ON MASSES OF HEAVIEST NUCLEI*

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Dedicated to Wojciech Królikowski in honour of his 70th birthday

Nuclear masses of heaviest nuclei are studied theoretically within a macroscopic–microscopic approximation. Effect of various approaches to the macroscopic part of the mass on the quality of description of already known masses, and also on the masses of nuclei expected to be synthesized in a near future, is analyzed. Even-even nuclei with proton number Z =82–116 and neutron number N =126–176 are considered.

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1. Introduction

Calculation of mass of a very heavy nucleus is important for a prediction of such properties of the nucleus as α-decay energy and α-decay half-life, the knowledge of which is helpful in the identification of the synthesized nucleus and, generally, in projecting the experiment of its synthesis. It is also important for prediction of the excitation energy of a synthesized compound nucleus, which determines the probability of the synthesis.

The objective of the present paper is to study theoretically masses of very heavy nuclei within a macroscopic–microscopic model of a nucleus. More specifically, it is aimed to study the effect of using various approaches to the macroscopic part of the mass on the masses of nuclei, which are expected to be synthesized in a near future. One should mention here that a comparison between various microscopic descriptions of nuclear mass [1]

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shows that the macroscopic–microscopic approach gives, up to now, the best reproduction of measured masses.

The microscopic part (shell correction) of the mass is taken here from [2] (*cf.* also [3]), where it has been calculated with the use of a 7–dimensional deformation space. That calculation was an extension of an earlier analysis [4] of mass, done for a smaller range of heavy nuclei and exploiting a smaller (3–dimensional) deformation space.

The macroscopic (smooth) part of the mass is taken in the present paper in the so called Yukawa–plus–exponential (or finite-range liquid drop) form [5], often used for a long time (*e.g.* [6, 4, 7]). However, the Thomas–Fermi smooth part, studied very recently [8, 9], is also tried.

Parameters of the studied variants of the macroscopic part of mass are adjusted to measured masses [10] of 77 heaviest even–even nuclei with proton number $Z = 82-106$ and neutron number $N = 126-156$. With those parameters, masses and some other properties of a few superheavy nuclei, planned to be synthesized in a near future, are calculated and compared between themselves. Only the Thomas–Fermi macroscopic part of mass is taken directly from [9] and is not varied in the present study.

Method of the analysis is described in Section 2. The results and the discussion of them are given in Section 3.

2. Method of the analysis

As already stated in the Intoduction, our analysis is performed within a macroscopic–microscopic model of a nucleus. Thus, the total mass is presented in the form

$$M(Z,N,\beta_\lambda^0) = M_{\rm macr}(Z,N,\beta_\lambda^0) + M_{\rm micr}(Z,N,\beta_\lambda^0)\,, \tag{1}$$

where the macroscopic (smooth) part of the mass, $M_{\rm macr}$, is described by a macroscopic model of a nucleus and the microscopic part, $M_{\rm micr}$, is given by a model describing its internal (shell) structure. Here, Z and N are proton and neutron numbers of the nucleus, and the deformation parameters β_λ^0 specify its equilibrium shape. The total mass may be also presented in the form

$$M(Z,N,\beta_\lambda^0) = M_{\rm macr}(Z,N,0) + M_{\rm sh}(Z,N,\beta_\lambda^0)\,, \tag{2}$$

where $M_{\rm sh}$, defined by this equation, is the shell correction to mass of a nucleus.

In the present paper, the shell correction $M_{\rm sh}$ is taken from [2], where it has been obtained by calculations performed in the 7–dimensional deformation space $\{\beta_\lambda\}$, $\lambda = 2,3,...,8$. Here, the commonly used deformation parameters β_λ are the coefficients in the expression of nuclear radius (in the intrinsic frame of reference) in terms of spherical harmonics $Y_{\lambda 0}$

$$R(\vartheta) = R_0(\beta_\lambda)\left[1 + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\vartheta)\right]. \tag{3}$$

The dependence of R_0 on the parameters β_λ is determined in this formula by the volume–conservation condition. The shell correction is based on the Woods–Saxon single-particle potential [11], describing the internal structure of a nucleus.

