparing Eq. (2) with Eq. (4), one notes that the residual correction ΔB is neglected in B_f^{WS4}. To better describe the fission barriers, we empirically write the residual correction (in MeV) as

$$\Delta B \approx -2.8 + 19 \exp(-\delta U^2/0.8). \tag{5}$$

In Fig. 4, we compare the results obtained using $B_f^{WS4} + \Delta B$ and those obtained using FRLDM [25]. The rms deviation is further reduced to 0.481 MeV, considering the residual correction given by Eq. (5). We note that the trend of the results obtained using FRLDM is similar to that obtained using WS4, for nuclei with $A \approx 210$ and $A > 240$. We also note that the mean values of the fission barrier heights obtained using the three macroscopic-microscopic approaches, *i.e.* $\langle B_f \rangle = (B_f^{FRLDM} + B_f^{WS4} + B_f^{WS4+\Delta B})/3$, also agree well with the empirical values, with an rms error of only 0.585 MeV. In the calculations of $\langle B_f \rangle$ we set a relatively larger weight for the WS4 model, considering its smaller rms error for describing known masses and empirical B_f. We would like to emphasize that the difference between the inner barrier heights and the outer ones for actinides ($Z \geqslant 90$) could result in some uncertainties in analyzing the model accur-

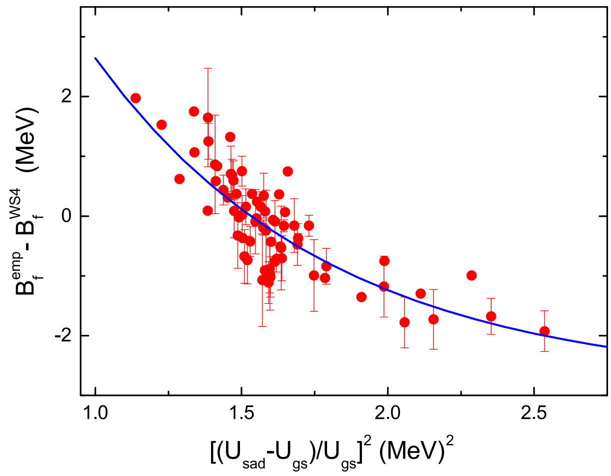

Fig. 3. (color online) Deviation $B_f^{emp} - B_f^{WS4}$ as a function of the ratio square of the shell correction. The error bars denote the difference between the inner barrier height and the corresponding outer barrier height for actinides [3]. The solid curve denotes the results obtained using Eq. (5).

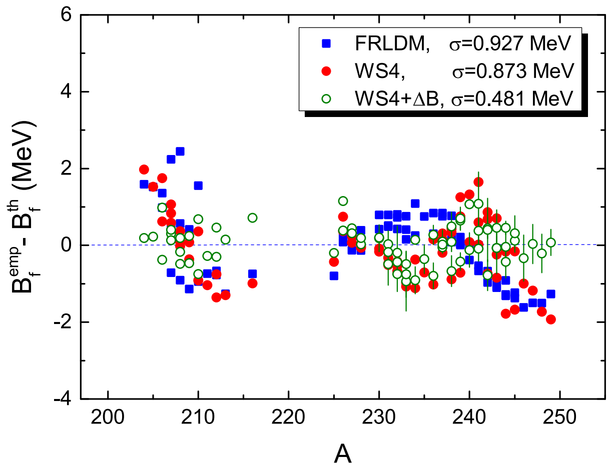

Fig. 4. (color online) The same as Fig. 2(a), but with the results of the finite-range liquid-drop (FRLDM) model [25] and $B_f^{WS4}+\Delta B$ for comparison. The error bars denote the difference between the inner barrier height and the corresponding outer barrier height for actinides [3].

