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Internal ionization accompanying K conversion: One-step theory

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A one-step theory of internal ionization accompanying K conversion has been developed. The ionization probability and the energy spectrum of the ejected electrons have been calculated using screened relativistic hydrogenic wave functions. It is shown that the probabilities calculated using the present model are in good agreement with the recent experimental values for the K-shell internal ionization accompanying K conversion. The calculated results predict that the ionization probability is dependent on the nuclear transition energy and on the multipolarity of the transition. The multipolarity dependence of the spectral shape of the ejected electrons has also been studied.

[RADIOACTIVITY ^{57}Fe, ^{95,96}Mo, ^{97}Tc, ^{109}Ag, ^{113,114}In, ^{131}Xe, ^{137}Ba, ^{141}Pr, ^{150}Sm, ^{169}Tm, ^{203}Tl; calculated internal ionization probability accompanying K conversion, ejected-electron spectrum.]

I. INTRODUCTION

During the internal-conversion process of an orbital electron, a second electron in the same atom can be ejected as a result of the sudden change in the central potential. A related process, known as internal ionization or electron shakeoff, has been studied theoretically and experimentally by many workers[1,2] for α decay, β decay, and electron capture. The internal ionization accompanying internal conversion is similar to that accompanying photoelectric effect or electron-impact ionization, because the nuclear charge does not change and the ionization process is due to the sudden change in the effective nuclear charge viewed by the atomic electron.

In a previous paper,[3] we calculated relativistically the shakeoff probability accompanying internal conversion within the framework of the sudden approximation. This approximation is based on a two-step model and corresponds to the case where the kinetic energy of the conversion electron is much greater than that of the shakeoff electron. Although this simple approach leads to probabilities which are in good agreement with recent experimental results, it does not take into account energy conservation. Furthermore, it is assumed that the ionization probability is independent of the kinetic energy of the conversion electron and of the multipolarity of the nuclear transition. In order to calculate more refined values of the internal-ionization probability and correct energy spectra of the ejected electrons, the one-step approach must be used, in which the two atomic electrons (a conversion electron and a shakeoff electron) are considered to be emitted simultaneously.

In the present work, we extend our previous theory[3] and estimate the K- and L-shell internal-ionization probabilities accompanying K-shell internal conversion and the ejected-electron spectra by the use of the one-step model. Calculations have been made using screened relativistic hydrogenic wave functions with screening constants determined from relativistic self-consistent-field (SCF) wave functions.

II. THEORETICAL MODEL

In order to simplify the problem, some assumptions have been made. First, antisymmetrization between the final two continuum electrons is not taken into account. As shown in our previous work,[3] in the internal-ionization process accompanying internal conversion the shakeoff electrons are concentrated in the very low-energy region. The most probable energy partition is that the shakeoff electron has a low kinetic energy and the conversion electron has an energy near that of the normal conversion line, forming a satellite line. Therefore, we may consider the effect of electron exchange in the final state to be small.

Second, we ignore the contribution of direct collisions. In addition to ionization due to the sudden change in the effective nuclear charge, there exists an alternative ionization mechanism which is usually referred to as direct collisions: Coulomb scattering of an atomic electron by the conversion electron. As discussed in a previous work,[3] the probability of this process is small when the nuclear transition energy is considerably higher than the binding energy of the atomic electron concerned.

Finally, we neglect K-electron ejection accom-

panying L-shell conversion. This process cannot be distinguished from its counterpart and the experimental observations include both contributions because the sum of the kinetic energies of the ejected electrons as well as the final state of the atom are the same. However, since the change in the effective nuclear charge seen by the K electron during L conversion is very small, this process is less probable than the L-electron ionization accompanying K conversion.

According to first-order perturbation theory, the probability that an orbital electron, initially in the state ψ_{2i}, makes a transition to a final state ψ_{2f} during internal conversion of a K-shell electron that goes from ψ_{1i} to ψ_{1f} can be written

$$w = 2\pi \left| \langle \psi_{1f}\psi_{2f}\psi_f(N) \mid H \mid \psi_{1i}\psi_{2i}\psi_i(N) \rangle \right|^2 \rho . \tag{1}$$

Here $\psi_i(N)$ and $\psi_f(N)$ are the initial and final nuclear wave functions, H represents the interaction between the nucleus and the electron via the electromagnetic field, and ρ is the density of final states. Throughout the present work, relativistic units ($\hbar = m = c = 1$) are used.

In ordinary K conversion, electron 2 is assumed to remain in its initial state and only electron 1 is ejected with a definite kinetic energy. The probability of K conversion is expressed as

$$w_K = \frac{1}{\pi} \sum \left| \langle \psi_{1f} \mid \Phi_{LM}^{(i)} + \vec{\alpha} \cdot \vec{A}_{LM}^{(i)} \mid \psi_{1i} \rangle \right|^2 |M_N|^2 p_0 W_0 . \tag{2}$$

Here p_0 and W_0 are the momentum and the total energy (including the rest mass) of the conversion electron, $\Phi_{LM}^{(i)}$ and $\vec{A}_{LM}^{(i)}$ are the magnetic ($i = m$) or electric ($i = e$) scalar and vector potentials of the radiation field corresponding to total angular momentum L and z component M, and M_N is the nuclear matrix element. The sum in Eq. (2) runs over all the initial and final states. Denoting the binding energy of the K-shell electron as B_K, the energy W_0 is

$$W_0 = k + 1 - B_K , \tag{3}$$

where k is the nuclear transition energy.

