

# Effect of potential-energy-model inaccuracies on predictions of fission-fragment mass distributions based on the Brownian shape-motion method

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**Background:** Most actinide nuclides fission asymmetrically. A common explanation was that this division benefited from leading to fragments in the vicinity of the doubly magic  $^{132}\text{Sn}$ . It was tacitly assumed that lighter nuclides would all fission symmetrically because a similar situation could not occur there. However, a weakly asymmetric mass distribution was found for some preactinides at energies about 10 MeV above the fission saddle point by Itkis *et al.* [Yad. Fiz. **52**, 944 (1990)] and Mulgin *et al.* [Nucl. Phys. A **640**, 375 (1998)]. A more recent experiment by Andreyev *et al.* performed in June 2008 [Andreyev *et al.*, Phys. Rev. Lett. **105**, 252502 (2010)] showed a strongly asymmetric mass distribution in fission of  $^{180}\text{Hg}$  at low excitation energies. This gave rise to a new focus on fission properties in the “below Pb” region. Möller and Randrup presented a comprehensive calculation, based on the Brownian shape-motion (BSM) method, of fission-fragment charge distributions [P. Möller and J. Randrup, Phys. Rev. C **91**, 044316 (2015)] which obtained that “a new region of asymmetry” appeared for approximately  $95 \leq N \leq 115$  and  $75 \leq Z \leq 94$ . Available experimental results at the time, except for the observation of symmetric fission of  $^{187}\text{Ir}$  by Itkis *et al.* [Yad. Fiz. **52**, 944 (1990)], agreed with these predictions apart for minor differences in the transition regions between predicted symmetric and asymmetric fission. It was argued [P. Möller and J. Randrup, Phys. Rev. C **91**, 044316 (2015)] that the inaccurate results for  $^{187}\text{Ir}$  were related to inaccuracies in the calculated potential-energy surface and that such inaccuracies are related to the (in)accuracies of the calculated ground-state masses for the corresponding mass splits.

**Purpose:** We expand on our previous discussion of a possible source of the difference between the experimental and theoretical fission-fragment mass distributions for  $^{187}\text{Ir}$  and furthermore investigate if such differences may occur for other fissioning nuclides in the below Pb and actinide regions.

**Methods:** It has been shown that all structure in the mass distributions obtained by use of the BSM method is entirely due to the structure of the potential-energy surfaces on which the random walks are executed. Therefore, to understand the discrepancy between the previous theoretical results and the experimental observations for  $^{187}\text{Ir}$  we focus on the accuracy of the calculated potential-energy surface.

**Results:** We find that in symmetric fission of  $^{187}\text{Ir}$  the corresponding calculated fragment ground-state masses are too high compared to experiment by about 2.5 MeV each so the scission potential energy is calculated to be too high by 5 MeV. We also find that this is the largest error that can occur for any scission configuration in heavy-element fission.

**Conclusions:** As earlier we pose that the reason that symmetric fission is not favored in the calculated fission-fragment distribution of  $^{187}\text{Ir}$  is that the potential-energy surface is overestimated by 5 MeV for symmetric splits. In the calculations a large error for symmetric splits extends only to nuclides a few nucleons beyond  $^{187}\text{Ir}$  and does not occur elsewhere. Therefore, to test this hypothesis of the origin of the discrepancy, it is of interest to map out in experiments how far this region of symmetric fission “within the predicted region of asymmetry” extends and if substantial discrepancies occur elsewhere.

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## I. INTRODUCTION

Fission below the actinide region has historically not been studied as extensively as fission of the heaviest nuclei. It was tacitly assumed that because of the absence of strong shell corrections in possible fragment splits of these nuclei they would all obey “liquid-drop” systematics, fission symmetrically, and therefore be fairly uninteresting for studying details of the fission process.