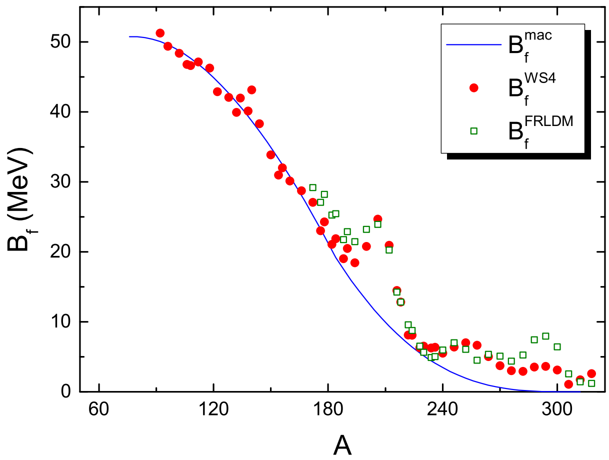

Fig. 5. (color online) Fission barrier heights for even-even nuclei which lie on or are the closest to the β-stability line (using Green's expression [37]).

acy. Compared with B_f^{WS4}, the rms deviation is reduced from 1.01 to 0.77 MeV for the 45 inner barriers of actinides with ΔB being considered, and the corresponding value is reduced from 0.92 to 0.48 MeV for the outer barriers.

Using the proposed approach, we systematically studied the fission barrier heights for stable nuclei. In Fig. 5, we show the predicted B_f for even-even nuclei which lie on or are the closest to the β-stability line (Green's expression [37], $N-Z=0.4A^2/(A+200)$, was arbitrarily adopted). The solid curve denotes the results of the macroscopic fission barrier B_f^{mac} given by Eq.(3). Evidently, the macroscopic barrier height approaches zero for super-heavy nuclei. For nuclei around ^{208}Pb, the fission barrier heights predicted with both FRLDM and WS4 models are significantly higher than those of B_f^{mac}, owing to the strong shell effects. For actinides with $A\approx 240$, the results obtained using WS4 are close to those obtained using FRLDM, with values of approximately 6 MeV. For super-heavy nuclei around ^{294}Cn, the results obtained using FRLDM are higher than those obtained using WS4, by approximately 4 MeV.

In addition, using the proposed approach we simultaneously investigated the fission barrier heights of unstable nuclei. In Fig. 6, we show the predicted barrier heights for isotopic chains of Pb, Ra, U and Cm. The pink squares denote the empirical barrier heights taken from Ref. [3]. For Pb isotopes, the fission barriers evidently decrease with the increasing distance from the doubly-magic nucleus ^{208}Pb. For Ra and U isotopes, all three approaches predict a peak at the neutron-deficient side with neutron number $N=126$. For ^{218}U, the predicted barrier height $B_f^{WS4+\Delta B}=5.30$ MeV, while the result obtained using FRLDM is 9.67 MeV. Very recently, the fission barrier heights for neutron-deficient nuclei ^{210}Fr and ^{210}Ra have been measured [38], and the reported values were $B_f(^{210}\mathrm{Fr})$ = 10.67 MeV and $B_f(^{210}\mathrm{Ra})$ = 8.54 MeV with uncertainty of 5%. The predicted values of $B_f^{WS4+\Delta B}$ were 11.50 MeV and 8.78 MeV for ^{210}Fr and ^{210}Ra, respectively. From Fig. 6(b), it is evident that the measured $B_f(^{210}\mathrm{Ra})$ (open circle) can be well reproduced using the WS4+ΔB calculations. For the neutron-rich side, the trend of the fission barrier height is also strongly affected by the shell corrections. In Fig. 7, we show the predicted B_f for nuclei with $Z=102$, 106, 119 and 120. For No and Sg isotopes, the peaks of the fission barrier heights at $N=152$ and $N=162$ can be clearly observed. The abrupt change of α-decay energies at neutron number of 152 and 162 owing to the shell effects can also be clearly observed for heavy and super-heavy nuclei [39].