On the other hand, when the i-shell electron is ejected with total energy W_2 accompanying K conversion, the probability is given by

$$w_{Ki} dW_2 = \frac{1}{2\pi^3} \sum \left| \langle \psi_{2f} \mid \psi_{2i} \rangle \right|^2 \times \left| \langle \psi_{1f} \mid \Phi_{LM}^{(i)} + \vec{\alpha} \cdot \vec{A}_{LM}^{(i)} \mid \psi_{1i} \rangle \right|^2 \times |M_N|^2 p_1 W_1 p_2 W_2 dW_2 , \tag{4}$$

where p_2 is the momentum of the shakeoff electron, and W_1 and p_1 are the energy and momentum of the conversion electron. The energy relation corresponding to Eq. (4) is expressed as

$$W_1 + W_2 = k + 2 - B_K - B_i - \delta . \tag{5}$$

Here B_i denotes the binding energy of the i-shell electron and δ is the shift of the binding energy of the i-shell electron resulting from the presence of a hole in the K shell.

Defining the differential internal conversion coefficient (ICC) for the nuclear transition energy k and the total energy of the ejected electron W ($1 \leq W \leq W_0$) as $\alpha^{(i)}(W)$, the internal-ionization probability per K conversion as a function of the ejected-electron energy is found from Eqs. (2) and (4) as

$$P_{Ki}(W_2) dW_2 = \frac{n_i}{2\pi^2} \left| \langle \psi_{2f} \mid \psi_{2i} \rangle \right|^2 \frac{\alpha^{(i)}(W_1)}{\alpha^{(i)}(W_0)} p_2 W_2 dW_2 , \tag{6}$$

where n_i is the number of electrons in the i shell. It should be noted that for the K shell n_i is taken to be unity, because only one electron is available in the internal-ionization process.

The total ionization probability per K conversion is given by

$$P_{Ki} = \int_1^{k+1-B_K-B_i-\delta} P_{Ki}(W_2) dW_2 . \tag{7}$$

Using relativistic hydrogenic wave functions in the Coulomb field,[4] the relevant expressions for the atomic matrix element for the ejection of a K- or L-shell electron, $\langle \psi_{2f} \mid \psi_{2i} \rangle$, were already given earlier [Eqs. (5) and (9) in Ref. 3].

The differential ICC in Eq. (6) can be expressed in the same form as the ordinary ICC ($W = W_0$). The analytical expressions for K-shell ICC have been derived by Rose *et al.*[5] and O'Connell and Carroll,[6,7] using relativistic hydrogenic wave functions in the Coulomb field of a point nucleus. By the use of the same wave functions as those for the atomic matrix element, the ICC's for the magnetic and electric multipole radiation are written in the expressions equivalent to those of Rose *et al.* and of O'Connell and Carroll.

III. ENERGY SHIFT, SCREENING CONSTANTS, AND NONRELATIVISTIC CALCULATIONS

A. Energy shift

The energy shift in Eq. (5) is defined as the energy difference between the binding energy of the electron in the presence of a K-shell vacancy and the normal binding energy. When final holes are present in the (nlj) and $(n'l'j')$ shells, the value of δ is estimated as[8,9]

TABLE I. Comparison of calculated probabilities per K conversion of K-electron ejection with measured probabilities.

Nuclide	Energy (keV)	Multipolarity	δ (eV)	Theoretical $P_{KK}\times 10^5$ REL [a]	LEV [b]	TSM [c]	Experimental $P_{KK}\times 10^5$	Method [d]	Ref.
^{57}Fe	122	$M1$	287	15.5	3.98	16.2	4–20	F	8
	136	$E2$	287	14.3	3.62	16.2			
^{95}Mo	204	$M1+25\%E2$	490	7.23	1.28	8.29			
^{96}Mo	778	$E2$	490	8.56	1.47	8.29			
^{97}Tc	96	$M4$	504	1.46	0.276	8.07	≤23	F	11
^{109}Ag	88	$E3$	557	0.916	0.160	7.36	68^{+5}_{-14} [e]	A	12
							<100	F	9
							15.3 ± 2.4	B	13
^{113}In	393	$M4$	585	3.93	0.605	7.07	<2 [f]	C	14
^{114}In	192	$E4$	585	2.06	0.330	7.07	<22 [g]	D	15
							<13 [g]	D	16
							1.7 ± 0.3 [h]	D	17
							12	B	18
^{131}Xe	164	$M4$	654	1.13	0.172	6.19	≃73 [e]	A	19
							11 ± 2 [e]	A	20
							<4	A	21
^{137}Ba	661	$M4$	682	3.76	0.498	6.03	18 ± 5 [i]	E	22
							<20	F	8
							7.1 ± 3.5	B	23
							<5	B	24
^{141}Pr	145	$M1$	719	4.32	0.556	5.74	≃10	B	18
^{150}Sm	334	$E2$	757	3.68	0.410	5.67			
^{169}Tm	...[j]	...[j]	847	1.39	0.134	5.60	7.6 ± 3.8	G	25
^{203}Tl	279	$E2+38\%M1$	1012	3.63	0.220	4.58	25	B	18
							4.0 ± 1.5	B	26