Only the macroscopic part of the mass, $M_{\rm macr}$, is studied in the present paper. It is taken in the form given by the Yukawa–plus–exponential model [5–7]. For even–even nuclei, studied in the present paper, this reads

$$\begin{aligned} M_{\rm macr}(Z,N,\beta_\lambda^0) &= M_H Z + M_n N - a_V(1-\kappa_V I^2)A \\ &+ a_S(1-\kappa_S I^2)A^{2/3}B_1(\beta_\lambda^0) + a_0 A^0 + c_1 Z^2 A^{-1/3} B_3(\beta_\lambda^0) - c_4 Z^{4/3} A^{-1/3} \\ &+ f(k_F r_p) Z^2 A^{-1} - c_a(N-Z) + W \mid I \mid -12A^{-1/2} + 10A^{-1} - a_{el} Z^{2.39}, \end{aligned} \tag{4}$$

where M_H is mass of the hydrogen atom, M_n is mass of neutron, $I = (N-Z)/A$ is the relative neutron excess, $A = Z + N$ is the mass number and the functions $B_1(\beta_\lambda)$ and $B_3(\beta_\lambda)$ describe the dependence of the surface and Coulomb energies, respectively, on the deformation β_λ. The quantities c_1 and c_4 appearing in the Coulomb and the Coulomb exchange correction energies, respectively, are

$$c_1 = \frac{3}{5}\frac{e^2}{r_0}, \qquad c_4 = \frac{5}{4}\left(\frac{3}{2\pi}\right)^{2/3} c_1, \tag{5}$$

where e is the elementary electric charge and r_0 is the nuclear-radius parameter. The quantity $f(k_F r_p)$ appearing in the proton form-factor correction to the Coulomb energy has the form

$$f(k_F r_p) = -\frac{1}{8}\frac{e^2 r_p^2}{r_0^3}\left[\frac{145}{48} - \frac{327}{2880}(k_F r_p)^2 + \frac{1527}{1\,209\,600}(k_F r_p)^4\right], \tag{6}$$

where the Fermi wave number is

$$k_F = \left(\frac{9\pi Z}{4A}\right)^{1/3} r_0^{-1}, \tag{7}$$

and r_p is the proton root-mean-square radius. The last term in Eq. (4) describes the binding energy of electrons and $a_V, \kappa_V, a_S, \kappa_S, a_0, c_a, W$ are adjustable parameters. Thus, only two of these parameters (a_S and κ_S) appear at the term, which depends on deformation. The five remaining free parameters stand at the terms independent of the shape of a nucleus.

3. Results and discussion

3.1. Description of known masses of heaviest nuclei

Let us look first at the quality of description of known masses of heaviest nuclei, when few variants of the macroscopic part of mass are used. As stated in the Introduction, the same microscopic part of mass (*i.e.* the shell correction $M_{\rm sh}$, Eq. (2)), obtained by us in [2], is taken in all these cases.

3.1.1. Traditional macroscopic part

In this variant of the macroscopic part, it is taken in the form specified in Section 2, Eq. (4), and used in many studies (*e.g.* [6, 4, 2, 7]). Only the parameters of this part differ from one paper to another, depending on which shell correction is added to it.

TABLE I

Values of the parameters of the macroscopic part of mass (see text).

a_V MeV	κ_V –	a_0 MeV	c_a MeV	W MeV	κ_S –	rms MeV	ref. –	no. –
(15.994)	(1.927)	(4.40)	(0.212)	(36.00)	(2.30)	0.809	[6]	
(15.994)	(1.962)	(4.40)	(0.330)	(36.00)	(2.30)	0.791	[4]	
(16.001)	(1.922)	(2.62)	(0.103)	(30.00)	(2.34)	1.053	[7]	
(15.994)	1.944	(4.40)	0.283	(36.00)	(2.30)	0.490	[2]	
(15.994)	(1.944)	4.42	(0.283)	(36.00)	(2.30)	0.489	[2]	
(15.994)	1.990	11.04	0.572	(36.00)	(2.30)	0.264	[2]	(1)
(15.994)	2.013	22.60	0.648	(new)	(2.30)	0.249	present	(2)
15.964	2.060	22.42	0.930	(new)	(2.30)	0.245	present	
16.061	1.907	22.75	0	(new)	(2.30)	0.287	present	(3)
(15.994)	1.875	6.83	0.396	(36.00)	κ_V	0.304	present	
(15.994)	1.907	18.70	0.486	(new)	κ_V	0.282	present	
15.933	2.036	19.60	1.111	(new)	κ_V	0.261	present	(4)
(15.994)	1.800	8.90	0	(new)	κ_V	0.651	present	
16.039	1.807	17.61	0	(new)	κ_V	0.321	present	(5)

The results are shown in Table I. For each variant of the parameters, root-mean-square (rms) of the discrepancies between the calculated and experimental masses is given in the Table, as well as the reference from which the values of the parameters are taken. These values, which were not fitted in a given variant are put in parentheses. The cases, in which new (modified) Wigner term has been taken, are denoted by "new" in the column devoted to this term (W). For the cases, when $\kappa_S = \kappa_V$ is taken, the parameter κ_V is put in the column devoted to κ_S. These variants of the parameters, which have been selected to the discussion in Table II, are denoted by (1) to (5) in the last column.

