Inner-shell ionization during α decay of superheavy isotopes from the tennessine $^{293}_{117}$Ts and oganesson $^{294}_{118}$Og chains

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Presented here are calculations of probabilities of the K-, L-, and M-shell ionization during α decay of superheavy isotopes $^{293}_{117}$Ts, $^{289}_{115}$Mc, and $^{285}_{113}$Nh involved in the tennessine decay chain as well as $^{294}_{118}$Og, $^{290}_{116}$Lv, and $^{286}_{114}$Fl involved in the new oganesson decay chain. The ionization probabilities are of importance for handling data obtained by methods of the combined α, γ, and conversion-electron spectroscopy used in the superheavy element synthesis analysis. Relativistic calculations are based on the quantum mechanical model. Electron wave functions are determined by the Dirac-Fock method. The α-particle tunneling through the atomic Coulomb barrier is taken into account. Peculiarities of the K-, L-, and M-shell ionization are considered. Results demonstrate that the effect of tunneling through the Coulomb barrier for the L and M shells is of no significance as distinct from the K shell, where the inclusion of the tunneling leads to a considerable decrease of the ionization probability. The probability of ionization from higher shells is larger than that from inner shells. However, the change from the K shell to L shell is much more significant than the change from the L shell to M shell. It has been found that only monopole and dipole terms of the radiative field $L = 0, 1$ make a contribution to the K- and L_1-shell ionization probabilities while contributions of all multipoles $L \leqslant 4$ may be important for the L_2, L_3, and particularly for M_1–M_5 subshells.

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I. INTRODUCTION

Recent discoveries of superheavy elements tennessine $_{117}$Ts and oganesson $_{118}$Og provide a possibility to complete the seventh row of the periodic table of the elements. Names and symbols of the elements have been recommended by International Union of Pure and Applied Physics (IUPAP) [1]. Properties and features of the elements as well as the discovery history are described in Refs. [2,3]. Both elements have been synthesized at the Joint Institute for Nuclear Research (Dubna). The discovery of elements with atomic numbers $Z = 113, 115, 117$, and 118 has been confirmed in Ref. [1]. The investigation of the α-decay products of tennessine revealed two decay chains. The first chain is associated with α decay of the isotope $^{294}_{117}$Ts. The corresponding chain includes isotopes $^{290}_{115}$Mc, $^{286}_{113}$Nh, $^{282}_{111}$Rg, $^{278}_{109}$Mt, $^{274}_{107}$Bh, and the long-life isotope $^{270}_{105}$Db. The second chain is associated with α decay of another isotope $^{293}_{117}$Ts and contains $^{289}_{115}$Mc, $^{285}_{113}$Nh, and $^{281}_{111}$Rg. At present, the only isotope of oganesson $^{294}_{118}$Og has been detected. The observation of α-decay chain of the isotope has been reported in a recent paper [4]. The chain involves isotopes $^{290}_{116}$Lv, $^{286}_{114}$Fl, and $^{282}_{112}$Cn. An active search for new isotopes $^{295,296}_{118}$Og and their associated decay chains is in progress [4].

As was shown earlier (see, for example, Ref. [5]), α decay is accompanied by radiation of the daughter atom electrons in a wide range of energies from eV to several hundred keV. The electron emission may be induced by different atomic processes, in particular, the inner shell ionization, the conversion process, the atomic shell rearrangement, and so on. The inner shell ionization process makes a considerable contribution to the observed electron emission during α decay and therefore the assessment of the process probabilities is of importance for interpretation of spectra obtained in studies of the superheavy isotope decay properties.

The K-shell ionization during α decay was predicted by Migdal in Ref. [6]. Later the probability of the process was studied theoretically [7–10] and experimentally [10–13] for the $_{84}$Po, $_{86}$Rn, $_{90}$Th, $_{94}$Pu, and other isotopes. Levinger [14] foretold that the L-shell ionization probability increases considerably as compared with the K-shell one. The L-shell ionization probability during α decay of the $^{210}_{84}$Po was considered in Refs. [5,6,13,15,16]. The calculations used the H-like electron wave functions or wave functions with approximate consideration of the screening. In addition, in specific cases, multipole terms which contribute significantly to the ionization probability were not taken into account. For example, calculations [6,10,15] were carried out in the dipole approximation without considering monopole terms, which may have a dramatic impact on the ionization probability.

We calculated the ionization probabilities for the K shell during α decay of several $_{84}$Po isotopes and of $^{222}_{86}$Rn [17,18] and for the L shells [19] during α decay of $^{210}_{84}$Po isotopes. Our results were obtained on the basis of the quantum

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mechanical model put forward by Anholt [8] using the sudden approximation. The nuclear recoil effect was taken into account. The α-particle tunneling through the atomic Coulomb barrier was accurately considered. Refined formulas were developed in Ref. [17] to take proper account of the tunneling, which was shown to affect considerably the probability of the K-shell ionization. Electron wave functions were calculated by the relativistic Dirac-Fock (DF) method. The method permits us to take into account the nuclear field screening by atomic electrons as well as to include properly the exchange interaction between electrons [20,21]. Calculations were performed using our package of computer codes, RAINE [21].