[a] Relativistic theory.
[b] Modified Levinger theory with Slater screening constants.
[c] Two-step model.
[d] A, B, C, D, E, F, and G denote the x-ray–x-ray coincidence, x-ray–x′-ray coincidence, e^--e^- coincidence with solid-state detectors, e^--e^- coincidence using β-ray spectrometers, e^--e^-–x-ray triple coincidence, direct observation of the satellite line in conversion-electron spectrum, and direct observation of the satellite line in x-ray spectrum, respectively.
[e] Calculated from the ratio of the probability for double K-electron emission to the single γ-ray transition probability.
[f] Energy range 68–276 keV.
[g] Energy and angular distributions are assumed to be isotropic.
[h] Energy spectrum is assumed to be that of double internal conversion.
[i] Energy range 115-472 keV.
[j] There are many nuclear transitions which cause double K-electron ejection (see text).

$$\delta = E_T(\text{neutral}) + E_T\left[(nlj)^{-1}(n'l'j')^{-1}\right] - E_T(nlj)^{-1} - E_T(n'l'j')^{-1}, \quad (8)$$

where E_T is the total electronic energy.

In the present work, the numerical values of δ have been calculated for various combinations of the atomic shells using a nonrelativistic hfs program.[10] The results are listed in Tables I and II. The predicted values are in good agreement with the calculated and experimental results of Porter, Freedman, and Wagner[8] for the KL band in ^{57}Fe, and also of Walen, Briançon, and Valadares[9] for the KL band in ^{109}Ag.

B. Screening constants

In order to take into account the Coulomb interaction between electrons, a screening correction has been applied as in our previous work.[3] The nuclear charge Z is replaced by the effective charge $Z_{\text{eff}} = Z - \sigma$.

For bound electrons, the screening constant σ is determined according to the relation[27]

$$\sigma = Z(1 - \bar{r}_Z/\bar{r}_{\text{SCF}}), \quad (9)$$

where $\bar{r}_Z$ is the mean relativistic hydrogenic radius and $\bar{r}_{\text{SCF}}$ is the mean radial distance evaluated from the relativistic SCF wave functions.[28] The expression for $\bar{r}_Z$ is given by Eq. (12) in Ref. 3.

The screening constant for the continuum electrons is taken to be the same as that for the bound electron before ejection. Such choice seems to be realistic, because the greatest contribution to the atomic matrix element and the ICC is from the region near the mean radius of the bound electron.

TABLE II. Comparison of calculated probabilities per K conversion of the L_i-shell electron ejection ($\times 10^4$).

Nuclide	Energy (keV)	Shell	δ (eV)	REL[a]	LEV[b]	TSM[c]
^{57}Ne	122	L_1	74	9.16	11.6	9.20
		L_2	88	7.08	5.22	7.10
		L_3	88	13.8	10.4	13.9
	136	L_1	74	8.99	11.4	9.20
		L_2	88	7.00	5.18	7.10
		L_3	88	13.7	10.4	13.9
^{95}Mo	204	L_1	134	4.47	3.85	4.60
		L_2	161	3.56	1.77	3.63
		L_3	161	6.05	3.55	6.17
^{96}Mo	778	L_1	134	4.62	4.17	4.60
		L_2	161	3.63	1.96	3.63
		L_3	161	6.21	3.93	6.17
^{97}Tc	96	L_1	139	3.14	2.75	4.40
		L_2	167	2.55	1.34	3.30
		L_3	167	4.96	2.68	5.87
^{109}Ag	88	L_1	154	2.70	2.16	3.97
		L_2	186	2.19	1.07	2.95
		L_3	186	3.93	2.13	5.17
^{113}In	393	L_1	164	3.40	2.49	3.87
		L_2	197	2.55	1.18	2.80
		L_3	197	4.44	2.36	4.48
^{114}In	192	L_1	164	2.98	2.21	3.87
		L_2	197	2.30	1.07	2.80
		L_3	197	4.02	2.13	4.48
^{131}Xe	164	L_1	188	2.37	1.63	3.39
		L_2	225	1.92	0.797	2.54
		L_3	225	3.26	1.60	4.20
^{137}Ba	661	L_1	198	2.95	1.88	3.28
		L_2	237	2.27	0.894	2.46
		L_3	237	3.64	1.79	3.91
^{147}Pr	145	L_1	207	3.03	1.79	3.11
		L_2	250	2.30	0.839	2.33
		L_3	250	3.67	1.68	3.71
^{150}Sm	334	L_1	218	2.70	1.50	2.96
		L_2	263	2.07	0.711	2.22
		L_3	263	3.21	1.42	3.42
^{169}Tm	...[d]	L_1	243	2.40	1.16	2.74
		L_2	294	1.95	0.562	2.12
		L_3	294	2.75	1.12	2.94
^{203}Tl	279	L_1	299	2.35	0.803	2.54
		L_2	360	1.89	0.388	2.02
		L_3	360	2.29	0.777	2.41

[a] Relativistic theory

[b] Modified Levinger theory with Slater screening constants.

[c] Two-step model (Ref. 3).

[d] There are many nuclear transitions (see text).

Although two electrons are emitted simultaneously, the ejection mechanisms for these electrons are different. The ejected conversion electron is due to electromagnetic interactions, while the shakeoff electron is due to a sudden change of the Coulomb field when the conversion electron is emitted. Since these electrons are treated as distinguishable in the present model, we use the different screening constants for the final states in the two mechanisms. In the conversion process the screening constant for the final state is the same as that for the initial state, but for the shakeoff electron the screening constant for the final state should be determined taking into account the presence of the K-shell vacancy resulting from the internal conversion.