One can see in Table I that the rather old macroscopic part of [6], combined with our shell correction, gives a rather large rms value of the discrepancies between the calculated and measured values of mass: rms=0.809 MeV. The corresponding values of rms obtained with the macroscopic parts of the papers [4] and [7] are 0.791 MeV and 1.053 MeV, respectively. To minimize rms of the discrepancies, when our shell correction is used, the parameters of the macroscopic part have been varied in [2]. One can see that a much lower rms is obtained (0.490 MeV) already in the case, when only 2 parameters: κ_V and c_a are varied. An additional variation of the parameter a_0 (with κ_V and c_a fixed) decreases rms very little. Only a simultaneous variation of all 3 parameters: κ_V, c_a and a_0 results in a further significant decrease of rms (to 0.264 MeV). This indicates that the parameter a_0 is correlated with κ_V and c_a in minimization of the mass discrepancies.

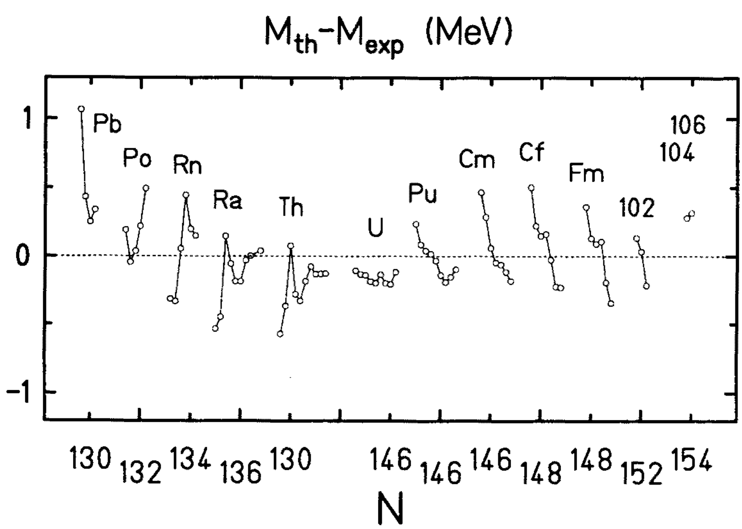

Fig. 1. Discrepancies between calculated and experimental masses in the case of traditional macroscopic part of the calculated mass. The scale in neutron number N is broken between neighboring elements, to make the figure more clear. Only the elements 104 and 106 have common scale. For each element, one neutron number is shown, to make the identification of isotopes possible.

The detailed structure of the discrepancy between the calculated and measured masses, obtained with this variant of the macroscopic part of mass, is given in Fig. 1. A rather complex structure of this discrepancy (*cf.* especially the Rn, Ra and Th isotopes) suggests that it is rather hard to expect to remove this discrepancy by a modification of only the macroscopic (smooth) part of the calculated mass.

3.1.2. Macroscopic part with a modified Wigner term

One may expect that the role of the Wigner term should be decreasing with increasing distance from the $N = Z$ line. Such an attenuated Wigner term was discussed a long time ago in [12] and also recently in [8]. In both these papers this term has been proposed in the form

$$W_a = -b\exp(-c \mid I \mid), \tag{8}$$

with $I = (N - Z)/A$ and $b > 0$, *i.e.* as an extra binding energy of nuclei with $N \approx Z$, attenuated with increasing $\mid I \mid$. Due to the interpretation of this term, it is called in [8] as the "congruence energy". A fit of its parameters to known masses of nuclei with $N \approx Z$ has resulted in the values: $b = 10$ MeV and $c = 4.2$ [8]. In this Subsection, we use this term instead of the Wigner term $W \mid I \mid$ appearing in Eq. (4) of Section 2.