Calculations [17,18] of the K-shell ionization probabilities for α decay of five $_{84}$Po isotopes and $^{222}_{86}$Rn were compared with experimental data [11,12] and with previous calculations [8]. Our results with consideration for the tunneling effect were shown to be in better agreement with the experiments than calculations [8]. Probabilities obtained without considering the tunneling presented also in Refs. [17,18] were close to results from Ref. [8]. Our values of the L-shell ionization probability during α decay of $^{210}_{84}$Po [19] agreed with experiments [13,15] better than calculations [9,16]. This gives a chance to use our approach for determination of the inner shell's ionization probability during α decay of superheavy nuclei. Calculations of the L-shell ionization probability were carried out in Ref. [19] for certain of isotopes from the first tennessine α decay chain, namely, for $^{294}_{117}$Ts, $^{286}_{113}$Nh, $^{278}_{109}$Mt, and $^{270}_{105}$Db.

In the present paper, the model mentioned above is used for calculations of the K-, L-, and M-shell ionization probabilities during α decay of isotopes from the second tennessine chain, $^{293}_{117}$Ts, $^{289}_{115}$Mc, and $^{285}_{113}$Nh, as well as from the oganesson chain, $^{294}_{118}$Og, $^{290}_{116}$Lv, and $^{286}_{114}$Fl. We calculate also the M-subshell ionization probability accompanying the α decay of $^{210}_{84}$Po, which has been studied experimentally [15]. A good agreement between the total M-shell probability [15] and our theoretical value suggests that calculations for the M_1–M_5 subshells of superheavy isotopes will be adequate.

Formulas and computational methods employed in calculations have been described in detail previously [17], so in Sec. II, we outline briefly only basic expressions underlying the calculations. In Sec. III, to confirm the validity of approximations in use, we compare ionization probabilities calculated for the K, L, and M shells during α decay of the $_{84}$Po isotopes and $^{222}_{86}$Rn with available experimental data. Next, we present new results obtained for the K-, L-, and M-shell ionization probability accompanying α decay of the superheavy isotopes listed above. Probabilities for different shells of superheavy elements are compared among themselves as well as with corresponding probabilities of heavy isotopes.

II. BASIC FORMULAS

According to Refs. [8,22], ionization from the daughter atom inner shell accompanying α decay is considered using the united atom approximation. The total amplitude of the ionization is treated as the sum of the standard semiclassical ionization amplitude and the quantum amplitude of the α-particle tunneling through the atomic Coulomb barrier. The α particle escaping from a nucleus is represented as a divergent wave, which is matched with an electron wave function at the point $r = R_{\rm nucl}$, where $R_{\rm nucl}$ is the nuclear radius. In this approximation, the differential probability $dP_i(E_f)/dE_f$ of the inner shell ionization accompanying α decay is expressed as [17]

$$\frac{dP_i(E_f)}{dE_f} = (Z_1\alpha)^2(2j_i+1)(2\ell_i+1) \times \sum_L \sum_{\kappa_f} \frac{(2j_f+1)(2\ell_f+1)}{(2L+1)^2}\left(C^{L0}_{\ell_i 0 \ell_f 0}\right)^2 \times W^2[\ell_i j_i \ell_f j_f; 1/2\, L]\left|\tilde{H}^{(L)}_{if}\right|^2. \quad (1)$$

Here Z_1 is the α-particle charge, α is the fine structure constant, ℓ and j are the orbital and total angular momenta of the emitted electron, respectively, L is the multipolarity of the radiative field, $\kappa = (\ell - j)(2j+1)$ is the relativistic quantum number, $C^{L0}_{\ell_i 0\ell_f 0}$ is the Clebsch-Gordan coefficient, and $W[\ell_i j_i \ell_f j_f; 1/2\, L]$ is the Racah coefficient. Subscripts i and f refer to the initial bound and final continuum electron state, respectively. The matrix element $\tilde{H}^{(L)}_{if} = H^{(L)}_{if}/Z_1$. We use relativistic units where the electron Compton wavelength $\hbar/m_0c$ serves as unit of length and the electron rest mass m_0c^2 serves as unit of energy. The total probability $P_i(Q_\alpha)$ of the ith-shell ionization at the α-particle energy Q_α is found as a result of integration of the differential probability $dP_i(E_f)/dE_f$ over the final electron energy E_f.

The matrix element $H^{(L)}_{if}$ without considering the α-particle tunneling through the atomic barrier may be written as

$$H^{(L)}_{if} = Z_1\left[\frac{1}{\omega}\int_0^\infty \sin(\omega t)\dot{R}(t)\frac{d\tilde{\mathcal{G}}^{(L)}_{if}(R)}{dR}dt - \delta_{L,1}\frac{Z_2}{M_2}I^{(1)}_{if}\int_0^\infty \cos(\omega t)\frac{1}{R^2(t)}dt\right] + iZ_1\left\{\frac{1}{\omega}\int_0^\infty \cos(\omega t)\dot{R}(t)\frac{d\tilde{\mathcal{G}}^{(L)}_{if}(R)}{dR}dt + \delta_{L,1}\frac{Z_2}{M_2}I^{(1)}_{if}\int_0^\infty \sin(\omega t)\frac{1}{R^2(t)}dt + \frac{1}{\omega}\left[\tilde{\mathcal{G}}^{(L)}_{if}(R_0) - \delta_{L,0}I^{(-1)}_{if}\right]\right\}, \quad (2)$$

where $\omega = E_f + \varepsilon_i$ is the electron transition energy and ε_i is the ith-shell eigenvalue. The time function $\dot{R}(t)$ is related to the α-particle trajectory over time $R(t)$ from the atomic Coulomb barrier with the radius R_0 to infinity in the following way:

$$\dot{R}(t) = v\left[1 - \frac{R_0}{R(t)}\right]^{1/2}. \quad (3)$$

Functions $R(t)$ and $\dot{R}(t)$ take the following values at the initial time moment $t=0$:

$$R(0)=R_0,\quad \dot{R}(0)=0\,. \tag{4}$$

In Eq. (3), v is the final velocity of the α particle,

$$v=[2(Q_\alpha-\omega)/\mu]^{1/2}, \tag{5}$$

where μ is the reduced mass for the α-particle mass M_1 and the daughter nucleus mass M_2. The Coulomb radius R_0 is determined as

$$R_0=\frac{Z_1Z_2\alpha}{Q_\alpha-\omega}, \tag{6}$$

where the daughter nucleus charge $Z_2=Z-Z_1$ and Z is the parent nucleus charge.