The screening constant for the shakeoff electron in the final continuum state is estimated by

$$\sigma_c = (\sigma_h/\sigma_S)\sigma , \tag{10}$$

where σ is determined from Eq. (9), and σ_h and σ_S are the Slater screening constants for the atom with the K-shell vacancy and for the ordinary atom, respectively.[29]

C. Nonrelativistic calculations

To compare with the relativistic theory, nonrelativistic calculations of the internal-ionization probability and the ejected-electron spectrum have been performed by the use of the modified Levinger theory. In the original theory of Levinger,[30] the probabilities for ejection of K- and L-shell electrons accompanying the change in the nuclear charge from Z to $Z \pm 1$ were expressed using nonrelativistic hydrogenic wave functions under some assumptions. We have extended his model for an arbitrary change in the effective nuclear charge and derived the analytical expressions for the ionization probabilities without any approximation.[3] The atomic matrix elements for K-, L_1-, and $L_{2,3}$-shell electron ejections are obtained from Eqs. (15), (16), and (17) in Ref. 3 by multiplying by a factor of $2\pi^2/pW$.

Using these matrix elements and Eq. (6), the nonrelativistic calculations have been made. All the screening constants in these calculations were estimated from Slater's recipe.[29]

IV. NUMERICAL RESULTS AND COMPARISON WITH EXPERIMENTS

We have calculated the internal-ionization probabilities per K conversion and the ejected-electron spectra for thirteen nuclides experimentally studied. The nuclear parameters for these nuclides are taken from Lederer, Hollander, and Perlman,[31] and the binding energies of the atomic electrons are from the table prepared by Bearden and Burr.[32] All the numerical calculations in the present work have been performed using the FACOM 230-75 computer in the Data Processing Center of Kyoto University.

A. Internal-ionization probability

The total K- and L_i-shell internal-ionization probabilities per K conversion, P_{KK} and P_{KL_i}

TABLE III. Nuclear parameters of the major transitions in ^{169}Tm used for calculations (taken from Ref. 31).

Energy (keV)	Relative γ-ray intensity (%)	Multipolarity	K-shell ICC
109.77	18	$M1$	2.1
130.51	11	$E2$	0.54
177.18	22	$M1+18\%E2$	0.52
197.97	35	$M1+7\%E2$	0.41
307.68	10	$E2$	0.048

($i=1,2,3$), have been calculated from Eq. (7). For the case of transitions with mixed multipolarities, the probability is obtained by

$$P=\frac{x\alpha^{(m)}P^{(m)}+(1-x)\alpha^{(e)}P^{(e)}}{x\alpha^{(m)}+(1-x)\alpha^{(e)}}, \tag{11}$$

where x is the fraction of the magnetic transition, and $\alpha^{(m)}$, $\alpha^{(e)}$ and $P^{(m)}$, $P^{(e)}$ are the ICC's and the internal-ionization probabilities for magnetic L-pole and electric $(L+1)$-pole transitions, respectively.

A special case is ^{169}Tm, in which there are many nuclear transitions which cause internal ionization accompanying K conversion. From the decay scheme,[31] the values of relative γ-ray intensities, multipolarities, and K-shell ICC's for several major radiations are obtained and shown in Table III. Using these values, the internal-ionization probability for this nuclide is given by

$$P=\frac{\sum_i \alpha_i I_i P_i}{\sum_i \alpha_i I_i}, \tag{12}$$

where α_i is the K-shell ICC, I_i is the relative γ-ray intensity, and P_i is the internal-ionization probability for the ith transition.

The probabilities found in the present numerical calculations are shown in Tables I and II. For comparison, the values obtained by the nonrelativistic calculations and those from the two-step model[3] are also listed. The columns labeled REL, LEV, and TSM correspond to relativistic theory, modified Levinger theory, and two-step relativistic theory, respectively.

As has been pointed out by us,[3] it can be seen from the tables that the relativistic effects do substantially increase the ionization probability. It is also clear that except for ^{96}Mo the REL values are less than the TSM values. The reduction of the probability becomes larger with decreasing nuclear-transition energy and with increasing multipolarity of the transition. A similar energy dependence has been reported in the case of internal ionization accompanying β^- decay[33] and electron capture.[34]

In Table IV the sum of L-shell internal-ionization probabilities per K conversion for all three L subshells are listed.

The experimental studies of the double-electron ejection accompanying K conversion have been summarized and discussed previously.[3] There are three mechanisms which cause simultaneous emission of two atomic electrons: (1) internal ionization, (2) double internal conversion (DIC), and (3) internal conversion of internal Compton effect (ICICE). These processes cannot be distinguished experimentally because of low probabilities. When comparison between the experimental and theoretical values is made, it should be noted that some experimental results were analyzed by using the energy and angular distributions of the DIC or ICICE process.

The experiments may be divided into seven categories: (A) x-ray–x-ray coincidence, (B) x-ray–x′ (hypersatellite)-ray coincidence, (C) e^--e^- coincidence with solid-state detectors, (D) e^--e^- coincidence using β-ray spectrometers, (E) e^--e^-–x-ray triple coincidence, (F) direct observation of the satellite line in the conversion-electron spectrum, and (G) direct observation of the satellite line in x-ray spectrum.