The discovery, in June of 2008, that fission of  $^{180}\text{Hg}$  at the particularly low excitation energies ( $E^* < 10$  MeV)

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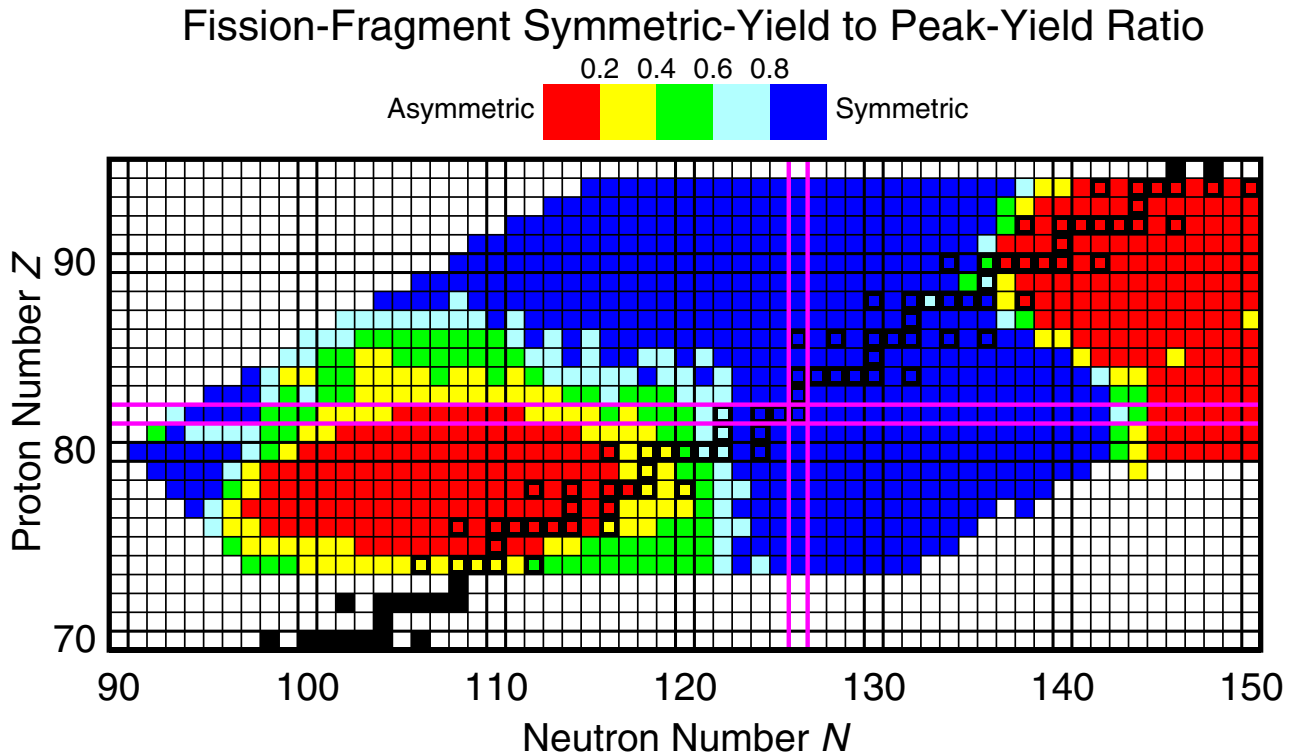


FIG. 1. Calculated symmetric-yield to peak-yield ratios for 987 fissioning systems. Black open squares indicate  $\beta$ -stable nuclei. These previously obtained results [1] show a new, contiguous region of asymmetric fission separated from the classical location of asymmetric fission in the actinides by an extended area of symmetric fission. The location of  $^{187}\text{Ir}$  is well inside the red region.

populated in  $\beta$  decay of  $^{180}\text{Tl}$  results in a well-developed asymmetric fragment mass distribution [2] put an abrupt end to this expectation.

Subsequently, experimental studies started to focus on nuclei in the below-Pb (and slightly above) region; some early studies are those of Refs. [3,4]. About two years after the asymmetric fission of  $^{180}\text{Hg}$  was observed, Randrup and Möller [5] developed the Brownian shape-motion (BSM) method, which allowed fission mass distributions to be calculated (for excitation energies above the barrier) for any fissioning compound nucleus. It was based on random walks on previously calculated five-dimensional (5D) potential-energy surfaces calculated as functions of five shape parameters [6,7].

The Brownian shape-motion model [5,8,9] in its initial implementation [5], had no *adjustable* parameters. There are two parameters, the strength of the bias potential and the critical neck radius at which we assume the fission-fragment mass asymmetry is frozen. Since it has been shown that the results are insensitive to a large range of these two parameters [8], they are not in the category of adjustable parameters. In the version of the model used subsequently, in particular in the large-scale calculation showing the extension of the “new region of asymmetry” [1] there are two adjustable parameters that govern the rate at which the shell effects dampen out with energy determined in Ref. [9]. The model has been extensively benchmarked, in Ref. [9] with respect to 70 charge yields measured at GSI [10], and in Ref. [11] with respect to new

and older data in the neutron-deficient Pb region. It is worth noting that the model has been extended and applied to additional fission properties such as neutron emission correlation with fission fragment masses [12], odd-even staggering, and fission-fragment isotopic yields [13–15].