For unknown super-heavy nuclei (SHN) with $Z=119$ and 120, the predicted fission barrier heights are presented in Fig. 7(c) and (d). Evidently, for the SHN with $Z=119$ and $A=297$, the barrier height predicted by the FRLDM is 7.94 MeV, which is higher than that obtained using the WS4 model by 2 MeV. We note that in the study of the fusion reaction ^{48}Ca+^{238}U [40], the negative of the shell correction energy (6.64 MeV) from the finite range droplet model (FRDM) [41] is taken as the fission barrier height of the compound nucleus, but multiplied by 0.7 in order to reproduce the maximal cross section for ^{283}Cn(3n) measured at an excitation energy of 35.0 MeV. The predicted value of $B_f^{WS4}=4.20$ MeV for ^{286}Cn, which is comparable with the result obtained using the FRDM multiplied by 0.7. Considering the reduction factor of 0.7 for the results obtained using the FRLDM, the fission barrier heights obtained using the two models are comparable for the SHN with $Z=119$ and $A=297$. For the SHN with $Z=120$, the largest value of $B_f^{WS4}=6.23$ MeV is located at $N=176$, which is consistent with the predic-

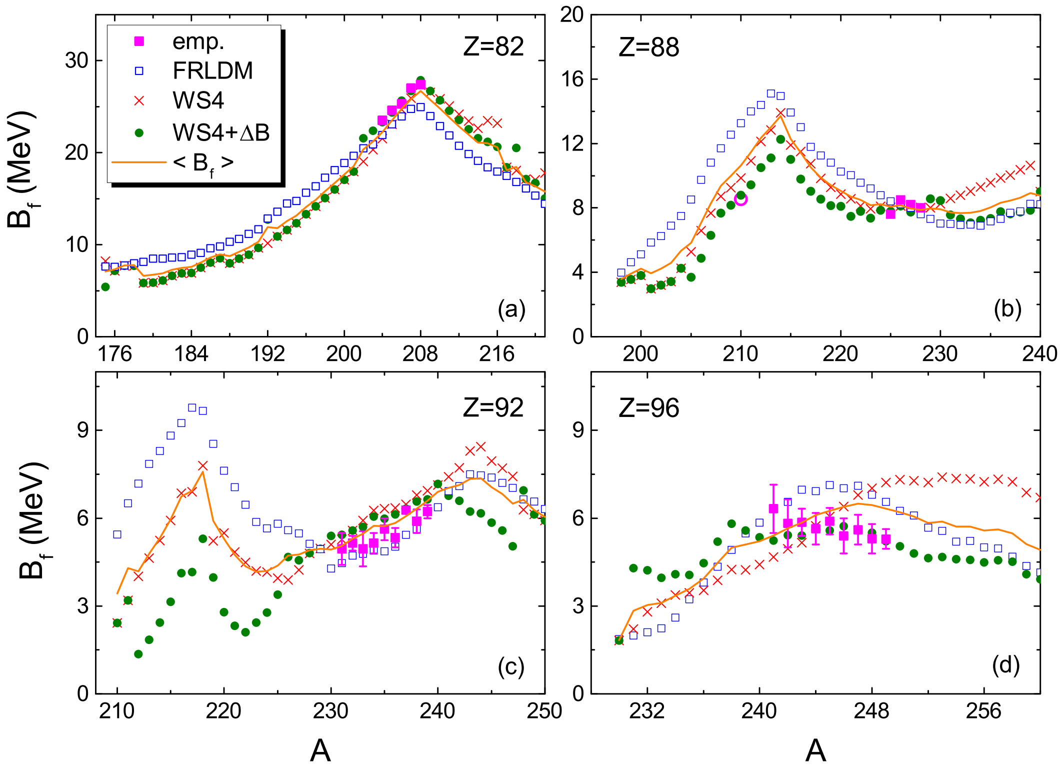

Fig. 6. (color online) Predicted fission barrier heights for isotopic chains of Pb, Ra, U and Cm. The open squares denote the results obtained using FRLDM. The crosses and the solid circles denote the results obtained using WS4 with Eq. (4) and those together with the residual correction ΔB, respectively. The solid curve denotes the mean value of the fission barrier heights $\langle B_{\rm f}\rangle$ obtained using the three approaches. The open circle in (b) denotes the measured $B_{\rm f}$ for ^{210}Ra taken from Ref. [38].