Table I summarizes the experimental results for double K-electron ejection. We have pointed out previously[3] that the reliable values in Table I are those obtained from the (B) -type experiments and that the experimental values of Briand *et al.*[23] for ^{137}Ba $[(7.1\pm3.5)\times10^{-5}]$ and of Desclaux *et al.*[26] for ^{203}Tl $[(4.0\pm1.5)\times10^{-5}]$ are in good agreement with the values calculated according to the two-step model. It is clear from the table that these values agree well with the present refined values, 3.76×10^{-5} and 3.63×10^{-5}, respectively.

After our previous work, four new experiments were reported. Khlyuchikov and Feoktistov[11] performed the (F) -type experiment for three nuclides, but could estimate the upper limit of the P_{KK} value only for ^{97}Tc. Their upper limit is much larger than our theoretical value.

By the (B) -type experiment, Nagy, Schupp, and Hurst[13] have recently obtained a P_{KK} value for ^{109}Ag, which is about a factor of 5 smaller than the previous measurement. Their value is an order of magnitude larger than the calculated value. It should be noted, however, that they could not observe the separate $K\alpha$ hypersatellite line. The intensity and the energy shift of this line were determined by least-squares fitting of the measured spectrum with a two-component Gaussian distribution. This procedure may introduce a large error in the intensity of the line. Furthermore, their experimental data should contain the contribution from the K-shell internal

TABLE IV. Comparison of calculated probabilities per K conversion of the L-electron ejection with measured ones ($\times 10^4$).

Nuclide	Energy (keV)	Theoretical REL[a]	Theoretical LEV[b]	Theoretical TSM[c]	Experimental	Method[d]	Ref.
^{57}Fe	122	30.1	27.3	30.2	90	F	8
	136	30.7	27.0	30.2	90	F	8
^{95}Mo	204	14.1	9.17	14.4	19	F	11
^{96}Mo	778	14.5	10.1	14.4	8.3	F	11
^{97}Tc	96	10.6	6.77	13.6	25	F	11
^{109}Ag	88	8.82	5.36	12.1	20	F	9
^{113}In	393	10.4	6.03	11.5	<1.8[e]	C	14
^{114}In	192	9.30	5.40	11.5	~3	D	35
					<2.6[f]	D	15
					<10[f]	D	16
^{131}Xe	164	7.55	4.02	10.1			
^{137}Ba	661	8.85	4.56	9.65	10	F	8
^{141}Pr	145	8.99	4.30	9.15			
^{150}Sm	334	7.98	3.63	8.60	≃4[g]	F	36
^{169}Tm	...[h]	7.10	2.84	7.80			
^{203}Tl	279	6.53	1.97	6.97			

[a] Relativistic theory.
[b] Modified Levinger theory with Slater screening constants.
[c] Two-step model (Ref. 3).
[d] Symbols are defined in Table I.
[e] Energy range 79–280 keV.
[f] Energy and angular distributions are assumed to be isotropic.
[g] Quoted from Ref. 2.
[h] There are many nuclear transitions (see text).

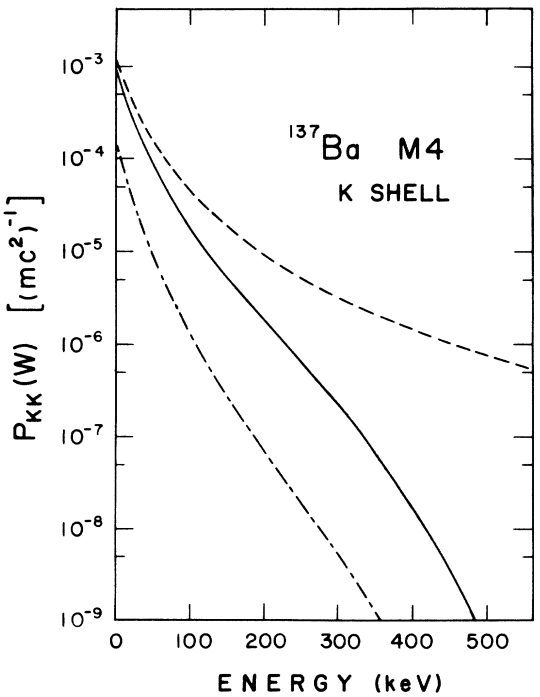

FIG. 1. Energy spectrum of electrons ejected from the K shell accompanying K conversion of the 661-KeV $M4$ transition in ^{137}Ba. The solid curve has been calculated from the present theory; the dashed curve from the two-step model; the dot-dashed curve from the modified Levinger theory with Slater screening constants.

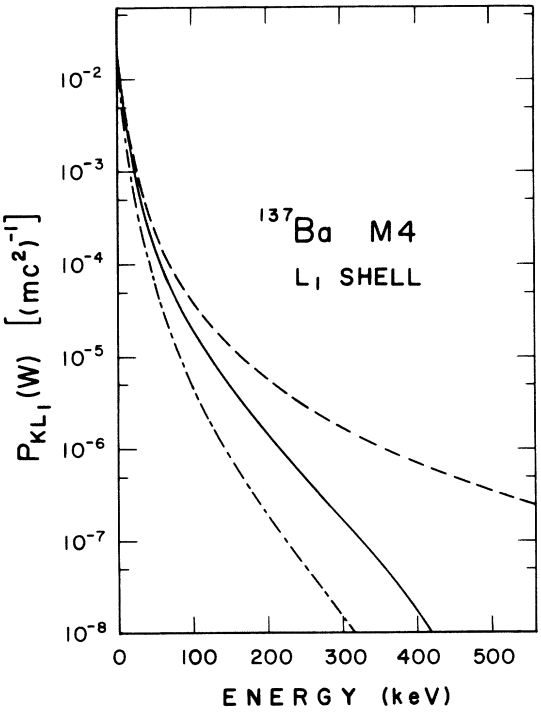

FIG. 2. Energy spectrum of electrons ejected from the L_1 shell accompanying K conversion of the 661-keV $M4$ transition in ^{137}Ba. The solid curve has been calculated from the present theory; the dashed curve from the two-step model; the dot-dashed curve from the modified Levinger theory with Slater screening constants.