There are few theoretical approaches to calculate fission-fragment mass distributions and other fission properties, that have so far been routinely applied to basically all fissioning systems and which show overall good quantitative agreement with observations. In contrast, after the initial sensitivity studies and benchmarking of the BSM method, it was applied to the calculation of fission-fragment mass yields for 987 nuclides in the region  $74 \leq Z \leq 94$ ,  $91 \leq N \leq 150$ . Adjacent to  $^{180}\text{Hg}$  the calculations showed a new contiguous region of asymmetric fission for approximately  $95 \leq N \leq 115$  and  $75 \leq Z \leq 85$  [1]. In the paper it was noted that the observation by Itkis *et al.* [17] and Mulgin *et al.* [18] of the symmetric fission of  $^{187}\text{Ir}$  contradicted the calculated results. It was proposed that the discrepancy was due to inaccuracies in the calculated 5D potential-energy surface for  $^{187}\text{Ir}$  for trajectories leading to symmetric division and that the magnitude of the inaccuracies of the calculated potential-energy surface could be related to the inaccuracies of the calculated ground-state masses of the corresponding fission fragments. The recent experimental paper by Duhri *et al.* [19] revisited in more detail the fission properties of  $^{187}\text{Ir}$  and commented on the discrepancy with respect to the studies in Ref. [1], which motivates us to present more detailed arguments for the proposed

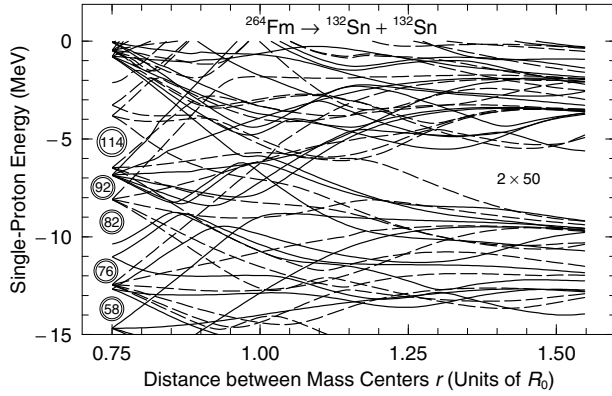


FIG. 2. Calculated single-particle levels for shape evolution from spherical shape to separated symmetric spherical fragments.

origin of the inaccuracy of the results for  $^{187}\text{Ir}$  and if this can occur for other fissioning nuclides.

## II. REGIONS IN THE NUCLEAR CHART WHERE THE BSM METHOD MAY BE INACCURATE

The BSM method is a random walk on 5D potential-energy surfaces previously calculated as functions of five nuclear shape “coordinates,” namely elongation, neck radius, left and right fragment ellipsoidal deformations, and mass (or equivalently volume) left-right fragment asymmetries. As implemented in the calculations shown in Fig. 1, all structures present in the fission-fragment mass distributions are consequences of the structures in the calculated potential-energy surfaces. Therefore, to shed light on the possible origin of the different experimental and theoretical results for the fission-fragment mass distributions for  $^{187}\text{Ir}$  and if they can occur elsewhere in the nuclear chart we need to understand the accuracy of the calculated potential-energy surfaces. However, the potential-energy surfaces consist of more than  $5 \times 10^6$  values corresponding to different shapes. Experimental values to compare to do not exist for these points except for the ground state, and to a lesser extent for the calculated fission-barrier saddle points and isomeric minima.