The relativistic radial form factor $\tilde{\mathcal{G}}^{(L)}_{if}(R)$ entering in Eq. (2) takes the form

$$\begin{aligned}\tilde{\mathcal{G}}^{(L)}_{if}(R)=&\frac{1}{R^{L+1}}\int_0^R r^L[G_i(r)G_f(r)+F_i(r)F_f(r)]dr\\&+R^L\int_R^\infty\frac{1}{r^{L+1}}[G_i(r)G_f(r)+F_i(r)F_f(r)]dr.\end{aligned} \tag{7}$$

Integrals $I^{(1)}_{if}$ and $I^{(-1)}_{if}$ are given by

$$I^{(1)}_{if}=\int_0^\infty r[G_i(r)G_f(r)+F_i(r)F_f(r)]dr, \tag{8}$$

$$I^{(-1)}_{if}=\int_0^\infty\frac{1}{r}[G_i(r)G_f(r)+F_i(r)F_f(r)]dr. \tag{9}$$

In Eqs. (7)–(9), $G(r)$ and $F(r)$ are the large and small components of the Dirac electron wave function multiplied by r. Electron wave functions are calculated by the DF method; that is, the bound and continuum wave functions represent the solutions of the DF equations with exact consideration of the exchange interaction between bound atomic electrons as well as between bound and free electrons [21]. The bound electron wave functions are normalized so that

$$\int_0^\infty\left[G_i^2(r)+F_i^2(r)\right]dr=1. \tag{10}$$

The continuum electron wave functions are normalized per unit energy range.

To take into account the α-particle tunneling through the atomic Coulomb barrier, the additional term $a^{(L)}_{if}(E_f)$ have to be included in the imaginary part of the matrix element $H^{(L)}_{if}$ [Eq. (2)]. The refined expression for the term was derived in our paper [17]. The expression is given by

$$\begin{aligned}a^{(L)}_{if}(E_f)=&-i\frac{R_0}{v}\int_{x_0}^1\frac{xdx}{\sqrt{x-x^2}}b^{(L)}_{if}(xR_0)\\&\times\exp\left\{-\omega\frac{R_0}{v}\left[\frac{\pi}{4}+\sqrt{x-x^2}\right.\right.\\&\left.\left.+\frac{1}{2}\arcsin(1-2x)\right]\right\},\end{aligned} \tag{11}$$

where

$$x_0=R_{\rm nucl}/R_0, \tag{12}$$

$$b^{(L=0)}_{if}(R)=\tilde{\mathcal{G}}^{(L=0)}_{if}(R)-I^{(-1)}_{if}, \tag{13}$$

$$b^{(L=1)}_{if}(R)=\tilde{\mathcal{G}}^{(L=1)}_{if}(R)+I^{(1)}_{if}\omega^2R\left(\frac{1}{Z_2}-\frac{\mu}{M_2Z_1}\right). \tag{14}$$

We present expressions for $a^{(L)}_{if}(E_f)$ only at $L=0$ and $L=1$ because as will be shown below (see Table II), the tunneling is important for the K-shell ionization and makes a minor contribution to the L_1-subshell ionization. In both cases, only the monopole and dipole terms contribute to ionization probabilities (see Table III).

III. RESULTS AND DISCUSSION

Probabilities of the inner shell ionization accompanying α decay were calculated in the framework of the model outlined above with allowance made for the α-particle tunneling through the atomic Coulomb barrier. All significant multipoles of the radiative field were taken into account. The relativistic electron wave functions were obtained by the self-consistent DF method.

To demonstrate the validity of this approach, we compare in Table I our theoretical ionization probabilities for the K-shell [17], L-shell [19], and M-shell (this work) electrons with available experimental data for various $_{84}$Po isotopes and for $^{222}_{86}$Rn. The K-shell ionization probabilities are presented for four Po isotopes and the differences between theory and experiment vary between 15% and 34%. This is a much better agreement than that obtained by Anholt [8], as has already been discussed in Ref. [17].

The ionization of the L subshells accompanying α decay of the $^{210}_{84}$Po isotope has been measured in Refs. [13,15]. The experimental results from Ref. [13] agree very well with our calculations for the L_1 and L_3 subshells, but the result for L_2 is nearly three times larger than our theoretical value. However, the experimental result for the L_2 subshell from the other paper [15] agrees well with our theory. We compare with the experiments also the total L-shell ionization probability

$$P_{L_{\rm tot}}=\sum_{i=1}^{3}P_{L_i}\,. \tag{15}$$

The theoretical total L-shell probability agrees satisfactory with both experimental values, the difference being 22% compared to Ref. [13] and 11% compared to Ref. [15]. As was shown in Ref. [19], our results for the L-subshells ionization probabilities during the $^{210}_{84}$Po α decay correlate better with experimental values than previous calculations [9,16].