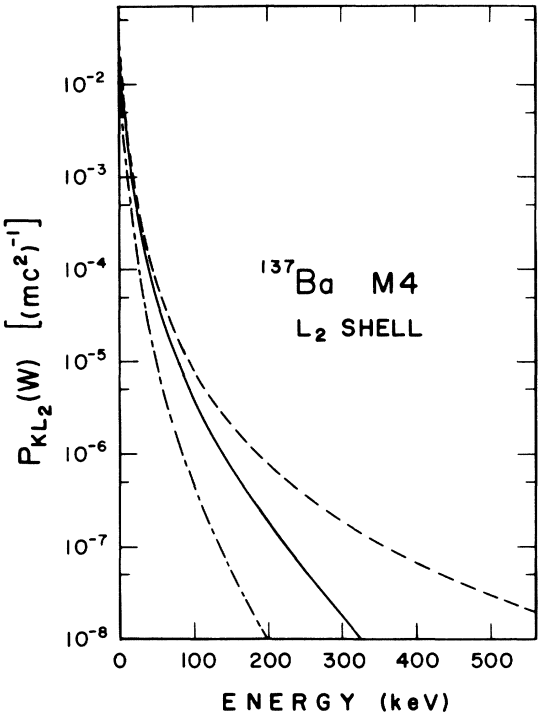

FIG. 3. Energy spectrum of electrons ejected from the L_2 shell accompanying K conversion of the 661-keV $M4$ transition in ^{137}Ba. The solid curve has been calculated from the present theory; the dashed curve from the two-step model; the dot-dashed curve from the modified Levinger theory with Slater screening constants.

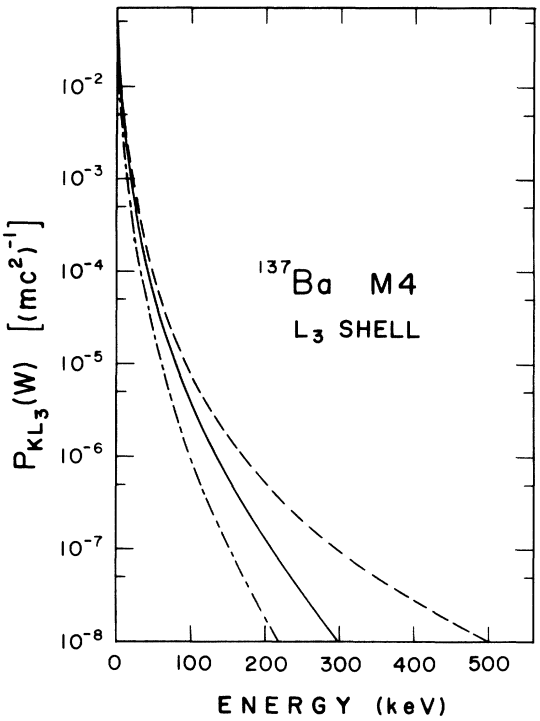

FIG. 4. Energy spectrum of electrons ejected from the L_3 shell accompanying K conversion of the 661-keV $M4$ transition in ^{137}Ba. The solid curve has been calculated from the present theory; the dashed curve from the two-step model; the dot-dashed curve from the modified Levinger theory with Slater screening constants.

ionization accompanying K capture of the parent nuclide ^{109}Cd. It is impossible to distinguish this process from the K-shell internal ionization due to K conversion, because in both processes double K vacancies are created in the daughter atom.

Ito, Isozumi, and Shimizu[24] have recently investigated double K-electron ejection in the decay of ^{137}Ba by triple-coincidence measurement. The K x-ray spectrum in coincidence with another K x ray and the ejected electrons was observed with a Si (Li) detector. However, these authors could not find the $K\alpha$ satellite line at the position reported by Briand *et al.*,[23] and estimated only the upper limit of the probability. The present numerical value is slightly smaller than this upper limit.

In the measurement of Javahery *et al.*,[25] the $K\alpha_1$ hypersatellite line in ^{169}Tm was observed with a curved-crystal spectrometer. The double K-hole creation probability was determined from the intensity of this line relative to that of the normal line. For this nuclide, there are many nuclear transitions which cause double K-electron ejection. The experimental result of Ref. 25 is larger than the theoretical value calculated for the transitions listed in Table III. It should be noted that the K-capture decay of the parent nuclide ^{169}Yb also causes double K-shell vacancies in the final atom and the (G) -type experiment contains both contributions.