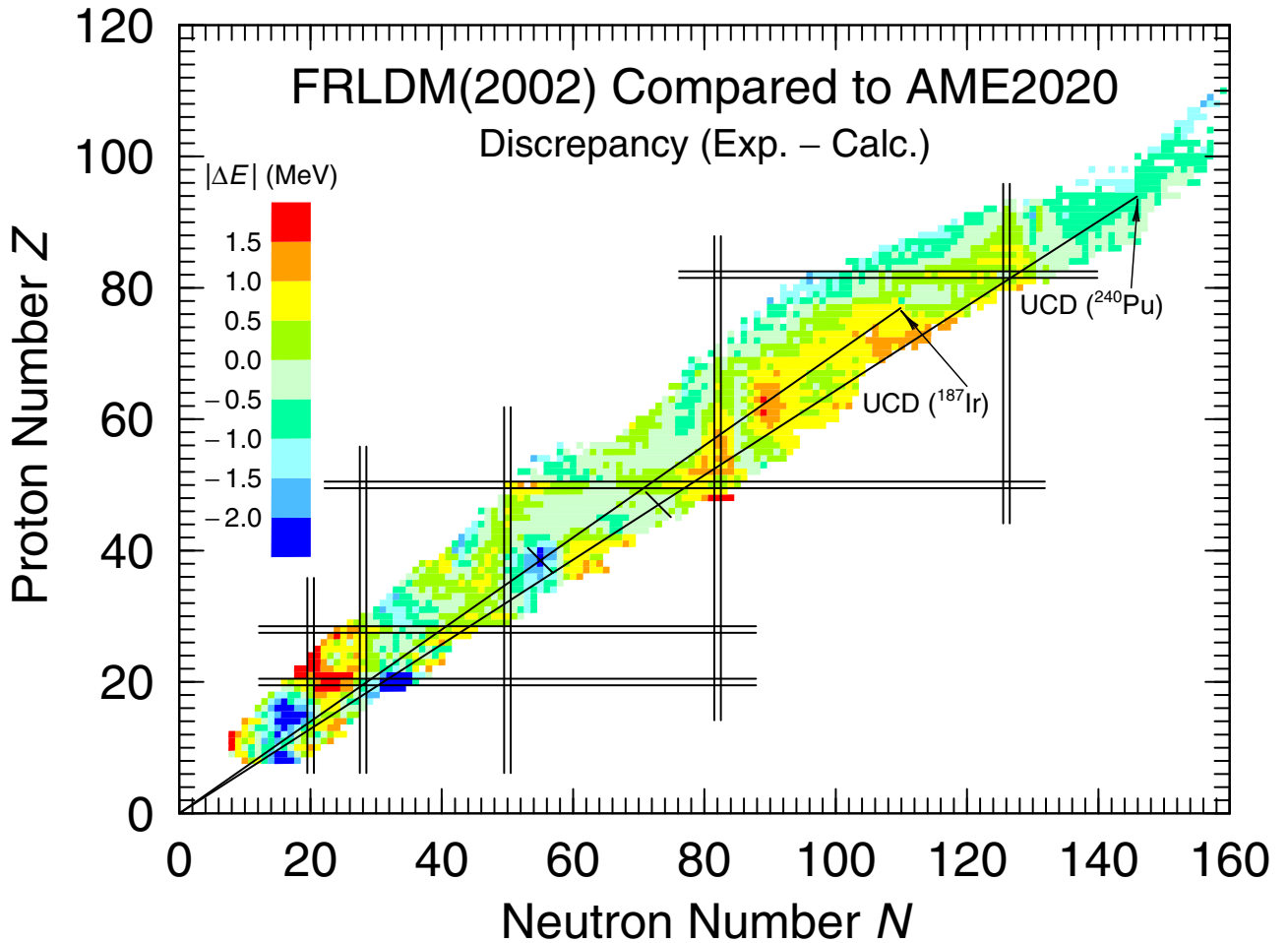


FIG. 3. Difference between experimental masses and theoretical masses calculated in the FRLDM2002 [16], which was the potential-energy model used to calculate the 5D potential-energy surfaces (it was the most current potential-energy model in the timeframe 2004–2006). Superimposed are the UCD lines for fission of  $^{187}\text{Ir}$  and  $^{240}\text{Pu}$  with symmetric fragment locations indicated by short black lines.

### A. Relation between 5D potential-energy surface accuracy and fission-fragment ground-state masses

At scission when the fission fragments have almost completely formed it is reasonable to assume that at this point the 5D potential-energy surface accuracy is closely related to the accuracy of the model as applied to the ground-state masses of the fragments involved. We furthermore know that in our model the level structure at scission appears long before the scission point, obviously where the nascent fragment shape is similar to the shapes at scission. This is seen in Fig. 2 (Fig. 7 in Ref. [20]), where the fragment  $Z = 50$  proton magic-number gap has almost fully developed already at  $r = 1.25$  which corresponds to the value at the fission isomeric shape; see Ref. [20] in which the potential-energy surfaces in Fig. 6 show this. Therefore it is reasonable to assume that the potential-energy surface already long before scission has inaccuracies the magnitude of which increases with increasing inaccuracies in the calculated masses of the corresponding fragments. These observations allow us to form an opinion where in the chart the calculated fission-fragment mass distributions are less accurate and in possible disagreement with experiment, as is the case for  $^{187}\text{Ir}$ .