One can see in Table I that a simultaneous variation of 3 parameters: κ_V, c_a and a_0 in the macroscopic part of the mass, when the traditional Wigner term $W \mid I \mid$ is replaced by the term W_a, Eq. (8), leads to rms= 0.249 MeV. Thus, this replacement slightly decreases (by 15 keV) rms of the discrepancies in the masses. Microstructure of these discrepancies is shown in Fig. 2. One can see that it is similar to that of Fig. 1.

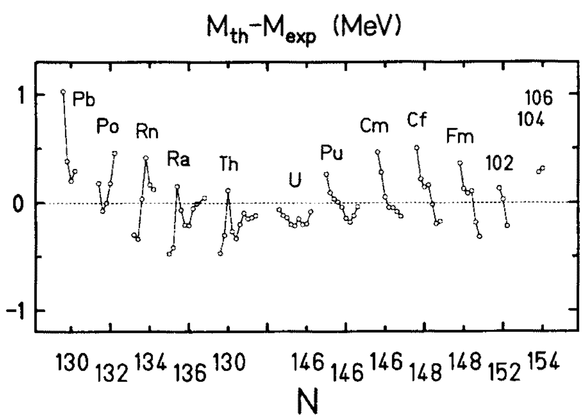

Fig. 2. Same as in Fig. 1, but for the case of the modified Wigner term.

The inclusion of a_V to varied parameters further decreases rms, but only a little (by 4 keV, to rms=0.245 MeV).

3.1.3. Macroscopic part without the charge-asymmetry term

It is interesting to see how much the quality of the description of mass is decreased when the charge-asymmetry term, $-c_a(N-Z)$, is removed. One can see in Table I that rms (0.287 MeV) is not much (by 42 keV) increased by this. Structure of the discrepancies between the calculated and measured masses, obtained in this case, is shown in Fig. 3. It is seen that the structure somewhat differs from that given in Fig. 2.

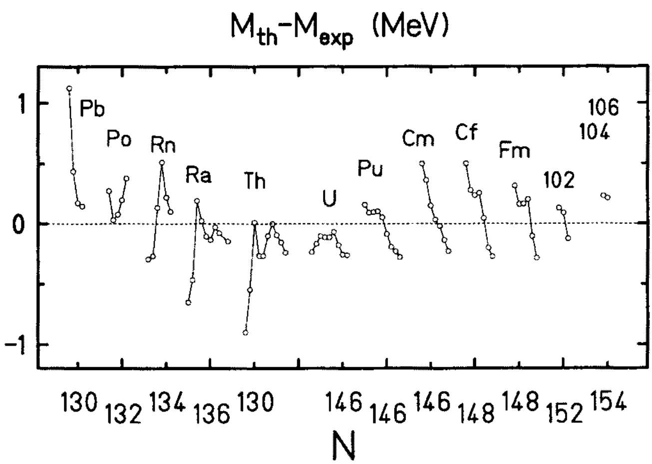

Fig. 3. Same as in Fig. 1, but for the case of the modified Wigner term and $c_a = 0$.

3.1.4. Macroscopic part with $\kappa_S = \kappa_V$

It is already a long time that the surface- and the volume-asymmetry parameters, κ_S and κ_V, respectively, are treated as independent quantities. This may be argued by a different structure of the surface and the interior of a nucleus. Still, it is interesting to see the role of this assumption in the description of masses of heaviest nuclei. To this aim, we have removed this assumption in few variants of the macroscopic part of mass.

One can see in Table I that putting the condition $\kappa_S = \kappa_V$ in the case of the macroscopic part with the old Wigner term and with 3 adjusted parameters: κ_V, a_0, c_a, one increases rms from 0.264 MeV to 0.304 MeV, *i.e.* by 40 keV. The same operation done in the case of the macroscopic part with the new Wigner term increases rms by 33 keV (from 0.249 MeV to

0.282 MeV) and by only 16 keV (from 0.245 MeV to 0.261 MeV) when 4 parameters: a_V, κ_V, a_0, c_a are adjusted. The respective increase of rms is 34 keV (from 0.287 MeV to 0.321 MeV) when 3 parameters: a_V, κ_V, a_0 are fitted in the macroscopic part with the new Wigner term and with $c_a = 0$ (*i.e.* without the charge-asymmetry term). Thus, the assumption that κ_S and κ_V are independent parameters does not seem to be very important for the description of masses of heaviest nuclei. Structure of the discrepancies between the calculated and experimental masses, obtained in the latter case (which corresponds to the last variant of the parameters in Table I) is shown in Fig. 4. It is rather similar to that of Fig. 3.