Twelve experiments for L-shell ionization accompanying K conversion are listed in Table IV. As has been described,[3] the (C)- and (D)-type experiments cannot be compared directly with the calculated values. In the experiment of Porter, Freedman, and Wagner,[8] the measured values for two transitions in ^{57}Fe are about 3 times larger than the calculated values, while the experimental value for ^{137}Ba is in good agreement with the theoretical one. The experimental results of Khlyuchikov and Feoktistov[11] are more complicated. The measured value for ^{95}Mo agrees with the value calculated according to the present model, but that for ^{96}Mo is smaller and that for ^{97}Tc is larger than the theoretical prediction. The experimental value of Briançon, Valadares, and Walen[9] for ^{109}Ag is 2 times larger than the theoretical value.

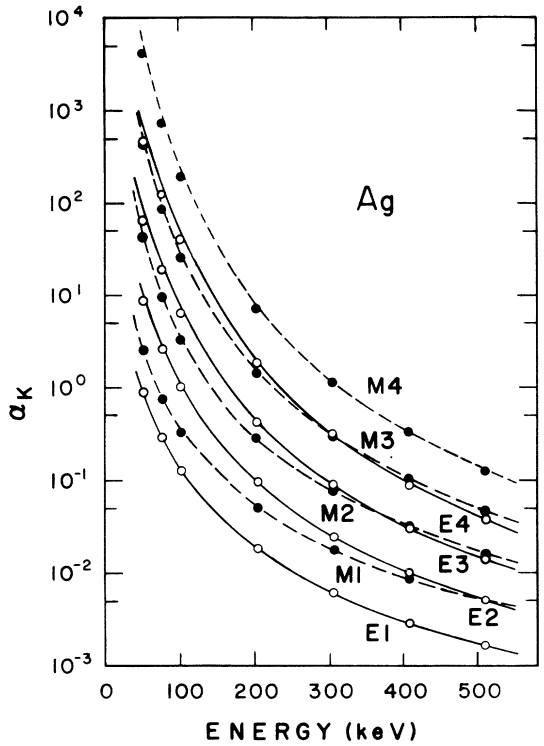

FIG. 5. The comparison of the K-shell internal conversion coefficients calculated from the present model for Ag ($Z=47$) with the values of Rose. Four lowest electric (solid line) and magnetic multipoles (dashed line) are considered. The values of Rose (Ref. 41) are shown by open and closed circles.

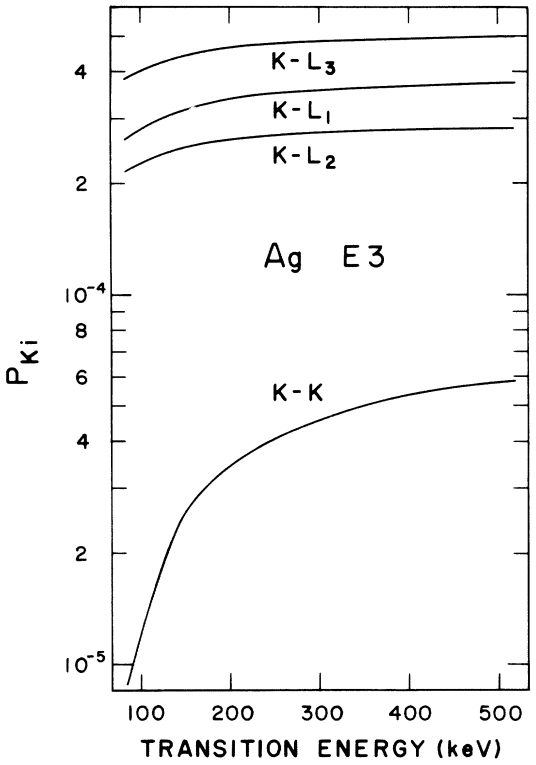

FIG. 6. The transition-energy dependence of the total internal ionization probabilities per K conversion for $E3$ transitions in Ag.

On the other hand, the experimental result of Prokofiev[36] for ^{150}Sm is about $\frac{1}{2}$ of the calculated value.

B. Spectral shape of ejected electrons

The energy distribution of the ejected electrons has been calculated using Eq. (6). The ejected-electron spectra from K and L_i shells ($i=1,2,3$) accompanying K conversion of 661-keV $M4$ transition in ^{137}Ba are shown in Figs. 1–4. For comparison, the nonrelativistic spectra calculated from the modified Levinger theory with Slater screening constants and those from the two-step theory are also plotted in the figures.

As can be seen from the figures, the relativistic spectrum is considerably different in shape from the nonrelativistic one, and the relativistic curve is always higher than the nonrelativistic curve. Furthermore, it is clear that the present theory results in quite different spectra from the two-step theory.[3] The difference between the present curve and other curves becomes large in the high-energy region.

It is very difficult to observe the electron spectrum ejected from the internal-ionization process, because these electrons are concentrated in the very low-energy region. However, from the conservation law of energy the complementary electron has an energy distribution which is just a mirror image of the low-energy spectrum. Therefore, it is advantageous to study the shape of the complementary-electron spectrum instead of the shakeoff-electron spectrum. Porter, Freedman, and Wagner[8] deduced the spectrum shapes of K-electron ejection accompanying K conversion in ^{57}Fe and ^{137}Ba by the (F) -type experiment. However, their spectrum is limited to a very narrow range (0–2 keV). In order to compare with our theory, a measurement over a wider-energy range is required.

V. DISCUSSION

The present model can yield internal-ionization probabilities which are in good agreement with the recent experimental results. However, for ^{109}Ag and ^{169}Tm the calculated values are considerably smaller than the measured values. It is interesting to note that these two nuclides have the following properties in common: (1) double K-shell vacancies can occur in the K-capture decay of

TABLE V. Multipolarity dependence of internal-ionization probabilities per K conversion ($\times 10^4$).