### B. Estimates of BSM method inaccuracies across the heavy-element region

We have called the mass model based on the parameters used in the potential-energy calculation FRLDM2002. It was not published, because it was an “interim” mass table, but the most current and best we had at the time the potential-energy calculations were carried out. For more details see Ref. [16]. For the most current mass tables see Ref. [21]. We compare in Fig. 3 FRLDM2002 to experimental masses. In the figure we also show two unchanged charge distribution (UCD) lines, one for fission of  $^{240}\text{Pu}$  and the other for  $^{187}\text{Ir}$ . UCD means that the  $N/Z$  ratio in the fragments is the same as in the fissioning system. This assumption is used in the standard version of the BSM method in order to partition the neutrons and protons between the two fragments for a given mass split. The location of the symmetric split is indicated by short lines crossing the UCD lines. When we discuss errors along the UCD line and when this line does not locate on integer proton or neutron numbers we take the average error of the most nearby masses (with integer  $Z$  and  $N$ ).

For fission of  $^{187}\text{Ir}$  symmetric fission leads to fragments for which the masses are calculated to be too high by about 2.5 MeV. Since the symmetric fission configuration consists of two such fragments we find that the potential-energy surface is too high by about 5 MeV for the symmetric fission configuration for  $^{187}\text{Ir}$ . In contrast, for symmetric fission of  $^{240}\text{Pu}$  the mass discrepancy at symmetry is almost zero. We illustrate in Figs. 4 and 5 the potential-energy accuracy determined in this way along all UCD lines of six representative fissioning systems, namely  $^{180}\text{Hg}$ ,  $^{187}\text{Ir}$ ,  $^{210}\text{Po}$ ,  $^{226}\text{Th}$ ,  $^{240}\text{Pu}$ , and  $^{258}\text{Fm}$ . This type of plot shows if a particular asymmetric mass split might be favored (positive deviation) or disfavored compared to a more accurate potential-energy surface. At each fragment split  $A_f$  the plotted error is the sum of the calculated mass error of the two fragments. We note immediately that the largest

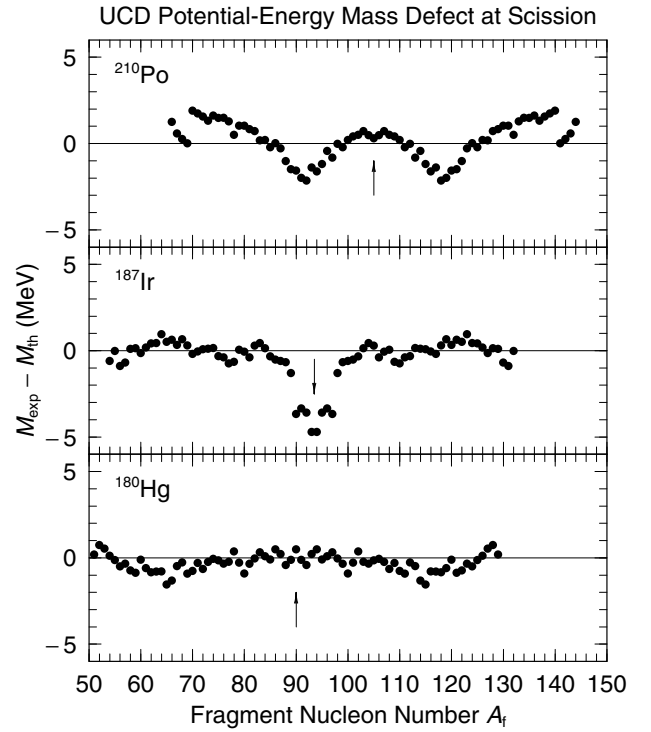


FIG. 4. Difference between experimental masses and calculated ground-state masses for a range of mass splits in fission along the UCD lines for three representative compound systems in the below Pb region. The thin arrows show the locations of symmetric splits.