The total M-shell ionization probability

$$P_{M_{\rm tot}}=\sum_{i=1}^{5}P_{M_i} \tag{16}$$

during α decay of $^{210}_{84}$Po was also measured in Ref. [15]. As is seen from Table I, our value of $P_{M_{\rm tot}}$ is in excellent agreement with the experimental value, the difference being less than 5%.

TABLE I. Comparison between our calculations of ionization probabilities $P_i(Q_\alpha)$ for the K [17], L [19], and M shells (this paper) during α decay of the $_{84}$Po and $^{222}_{86}$Rn isotopes and available experimental values.

Isotope	Shell	Q_α (MeV)	Our calculations	Experiment	Ref.
$^{210}_{84}$Po	K	5.305	3.00×10^{-6}	$(2.58 \pm 0.08) \times 10^{-6}$	[11]
$^{218}_{84}$Po	K	6.002	4.31×10^{-6}	$(3.73 \pm 0.25) \times 10^{-6}$	[12]
$^{216}_{84}$Po	K	6.777	5.93×10^{-6}	$(4.42 \pm 0.4) \times 10^{-6}$	[11]
$^{214}_{84}$Po	K	7.687	8.02×10^{-6}	$(6.1 \pm 0.3) \times 10^{-6}$	[12]
$^{222}_{86}$Rn	K	5.490	2.94×10^{-6}	$(2.36 \pm 0.22) \times 10^{-6}$	[12]
$^{210}_{84}$Po	L_1	5.403	3.08×10^{-4}	$(3.05 \pm 0.46) \times 10^{-4}$	[13]
$^{210}_{84}$Po	L_2	5.403	8.78×10^{-5}	$(2.83 \pm 0.45) \times 10^{-4}$	[13]
				$(0.62 \pm 0.06) \times 10^{-4}$	[15]
$^{210}_{84}$Po	L_3	5.403	2.46×10^{-4}	$(2.32 \pm 0.5) \times 10^{-4}$	[13]
$^{210}_{84}$Po	L_{tot}	5.403	6.42×10^{-4}	$(8.20 \pm 0.5) \times 10^{-4}$	[13]
				$(7.25 \pm 1.18) \times 10^{-4}$	[15]
$^{210}_{84}$Po	M_{tot}	5.403	1.75×10^{-2}	$(1.84 \pm 0.37) \times 10^{-2}$	[15]

Note. Two experimental values obtained in Refs. [13] and [15] are given for the L_2-subshell ionization probability as well as for the total L-shell probability.

Consequently, the calculated ionization probabilities for inner shells of daughter atoms during α decay of the heavy $_{84}$Po and $^{222}_{86}$Rn isotopes are in reasonable agreement with available experimental data. This makes it possible to apply the model to calculations of $P_i(Q_\alpha)$ for superheavy isotopes.

First, we consider the tunneling impact on the inner shell ionization accompanying α decay of superheavy isotopes. As was shown in Ref. [17], taking into account the α-particle tunneling through the atomic Coulomb barrier decreases significantly, up to $\gtrsim$40%, the probability of the K-shell ionization during α decay of the $_{84}$Po isotopes. As the α-particle energy Q_α is lower, the more significant the tunneling effect becomes. For superheavy isotopes, values of $P_i(Q_\alpha)$ calculated with and without consideration for the tunneling effect are presented in Table II for ionization of the K, L, and M shells during α decay of isotopes $^{285}_{113}$Nh, $Q_\alpha = 9.48$ MeV, and $^{286}_{114}$Fl, $Q_\alpha = 10.21$ MeV.

Table II demonstrates that the tunneling affects considerably the K-shell ionization probability for superheavy elements. Taking account of the tunneling decreases the probability $P_K(Q_\alpha)$ by 41% during α decay of $^{285}_{113}$Nh at $Q_\alpha = 9.48$ MeV and by 27% during α decay of $^{286}_{114}$Fl at $Q_\alpha = 10.21$ MeV. The effect is enhanced as the α-particle energy decreases. In the rest cases, the most tunneling effect is equal to 1.4% for the L_1-shell ionization probability. For other subshells, the effect does not exceed 0.5%. We do not list the data for the M_2–M_5 subshells because a tunneling consideration has no effect on them. Consequently, the tunneling effect should be necessarily included in calculations of the K-shell ionization probability and should be desirable included in the L_1-subshell calculations.

As was mentioned above, the necessary multipole contributions were not taken into account in a number of previous calculations for heavy isotopes. In this connection, it is of interest to estimate significant multipole contributions to the ionization probabilities for various inner subshells of superheavy isotopes. It has been found [17,18] that the main contribution, ≈80%, to the K-shell ionization probability during α decay of polonium isotopes is made by monopole terms of the radiative field. Dipole terms contribute the rest ≈20%. This may break down for superheavy isotopes and for higher shells. Relative contributions of the various multipoles to the ionization probability $P_i(Q_\alpha)$ accompanying α decay of isotopes $^{285}_{113}$Nh and $^{294}_{118}$Og are presented in Table III for the K, L, and M shells.

Table III shows that for the K shell of superheavy elements, monopole terms $L = 0$ contribute to the probability $P_K(Q_\alpha)$ more than 90%, and the rest of the probability is associated with dipole terms $L = 1$. There is nearly the same multipole distribution for the L_1 shell. However, for the L_2 shell, the main contribution (≈90%) is distributed among monopole and dipole terms as well as an essential contribution ($\gtrsim$10%)

TABLE II. Probabilities $P_i(Q_\alpha)$ of the inner shell ionization accompanying α decay of superheavy isotopes calculated with and without considering the α-particle tunneling through the atomic Coulomb barrier.