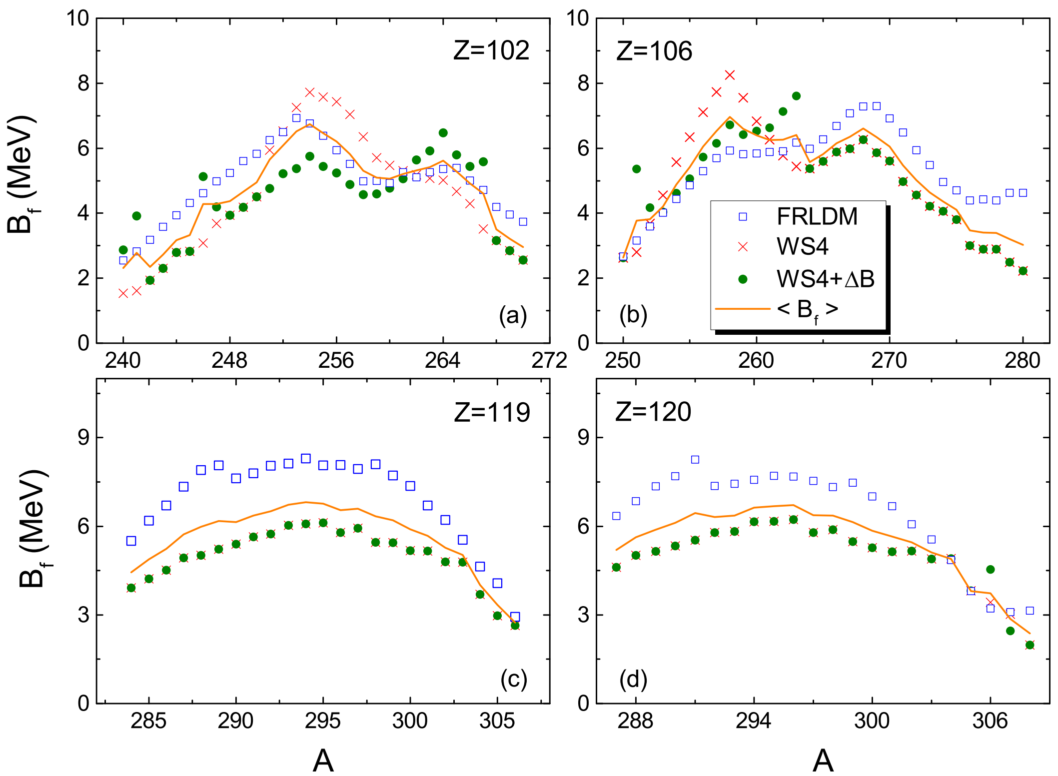

Fig. 7. (color online) The same as Fig. 6, but for heavier nuclei.

tions of Warsaw's macroscopic-microscopic calculations [24].

IV. SUMMARY

Based on the WS4 mass model with which the known masses can be reproduced with an rms error of ~0.3 MeV and the known α-decay energies of SHN can be reproduced with deviations smaller than 0.5 MeV, the fission barrier heights of heavy and superheavy nuclei were systematically studied. Considering the shell corrections, the macroscopic deformation energy and a phenomenological residual correction, the fission barrier heights for nuclei with $Z \geqslant 82$ were well described, with an rms error of only 0.481 MeV. We note that in addition to the shell correction at the ground state, the shell correction at the saddle point and its relative value were also important for accurate description of the barrier height. From the predicted fission barriers for isotopic chains of Pb, Ra, No and Sg, we note that the influence of the shell effect on the barrier height was evident. For Ra and U isotopes, all three approaches predicted a peak at the neutron-deficient side with $N = 126$. For No and Sg isotopes, the peaks of the barrier heights at $N = 152$ and $N = 162$ were clearly observed. With the predicted fission barriers, the evaporation residual cross sections in the fusion reactions searching for new neutron-deficient isotopes [42] and the reactions leading to the synthesis of super-heavy nuclei [43] can be analyzed more accurately.

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The table of the fission barriers with the WS4 model is available from http://www.imqmd.com/mass/BfWS4.txt

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