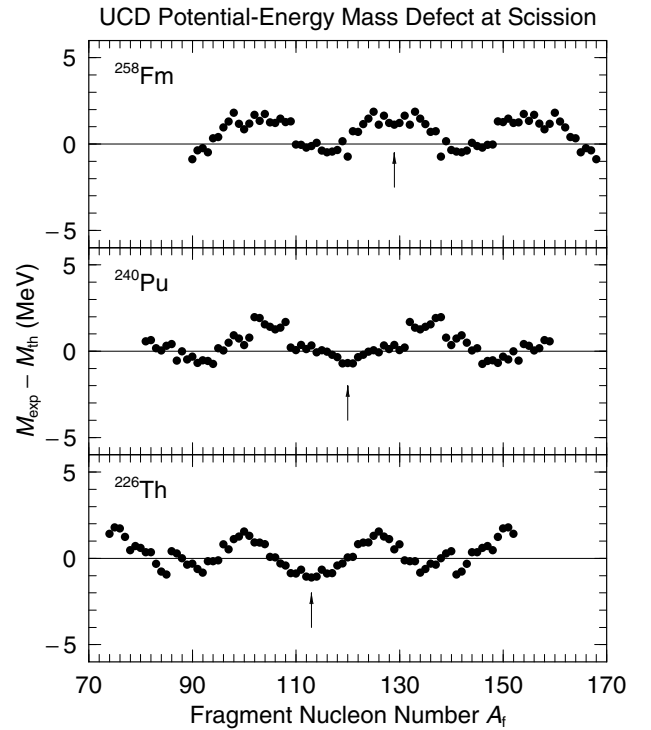


FIG. 5. Difference between experimental masses and calculated ground-state masses for a range of mass splits in fission along the UCD lines for three representative compound systems in the “classical region of asymmetry” (actinide region). The thin arrows show the locations of symmetric splits.