Shell	$^{285}_{113}$Nh, $Q_\alpha = 9.48$ MeV		$^{286}_{114}$Fl, $Q_\alpha = 10.21$ MeV	
	Tunneling	No tunneling	Tunneling	No tunneling
K	5.74×10^{-6}	9.74×10^{-6}	7.16×10^{-6}	9.76×10^{-6}
L_1	2.95×10^{-4}	2.99×10^{-4}	3.15×10^{-4}	3.19×10^{-4}
L_2	5.67×10^{-5}	5.68×10^{-5}	6.40×10^{-5}	6.41×10^{-5}
L_3	1.09×10^{-4}	1.09×10^{-4}	1.17×10^{-4}	1.17×10^{-4}
M_1	8.73×10^{-4}	8.77×10^{-4}	8.99×10^{-4}	9.03×10^{-4}

TABLE III. Relative contributions (in %) of various multipoles L to probabilities of ionization $P_i(Q_\alpha)$ accompanying α decay of isotopes $^{285}_{113}$Nh and $^{294}_{118}$Og.

Isotope	$^{285}_{113}$Nh, $Q_\alpha = 9.48$ MeV						$^{294}_{118}$Og, $Q_\alpha = 11.65$ MeV					
Shell/ L	0	1	2	3	4	$\geqslant 5$	0	1	2	3	4	$\geqslant 5$
K	91.7	8.2	0.1				93.4	6.6				
L_1	89.4	10.1	0.5				91.1	8.4	0.4			
L_2	58.9	26.8	13.8	0.5			70.4	19.9	9.4	0.3		
L_3	14.8	50.0	31.8	3.4			16.4	49.2	30.7	3.7		
M_1	74.5	11.6	10.5	3.2	0.2		78.5	9.8	8.9	2.7	0.1	
M_2	60.7	26.3	6.3	5.3	1.4		66.9	22.6	5.1	4.3	1.1	
M_3	21.6	40.3	23.4	8.5	5.8	0.4	22.3	38.2	24.6	8.1	6.2	0.6
M_4	24.9	35.0	21.6	10.4	6.0	2.1	26.8	34.4	20.8	10.1	5.8	2.1
M_5	23.7	35.3	21.1	11.1	6.3	2.5	24.9	35.2	20.3	10.8	6.1	2.7

is made by quadrupole terms $L = 2$. For the L_3 shell, the most considerable contributions are associated with the dipole ($\approx$50%) and quadrupole ($\gtrsim$30%) terms. In addition, there exists even a small octupole $L = 3$ contribution, $\lesssim$4%.

Another multipole distribution occurs for the M shell. The M-subshell ionization probabilities are smeared over multipoles as compared with the K and L shells. For the M_1 shell probability, although the main contribution ($\gtrsim$75%) is made by the monopole term, the dipole and quadrupole terms constitute $\approx$10% each. There exists a small fraction of octupole terms, $\gtrsim$3%. For the M_2 shell, multipoles $L = 0$ and $L = 1$ contribute about 90% and $L = 2$ and $L = 3$ comprise $\gtrsim$10%. The M_3-shell probability includes multipoles to $L = 4$. The M_4- and M_5-shell probabilities include contributions of all multipoles up to $L = 5$. From the results obtained, it may be deduced that probabilities $P_i(Q_\alpha)$ for each a higher shell involve the higher multipole contributions. In addition, the low-multipole contributions increase with the α-particle energy and the nuclear charge.

New calculations of the ionization probability for the K, L, and M shells during α decay of the tennessine isotope $^{293}_{117}$Ts and isotopes entering into the relevant decay chain are presented in Table IV. Table V lists ionization probabilities for oganesson $^{294}_{118}$Og and isotopes from its decay chain.

One can see from Tables IV and V that the ionization probability significantly increases for higher shells. In order to clarify the effect, let us consider differential probabilities $dP_i(E_f)/dE_f$ exhibited in Fig. 1 for the K-, L-, and M-shell ionization accompanying α decay of $^{294}_{118}$Og at $Q_\alpha = 11.65$ MeV. A comparison of relevant curves reveals the difference between the probabilities for various shells. In particular, at high energies of a free electron $E_f \gtrsim 100$ keV, curves $dP_i(E_f)/dE_f$ diminish more rapidly for higher subshells. For example, the drop is more pronounced for the probability of the L subshells and especially of M subshells than for the K shell. This permits calculations of differential probabilities for the L and M shells to be carried out to $E_f \lesssim 1000$ keV while the probability for the K shell are performed up to $E_f \approx 2000$ keV.

In contrast, differential probabilities are seen from Fig. 1 to increase for higher shells at low energies $E_f \lesssim 10$ keV. The low-energy range makes a main contribution to the probability $P_i(Q_\alpha)$. This has been demonstrated in Fig. 4 from Ref. [17], where the formation region for the K-shell ionization

TABLE IV. Probabilities $P_i(Q_\alpha)$ of the K-, L-, and M-shell ionization accompanying α decay of isotopes from the tennessine α-decay chain.