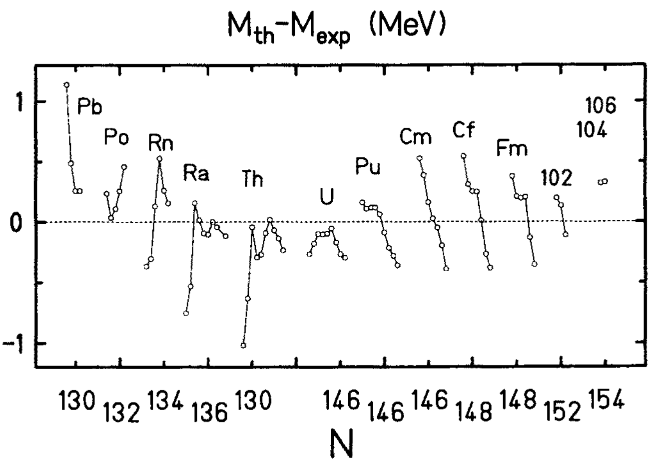

Fig. 4. Same as in Fig. 1, but for the case of the modified Wigner term, $c_a = 0$ and $\kappa_S = \kappa_V$.

3.1.5. Thomas–Fermi macroscopic part

As already stated in the Introduction, the Thomas–Fermi macroscopic part of mass is taken directly from [9] and is not varied in the present paper. The parameters of it have been adjusted to the other shell correction [7] than ours. Due to this, rms obtained with this macroscopic part and our shell correction is large: 1.429 MeV. The corresponding discrepancies between the calculated and experimental masses are shown in Fig. 5. One can see that a readjustment of the parameters of the Thomas–Fermi macroscopic part is necessary, if used with our shell correction. It is interesting to note some similarity between the microstructure of the discrepancies in Fig. 5 and that in Fig. 3.

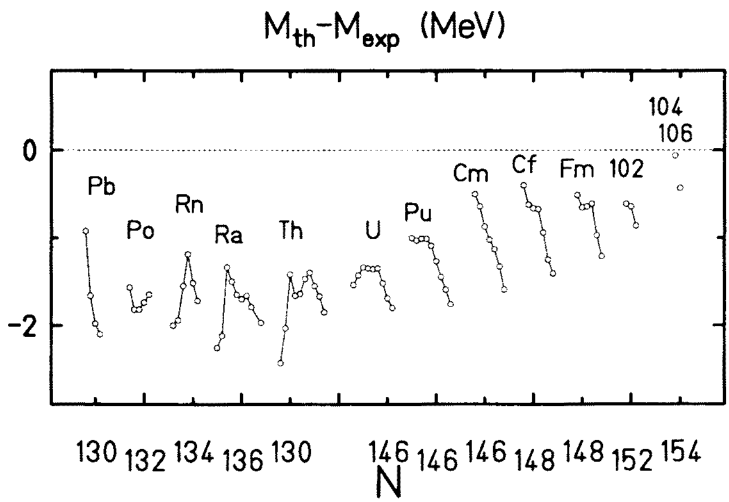

Fig. 5. Same as in Fig. 1, but for the case of the Thomas–Fermi macroscopic part of the calculated mass.

3.2. Predictions for yet unknown nuclei

For the discussion of the effect of changes in the macroscopic part of mass on the properties of yet unobserved nuclei, three nuclei have been chosen: $^{276}112$, $^{288}114$, $^{292}116$. These are the nuclei, which are planned to be synthesized in a near future [13, 14], or are close to those nuclei. Three quantities are calculated: mass M, α-decay energy Q_α and logarithm of the α-decay half-life (given in seconds), $\log_{10}T_\alpha(s)$. Six variants of the macroscopic part are taken for the discussion. Five of them are denoted by (1)–(5) in the last column of Table I and the sixth one is the Thomas–Fermi macroscopic mass.