Multipolarity	P_{KK}	P_{KL_1}	P_{KL_2}	P_{KL_3}
$E1$	0.743	3.43	2.53	4.01
$E2$	0.589	3.26	2.44	3.89
$E3$	0.479	3.11	2.36	3.77
$E4$	0.398	2.98	2.29	3.66
$M1$	0.644	3.33	2.48	3.94
$M2$	0.530	3.18	2.40	3.83
$M3$	0.444	3.07	2.33	3.73
$M4$	0.376	2.95	2.27	3.64

the parent atom, and (2) the B_K/k value is large.

In a recent paper,[37] we have developed the theory for the double K-hole creation probability per K capture, $P(2)$, based on model similar to that of the present work. From our theory, the $P(2)$ values for ^{109}Cd and ^{169}Yb can be estimated to be 3.47×10^{-5} and 0.842×10^{-5}, respectively. Using the $P(2)$ and P_{KK} values and the nuclear parameters for ^{109}Cd and ^{109}Ag,[38] the relative probability for double to single K-hole creation is calculated as 2.5×10^{-5}. This value is still smaller than the experimental result.[13]

For the case of ^{169}Tm, Javahery *et al.*[25] derived from the decay scheme[31] a value of 40% for the fraction of the $K\alpha_1$ line due to electron capture and 60% due to internal conversion. Using the $P(2)$ value obtained above and the P_{KK} value in Table I, the relative intensity of the $K\alpha_1$ hypersatellite line is found to be 1.2×10^{-5}. This is about 5 times smaller than the experimental value.

According to Feinberg,[39] the relative probability of direct collision to shakeoff in β^- decay is approximately equal to B_K/E_0, where E_0 is the kinetic energy of the β particle. The large double K-hole creation probability for these two nuclides may suggest that the direct-collision process neglected in the present work plays an important role when the B_K/k value is large. A similar situation has already been pointed out in the case of the internal ionization accompanying low-energy β^- decay.[40]

As can be seen in Tables I and II, the calculated probabilities depend on the multipolarity of the nuclear transition. Since this dependence comes from the differential ICC, $\alpha^{(i)}(W)$, the validity of our screening constants in the calculation of the differential ICC has been tested by comparing the ordinary ICC values calculated from our model, $\alpha^{(i)}(W_0)$, with the precise values of Rose.[41] The results for Ag ($Z=47$) are shown in Fig. 5. It can be seen from the figure that our model can yield reasonable ICC's.

The ionization probabilities as a function of the nuclear transition energy have been studied for $E3$ transitions in Ag. The calculated results are shown in Fig. 6. The probability increases with increasing transition energy and gradually approaches a constant value. The probability for an L_i shell is less sensitive to change in the nuclear transition energy than that for the K shell.

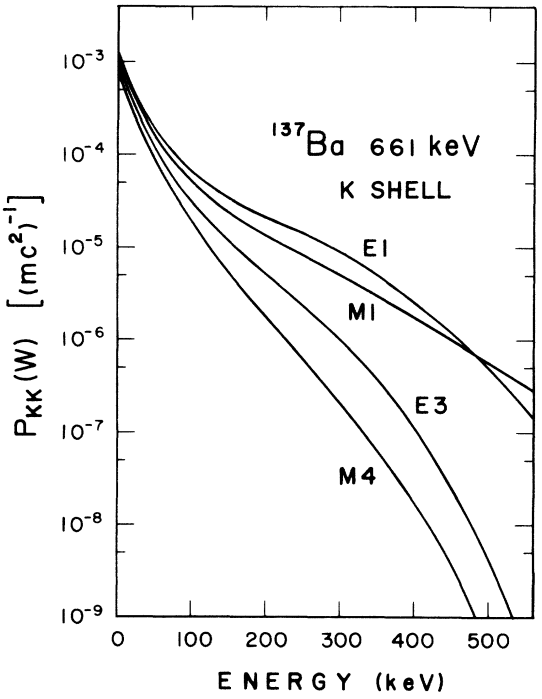

FIG. 7. The multipolarity dependence of the energy spectrum of ejected electrons from K shell accompanying K conversion of 661-keV transition in ^{137}Ba.

The multipolarity dependence of the probabilities and the ejected-electron spectrum have been investigated for the 661-keV transition in ^{137}Ba. The calculated results in Table V indicate that the ionization probability decreases with increasing multipolarity. It is interesting to note that for $M1$ and $E1$ transitions the probabilities in the present model are larger than according to the two-step model.

In Fig. 7, the effect of multipolarity on the ejected-electron spectrum is shown. It is clear from the figure that the spectrum shape is dependent on the multipolarity of the transition. This is because the differential ICC as a function of the ejected-electron energy changes remarkably with the multipolarity.

In conclusion, we have refined our previous model. The internal-ionization probability accompanying K conversion and the spectral shape of the ejected electrons have been calculated in the one-step treatment, taking into account the multipo-

larity of the transition. It is shown that the calculated probabilities are in good agreement with the recent experimental results. The present theory indicates that the ionization probability as well as the energy spectrum of the ejected electrons are strongly dependent both on the nuclear transition energy and on the multipolarity of the transition. In order to make a comparison between theory and experiment in more detail, new experimental data with high precision are needed.

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