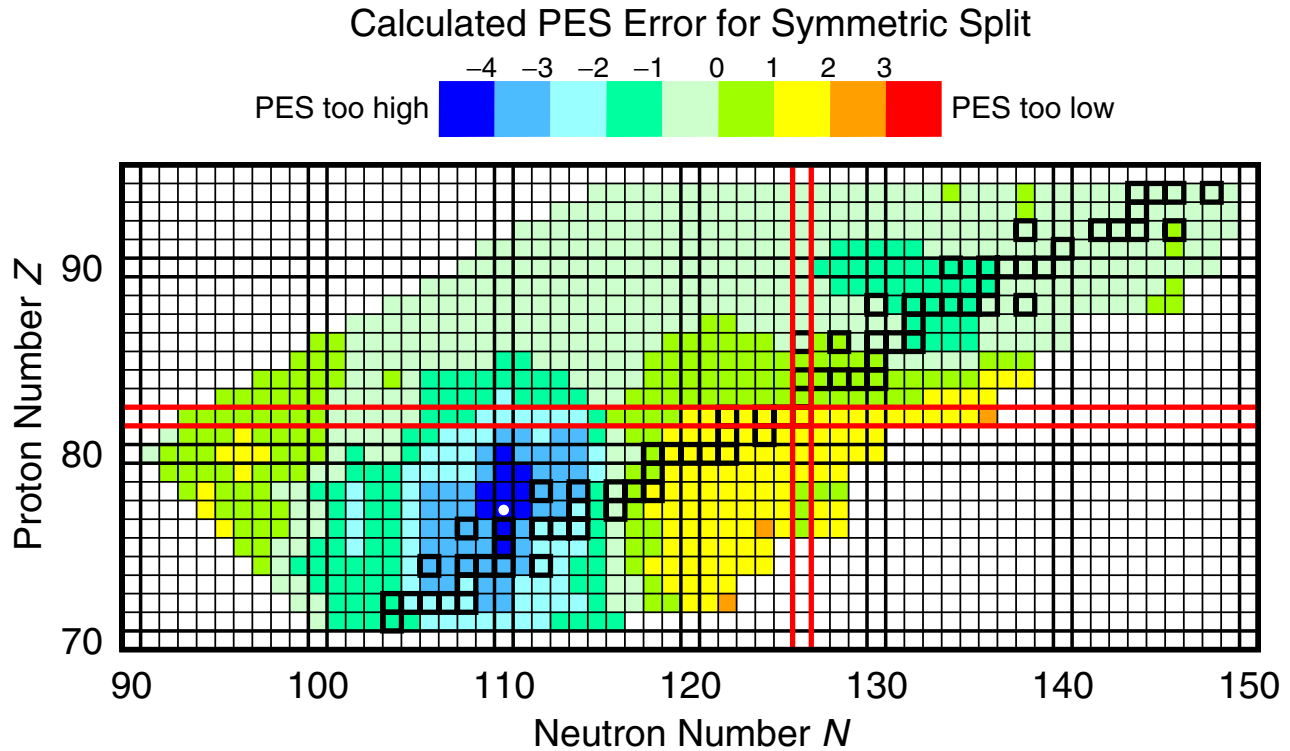


FIG. 6. Difference between experimental masses and calculated ground-state masses for symmetric mass splits for fission of compound systems in the below Pb region and extending into the beginning of the actinide region. The location of the compound fissioning nuclide  $^{187}\text{Ir}$  is indicated by a white circle. Open black squares indicate experimentally known  $\beta$ -stable nuclides.

deviation is for symmetric split of  $^{187}\text{Ir}$ , namely  $\approx -5$  MeV. With our definition of potential-energy surface accuracy at scission this is actually the largest deviation that can occur for symmetric scission points for any nuclide in the region  $Z \geq 70$  and  $N \geq 90$  because there are no larger mass errors in the FRLDM2002 mass model in the regions where the fission fragments “land.” Because at each division we have added the error of the light and heavy fragment the sum can be small when the individual fragment errors are large when they are of opposite sign and roughly cancel each other.

We show in Figs. 6 and 7 the potential-energy accuracy at symmetric scission configurations for all heavy nuclei when experimental masses for the fragments are available. As surmised just above, the largest deviations occur in the vicinity of the location of the symmetric split of  $^{187}\text{Ir}$ . We also notice that in the heavier region from the actinide to the superheavy region the errors in the landing locations for symmetric fission are consistently much smaller. This is also to be expected because fission fragments in symmetric fission of these heavy nuclides land in a heavier mass region where the mass-model error is considerably smaller than in the landing region in fission of rare-earth nuclides. As a consequence, no major difference between calculated results and experimental observations was observed for fission of actinides, as benchmarked in Refs. [5,9]. However, some larger deviations in detailed, calculated fission-fragment charge distributions that include descriptions of odd-even staggering are visible in results in Ref. [14], in particular near  $Z = 36$  in the light fragment peak

in fission of uranium isotopes. It was pointed out that this deviation also occurs because the corresponding light fragments land in the region of large mass-model deviations centered at  $Z = 40$  and  $N = 56$ .

### III. SUMMARY AND CONCLUSIONS

The actinide region of asymmetric fission was extensively studied for close to a century. In contrast, the extent of the preactinide asymmetric-fission “island” is under very active research only since the time of the experiment of Andreyev *et al.* in 2008 [2], which demonstrated the occurrence of a well-developed asymmetric split for fission at low excitation energies of the neutron-deficient nuclide  $^{180}\text{Hg}$ . In 2015 the BSM method, which gave realistic results for actinide fission, in a large-scale calculation predicted a new contiguous region of asymmetric fission in the “rare-earth” (also referred to as below-Pb) region. These predictions were found to be overall consistent with the numerous experimental studies going on in parallel since the communication by Andreyev *et al.* [2]. However, recently, from the experimental side, Dhuri *et al.* [19] emphasized the clear discrepancy between the model and measurements for  $^{187}\text{Ir}$ . The calculation showed a well-developed asymmetric fission-fragment mass distribution at low excitation energy, whereas experiments are dominantly symmetric.

Symmetric fission fragments in the fission of  $^{187}\text{Ir}$  land in an area where the mass-model errors and consequently the