Isotope	$^{293}_{117}$Ts	$^{289}_{115}$Mc	$^{285}_{113}$Nh
Shell/Q_α(MeV)	11.03	10.31	9.48
K	8.83×10^{-6}	7.29×10^{-6}	5.74×10^{-6}
L_1	3.40×10^{-4}	3.18×10^{-4}	2.95×10^{-4}
L_2	7.44×10^{-5}	6.54×10^{-5}	5.68×10^{-5}
L_3	1.14×10^{-4}	1.13×10^{-4}	1.09×10^{-4}
L_{tot}	5.29×10^{-4}	4.96×10^{-4}	4.61×10^{-4}
M_1	9.29×10^{-4}	9.02×10^{-4}	8.73×10^{-4}
M_2	7.75×10^{-4}	7.48×10^{-4}	7.20×10^{-4}
M_3	9.85×10^{-4}	1.02×10^{-3}	1.04×10^{-3}
M_4	1.40×10^{-3}	1.45×10^{-3}	1.46×10^{-3}
M_5	2.26×10^{-3}	2.32×10^{-3}	2.36×10^{-3}
M_{tot}	6.35×10^{-3}	6.44×10^{-3}	6.45×10^{-3}

TABLE V. Probabilities $P_i(Q_\alpha)$ of the K-, L-, and M-shell ionization accompanying α decay of isotopes from the oganesson α decay chain.

Isotope	$^{294}_{118}$Og	$^{290}_{116}$Lv	$^{286}_{114}$Fl
Shell/Q_α(MeV)	11.65	10.80	10.21
K	1.04×10^{-5}	8.34×10^{-6}	7.16×10^{-6}
L_1	3.58×10^{-4}	3.32×10^{-4}	3.15×10^{-4}
L_2	8.23×10^{-5}	7.10×10^{-5}	6.41×10^{-5}
L_3	1.19×10^{-4}	1.16×10^{-4}	1.17×10^{-4}
L_{tot}	5.60×10^{-4}	5.19×10^{-4}	4.96×10^{-4}
M_1	9.52×10^{-4}	9.19×10^{-4}	8.99×10^{-4}
M_2	8.01×10^{-4}	7.66×10^{-4}	7.47×10^{-4}
M_3	9.86×10^{-4}	1.01×10^{-3}	1.05×10^{-3}
M_4	1.41×10^{-3}	1.44×10^{-3}	1.50×10^{-3}
M_5	2.27×10^{-3}	2.32×10^{-3}	2.40×10^{-3}
M_{tot}	6.42×10^{-3}	6.45×10^{-3}	6.59×10^{-3}

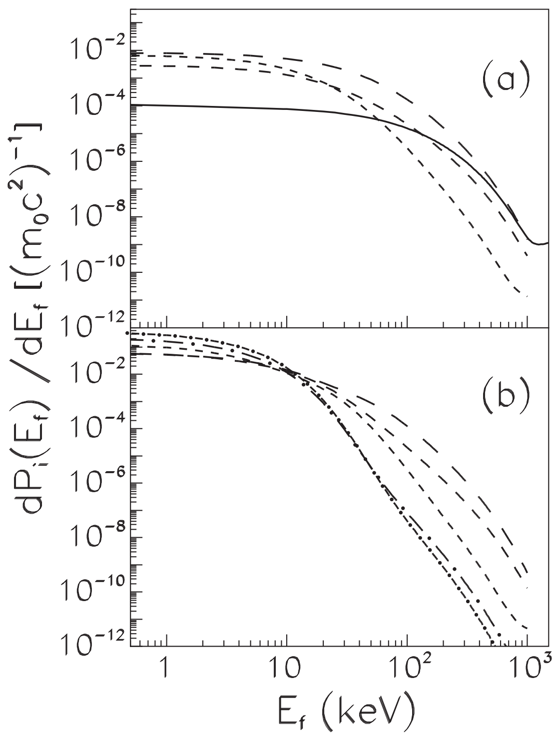

FIG. 1. The differential probability $dP_i(E_f)/dE_f$ of ionization during α decay of $^{294}_{118}$Og at $Q_\alpha = 11.65$ MeV for the K, L (a) and M (b) shells vs the continuum electron energy E_f. (a) Solid, the K shell; large dashed, the L_1 subshell; middle dashed, L_2; small dashed, L_3. (b) large dashed, M_1; middle dashed, M_2; small dashed, M_3; large chain, M_4; small chain, M_5.

probability during α decay of $^{212}_{84}$Po has been displayed. Consequently, the total probabilities $P_i(Q_\alpha)$ should also increase for higher shells.

As is seen from Tables IV and V, the total ionization probability $P_{L_{\rm tot}}(Q_\alpha)$ [Eq. (15)] exceeds considerably the probability $P_K(Q_\alpha)$, while the total probability for the M shell $P_{M_{\rm tot}}(Q_\alpha)$ [Eq. (16)] exceeds $P_{L_{\rm tot}}(Q_\alpha)$ far less. Let us denote the relevant ratios by

$$\begin{aligned} A_{L,K} &= P_{L_{\rm tot}}(Q_\alpha)/P_K(Q_\alpha),\\ A_{M,L} &= P_{M_{\rm tot}}(Q_\alpha)/P_{L_{\rm tot}}(Q_\alpha)\,. \end{aligned} \qquad (17)$$

We list ratios $A_{L,K}$ and $A_{M,L}$ for superheavy isotopes as well as for $^{210}_{84}$Po and $^{222}_{86}$Rn in Table VI. As is seen, the ratios decrease smoothly with a rise in the α-particle energy Q_α, even for a set of various isotopes, that is, the ratios depend mainly on the energy Q_α. In addition, Table VI shows that the ratio $A_{L,K}$ exceeds $A_{M,L}$ by a factor of $\approx$5 for superheavy isotopes and by a factor of $\approx$7 for heavy ones for which energies Q_α are well lower.