The results obtained with the variant (1) are:

M=150.19 MeV, 173.67 MeV, 187.16 MeV;

Q_α =12.13 MeV, 10.32 MeV, 11.07 MeV;

$\log_{10}T_\alpha(s) = -5.81, -0.85, -2.26,$

for $^{276}112$, $^{288}114$, $^{292}116$, respectively. Changes of mass corresponding to the changes of parameters from variant (1) to variants (2), (3), (4), (5) do not exceed (in absolute values): 0.28 MeV, 0.06 MeV, 0.07 MeV for the three nuclei, respectively. The respective numbers for Q_α are: 0.05 MeV, 0.02 MeV, 0.02 MeV, and for $\log_{10}T_\alpha(s)$: 0.10, 0.06, 0.03. Structure of the changes is illustrated in Table II for the case of the heaviest nucleus considered: $^{292}116$. Thus, the changes are rather small. In particular, the changes of $\log_{10}T_\alpha$ do not exceed 0.10, which correspond to changes of the half-life T_α, itself, by less than a factor of 1.26. The largest changes are obtained for the lightest (and, simultaneously, with the smallest neutron excess) nucleus $^{276}112$, of all the three nuclei considered.

TABLE II

Changes in predicted mass, α-decay energy and logarithm of α-decay half-life of the nucleus $^{292}116$

Variant –	δM MeV	δQ_α MeV	$\delta\log_{10}T_\alpha$ –
(1)	0	0	0
(2)	-0.04	-0.01	0.03
(3)	0.02	-0.01	0.03
(4)	0.05	-0.01	0.02
(5)	-0.07	-0.02	0.03
(T–F)	-0.46	-0.02	0.04

Concerning the changes when the Thomas–Fermi macroscopic part of mass is taken instead of that corresponding to the variant (1) of parameters, they are:

$\delta M = -0.61$ MeV, -0.44 MeV, -0.46 MeV;
$\delta Q_\alpha = -0.04$ MeV, 0.03 MeV, -0.02 MeV;
$\delta\log_{10}T_\alpha = 0.08, -0.08, 0.04,$

for the nuclei $^{276}112$, $^{288}114$, $^{292}116$, respectively. Thus, even in this case, the changes δQ_α and $\delta\log_{10}T_\alpha$ are not large. Only the changes of mass, δM, are rather large. However, as stated already above, one should not use this macroscopic part of mass with our shell correction, without readjustment of its parameters.

In conclusion, one can say that predictions for such properties of superheavy nuclei as the α-decay energy and the α-decay half-life are not very sensitive to changes in the "classical" (finite-range liquid drop) macroscopic part of mass, given by Eq. (4).

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REFERENCES

[1] Z. Patyk, A. Baran, J.F. Berger, J. Dechargé, J. Dobaczewski, R. Smolańczuk, A. Sobiczewski, *Acta Phys. Pol.* **B27**, 457 (1996).
[2] R. Smolańczuk, A. Sobiczewski, Proc. XV EPS Conf. on nuclear physics: *Low Energy Nuclear Dynamics*, ed. by Yu. Ts. Oganessian, R. Kalpakchieva and W. von Oertzen, St. Petersburg (Russia) 1995, World Scientific, Singapore 1995) p.313.
[3] A. Smolańczuk, J. Skalski, A. Sobiczewski, Proc. Int. Workshop: *Extremes of Nuclear Structure*, Hirschegg (Austria) 1966, in press.
[4] Z. Patyk, A. Sobiczewski, *Nucl. Phys.* **A533**, 132 (1991).
[5] H.J. Krappe, J.R. Nix, A.J. Sierk, *Phys. Rev.* **C20**, 992 (1979).
[6] P. Möller, J.R. Nix, *Nucl. Phys.* **A361**, 117 (1981); *At. Data Nucl. Data Tables* **26**, 165 (1981).
[7] P. Möller, J.R. Nix, W.D. Myers, W.J. Swiatecki, *At. Data Nucl. Data Tables* **59**, 185 (1995).
[8] W.D. Myers, W.J. Swiatecki, Report LBL–37363, Berkeley 1995.
[9] W.D. Myers, W.J. Swiatecki, Report LBL–36803, Berkeley 1994.
[10] G. Audi, A.H. Wapstra, *Nucl. Phys.* **A565**, 1 (1993).
[11] S. Ćwiok, J. Dudek, W. Nazarewicz, J. Skalski, T. Werner, *Comput. Phys. Commun.* **46**, 379 (1987).
[12] W.D. Myers, W.J. Swiatecki, *Nucl. Phys.* **81**, 1 (1966).
[13] S. Hofmann *et al.*, private communication 1995.
[14] Yu.A. Lazarev, Yu.Ts. Oganessian, private communication 1995.