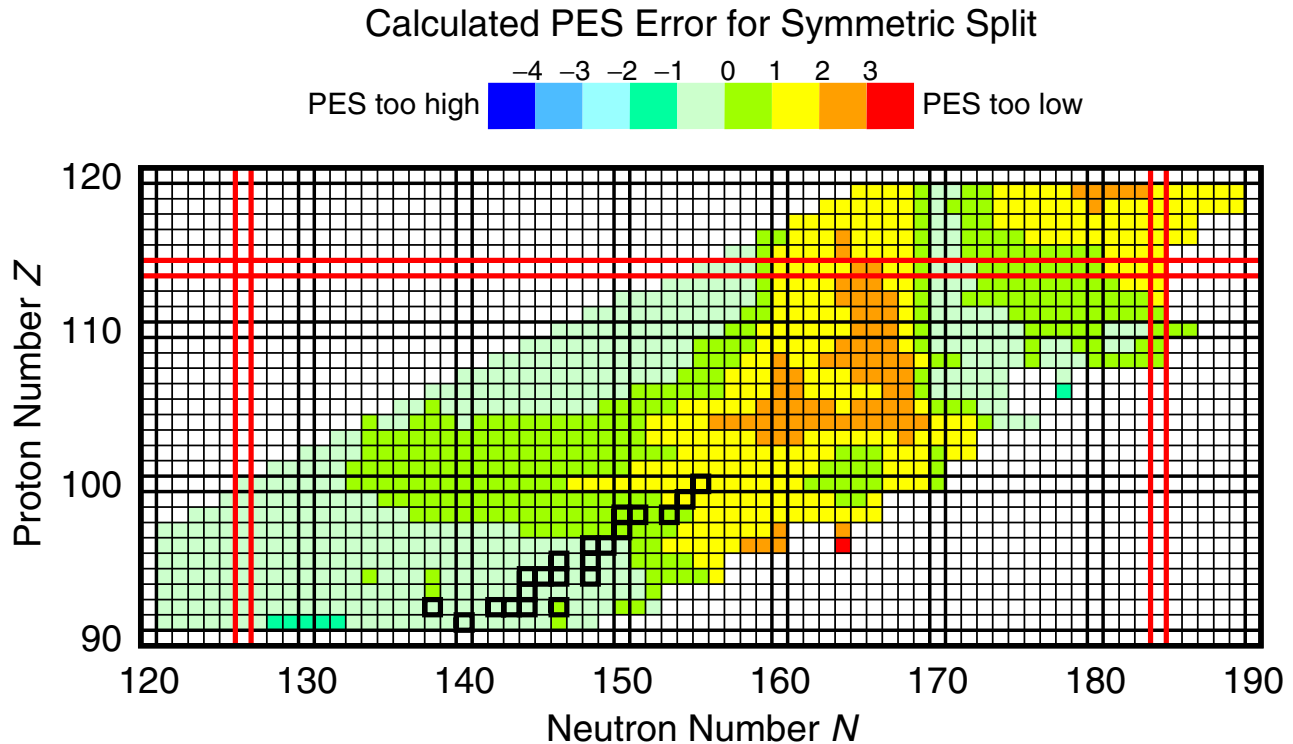


FIG. 7. Difference between experimental masses and calculated ground-state masses for symmetric mass splits for fission of compound systems in the region of the heaviest elements. Open black squares indicate experimentally known  $\beta$ -stable nuclides.

potential-energy errors near scission are unusually large. It is well known for more than half a century that in nuclei with proton number near  $Z = 40$  and  $N = 56$  the corresponding spherical level gaps open up. These two gaps become much larger than has so far been obtained in global single-particle models. In nuclei symmetric fission leading to fragments near these nucleon numbers is therefore unusually favored relative to theory. Errors in the calculated 5D potential-energy surfaces leading to fragment splits away from this region for any other fissioning nuclei are probably less than half of this error, that is less than half the 5 MeV we see in the potential-energy surface corresponding to symmetric division of  $^{187}\text{Ir}$ . Only a few fissioning systems can have *both* fragments land in this region of large errors (and it must obviously be symmetric fission) which are seen in Fig. 3. In Figs. 4 and 5 there are deviations of up to  $\pm 2$  MeV for  $^{180}\text{Hg}$ ,  $^{210}\text{Po}$ ,  $^{226}\text{Th}$ ,  $^{240}\text{Pu}$ , and  $^{258}\text{Fm}$ . However, BSM method calculations of fission-

fragment mass distributions for these nuclides agree quite well with experiment [5,9,22]. Therefore local inaccuracies up to this magnitude do not seem to make the calculated fragment distributions inaccurate. Our discussions in this paper showed that larger calculated 5D potential-energy surface inaccuracies occur only in the vicinity of  $^{187}\text{Ir}$ . Therefore we expect that calculated fragment mass distributions will agree with (future) experiments elsewhere.

#### ACKNOWLEDGMENT

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#### DATA AVAILABILITY

The data that support the findings of this article are openly available [21].

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