So, in the general case, we can expect an enhancement of the ionization probability for each subshell with a higher principal quantum number n as well as for the sum of the subshells

$$\begin{aligned} P_{i\equiv(n+1)\kappa}(Q_\alpha) &> P_{i\equiv n\kappa}(Q_\alpha),\\ \sum_\kappa P_{i\equiv(n+1)\kappa}(Q_\alpha) &> \sum_{\kappa'} P_{i\equiv n\kappa'}(Q_\alpha). \end{aligned} \qquad (18)$$

However, the probability enhancement $A_{(n+1),n} = \sum_\kappa P_{i\equiv(n+1)\kappa}(Q_\alpha)/\sum_{\kappa'} P_{i\equiv n\kappa'}(Q_\alpha)$ decreases by several multiples as n increases:

$$A_{(n+2),(n+1)} < A_{(n+1),n}\,. \qquad (19)$$

It is well to bear in mind that regularities (18) and (19) are true only for the inner shell ionization.

A qualitative consideration of the regularities [Eqs. (18) and (19)] can be performed if it is treated that the inner shells ionization during α decay is caused by the direct collision of α particle with the ith-shell electron [23]. Differences in behavior of the collisional-ionization cross sections for the K, L, and M shells provide insight into differences in probabilities of ionization from the shells.

For heavy and superheavy isotopes, the ratio of the α-particle velocity to the inner-shell electron orbital velocity $\tilde{v}_i = v_\alpha/v_i$ can be approximately estimated as

$$\tilde{v}_{i\equiv K} \approx 0.1;\quad \tilde{v}_{i\equiv L} \approx 0.2;\quad \tilde{v}_{i\equiv M} \approx 0.4\,. \qquad (20)$$

Provided that $\tilde{v}_i \lesssim 1$, we can conveniently use the simple fit expression for the collisional-ionization cross section $\sigma(i, \tilde{v}_i)$ obtained within the Born approximation by Kaganovich *et al.* [24],

$$\begin{aligned} \sigma(i,\tilde{v}_i) = \pi a_0 \frac{E_0^2 Z_1^2}{I_i^2 \tilde{v}_i^2}\big[0.283\ln\big(\tilde{v}_i^2+1\big)+1.26\big]\\ \times \exp\left[-\frac{1.95}{\tilde{v}_i\big(1+1.2\tilde{v}_i^2\big)}\right], \end{aligned} \qquad (21)$$

where $a_0 = \hbar^2/m_0e^2$, $E_0 = m_0v_0^2 = 27.2$ eV, and I_i is the ionization potential. Equation (21) is claimed in Ref. [24] to yield cross-section values which agree with the exact calculations within 20% for $0.2 \lesssim \tilde{v}_i \lesssim 1$.

In Eq. (21), the factor $1/I_i^2$ associated with the ionization potential increases the cross section $\sigma(i, \tilde{v}_i)$ by $\lesssim$2 orders of magnitudes for each higher shell. The exponential factor $\exp\{-1.95/[\tilde{v}_i(1+1.2\tilde{v}_i^2)]\}$ increases the value of $\sigma(i, \tilde{v}_i)$ by several orders. Factors $1/\tilde{v}_i^2$ and $[0.283\ln(\tilde{v}_i^2+1)+1.26]$ influence the cross section only moderately. Consequently, the ionization cross section $\sigma(i, \tilde{v}_i)$ grows in magnitude for

TABLE VI. Ratios $A_{L,K}$ and $A_{M,L}$ [Eqs. (17)] for the heavy and superheavy isotopes.

Isotopes	$^{210}_{84}$Po	$^{222}_{86}$Rn	$^{285}_{113}$Nh	$^{286}_{114}$Fl	$^{289}_{115}$Mc	$^{290}_{116}$Lv	$^{293}_{117}$Ts	$^{294}_{118}$Og
Q_α (MeV)	5.403	5.49	9.48	10.21	10.31	10.8	11.03	11.65
$A_{L,K}$	201.9	199.2	80.3	69.3	68.2	62.4	59.9	53.8
$A_{M,L}$	27.3	26.8	14.0	13.3	12.9	12.4	12.0	11.5

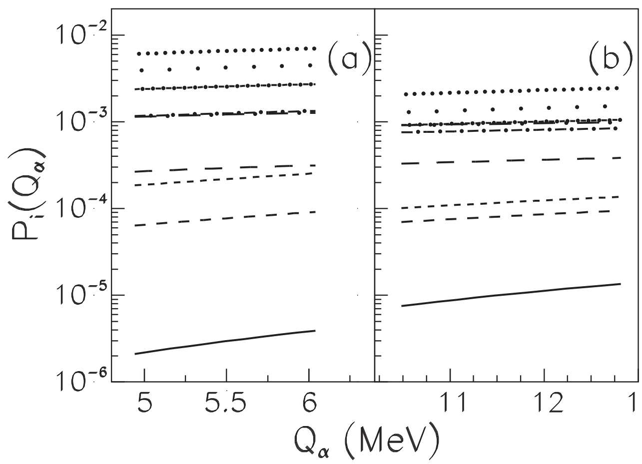

FIG. 2. The probability of ionization $P_i(Q_\alpha)$ during α decay of $^{222}_{86}$Rn (a) and $^{294}_{118}$Og (b) vs the α-particle energy Q_α for the K, L_i, and M_i subshells. Solid, the K shell; long-dashed, the L_1 subshell; middle-dashed, L_2; short-dashed, L_3; long-chain, M_1; middle-chain, M_2; short-chain, M_3; rare-dot, M_4; frequent-dot, M_5.

each a higher shell [see Eq. (18)]. However, in keeping with Eqs. (20), the enhancement of the exponential factor decreases drastically for higher shells, so it is the factor which is responsible also for regularity (19), i.e., in our case, for the fact that the ratio $\sigma(L, \tilde{v}_L)/\sigma(K, \tilde{v}_K)$ is much larger than the ratio $\sigma(M, \tilde{v}_M)/\sigma(L, \tilde{v}_L)$. This can be easily verified for heavy and superheavy isotopes.

The α-particle energy Q_α is not necessarily known with a satisfactory accuracy. Because of this, it is useful to consider the variation of the inner shell ionization probability with the α-particle energy. In Fig. 2, the dependence $P_i(Q_\alpha)$ is displayed under the energy change by $\pm 10\%$. Figure 2(a) refers to the K-, L-, and M-subshell ionization during the α decay of the heavy isotope $^{222}_{86}$Rn, where Q_α changes through the range $4.941 \leqslant Q_\alpha \leqslant 6.039$ MeV. Figure 2(b) refers to the inner shell ionization during α decay of superheavy isotope $^{294}_{118}$Og, where Q_α changes through the range $10.485 \leqslant Q_\alpha \leqslant 12.815$ MeV.

As is seen from Fig. 2, all ionization probabilities grow slowly with increase in α-particle energy. The reason is also understood by reference to Eq. (21). Although a small enhancement of energy Q_α and hence of the velocity ratio $\tilde{v}_i$ decreases somewhat the magnitude of $1/\tilde{v}_i^2$, the exponential factor increases significantly, resulting in an enhancement of cross section $\sigma(i, \tilde{v}_i)$ as the energy Q_α increases.

The K-shell ionization probability (solid curves) increases more rapidly than the L- and M-shell probabilities. For both isotopes, the energy change of 10% brings the $\gtrsim$30% change in P_K and the 15–18% change in P_{L_2} and P_{L_3}. The ionization probabilities for the rest shells, including P_{L_1}, change by 5–9%. Consequently, Fig. 2 shows that the inner shell ionization probabilities except for the K shell depend rather slightly on a comparatively small change of the α-particle energy Q_α.

Figure 2 also demonstrates distinctions between magnitudes of the ionization probabilities for different shells as well as between appropriate shells of different isotopes. In particular, probabilities P_{L_1} and P_{L_2} for $^{222}_{86}$Rn are close to the corresponding probabilities for $^{294}_{118}$Og. However, there is a considerable difference between probabilities of the L_3-subshell ionization, with P_{L_3} being closer to P_{L_1} for $^{222}_{86}$Rn and P_{L_3} being closer to P_{L_2} for $^{294}_{118}$Og. It is also notable that for $^{222}_{86}$Rn, probabilities of the M_1- and M_2-subshell ionization merge while P_{M_3} lies markedly higher. However, for $^{294}_{218}$Og, the M_1 and M_3 probabilities practically merge while P_{M_2} lies slightly lower. In addition, the magnitude of P_K for $^{222}_{86}$Rn is less than P_K for $^{294}_{118}$Og. However, magnitudes of the M-subshell probabilities, especially $P_{M_3}-P_{M_5}$, for $^{222}_{86}$Rn are much larger than for superheavy isotope $^{294}_{118}$Og. This may be assigned to a difference between α-particle energies, because the ionization probability increases with the energy Q_α for the K and L shells and slightly decreases for the M_3, M_4, and M_5 subshells of various isotopes (see Tables I for the K shell of ^{210}Po as well as Tables IV and V).

IV. CONCLUSIONS

New data on probabilities of the K-, L-, and M-shell ionization accompanying α decay of superheavy isotopes $^{293}_{117}$Ts, $^{289}_{115}$Mc, $^{285}_{113}$Nh, $^{294}_{118}$Og, $^{290}_{116}$Lv, and $^{286}_{114}$Fl have been obtained. The isotopes are involved in α decay chains of tennessine and oganesson. Probabilities of the electron emission due to the inner shell ionization are of importance for interpretation of spectra obtained in study of decay properties of superheavy nuclei.

The calculations are based on the quantum mechanical treatment. Electron wave functions are calculated in the framework of the relativistic DF method with the exact consideration of the screening and the electron exchange interaction. The α-particle tunneling through the atomic Coulomb barrier is taken into account. All significant multipoles of the radiative field have been included. The calculated ionization probabilities are shown to be in a reasonable agreement with available experimental values for the K, L, and M shells during α decay of the $_{84}$Po and $^{222}_{86}$Rn isotopes.

Results of calculations have shown that the probability of ionization from higher shells is larger than that from inner shells. However, the change from the K shell to L shell is much more significant than the change from the L shell to M shell. The regularities found in the calculations are supported by a qualitative analysis.

As distinct from the K-shell ionization probability where the effect of the α-particle tunneling through the Coulomb barrier reaches $\gtrsim$40% for superheavy isotopes, the tunneling has a negligible effect on the L- and M-shell ionization probabilities.

The dominant contribution to the K- and L_1-shell ionization probability during α decay of superheavy isotopes, $\gtrsim$90%, is made by monopole terms and the rest is contributed by dipole terms. However, higher multipoles, up to $L = 4$, make considerable contributions to the L_2 and L_3 subshell probabilities and especially to the $M_{1\text{–}5}$ subshell ones.

Small variations in the α-particle energy affect moderately the L- and M-shell ionization probabilities. However, the K-shell ionization probability varies by $\gtrsim$30% under the 10% change in the α-particle energy.

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