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Intershell Tranition of Atomic Electrons during Inner-Shell Ionization by Heavy-Ion Impact

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Expressions for probabilities of electron transition between K and L shells during ion-atom collisions have been derived using the semiclassical approximation. The K-shell ionization cross sections by heavy-ion impact have been modified by taking into account the intershell transition probabilities of K- and L-shell electrons. The results indicate that the effect of the intershell transition on the K-shell ionization cross sections is small.

KEY WORDS: K-shell Ionization / Heavy-Ion Impact / Intershell Excitation Probability /

I. INTRODUCTION

In the course of K-shell ionization by heavy-ion bombardments, it is reasonable to consider that multi-electron transition process takes place. For example, we have observed[1] the evidence of multiple ionization by ^{14}N-ion impact on the targets from $Z_2=22$ to 32 in the low-energy region of $E_1/M_1=0.2$ MeV/amu, where E_1 and M_1 are the energy and mass of projectile, respectively. This fact indicates that multi-electron transition is important even for low-energy heavy-ion bombardments. For the case of multiple ionization process during ion-atom collision, extensive experimental and theoretical investigations have been reported. On the other hand, studies on the atomic electron transition to the vacant state during inner-shell ionization are scarse.

We can consider this process in two step; first a vacancy is produced due to a direct Coulomb ionization mechanism by a charged-particle impact and as a second step an electron in the other shell of the same atom moves to this vacancy by a collision-induced transition. In this way, the primary vacancy transfers to the second shell. When we observe only x rays emitted after the final vacancy is filled, this multi-step process cannot be separated from the direct Coulomb ionization of the second shell by the projectile. If the probability for the collision-induced transition is large, we must take into account the contribution from such a multi-step process in order to compare the theoretical ionization cross section with the experimental value.

The possibility for the electron transition during inner-shell ionization was first pointed out by McGuire *et al.*[2] They derived expressions of probabilities for $2s-2p$ excitation by proton impact, using the semicalssical approximation. Their intrashell

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transition probabilities are very small except for very low projectile energies. However, the probability is proportional to the square of the projectile charge Z_1 and this fact suggests that for heavy ions with large Z_1 the $2s-2p$ transition probabilities be significant.

We have applied the similar model[3] for L-subshell ionization cross sections by heavy-ion impact and shown that the large discrepancy between theory and experiment for L-subshell ionization cross sections by heavy-ion bombardments[4] can be well resolved by introducing the collision-induced intrashell transitions between three L subshells.

It is the purpose of the present work to estimate the effect of *a collision-induced intershell transition* between K and L shells on the K-shell ionization cross sections by heavy-ion impact. For this purpose, we consider two types of multi-step processes, *i. e.* the vacancy transition from K to L shell during K-shell ionization and that from L to K shell accompanying L-shell ionization. The K-shell ionization cross sections with and without the contributions from the multi-step process are calculated and compared with the experimental data.

II. THEORY

Within the framework of the semiclassical approximation, the amplitude for electron transition during ion-atom collision is given by

$$a_{if} = -i\int_{-\infty}^{\infty} V_{if}(R(t))\, e^{i\Delta Et}dt. \tag{1}$$

where $R(t)$ is the projectile coordinate, ΔE is the energy difference between two states, and $V_{if}(R(t))$ is the matrix element of the electron transition with the potential $Z_1/|R-r|$:

$$V_{if}(R(t)) = \int dr\, \varphi_f^*(r) \frac{Z_1}{|R(t)-r|} \varphi_i(r). \tag{2}$$

In Eq. (2) $\varphi_i(r)$ and $\varphi_f(r)$ are the electron wave functions for the initial and final states and r is the electron coordinate. Throughout the present work the atomic units $(e=m=\hbar)$ are used.

We use the nonrelativistic hydrogenic wave functions for K- and L-shell electrons and assume the straight-line trajectory for the projectile. Following the method of McGuire *et al.*,[2] we obtain the $1s-2s$ transition amplitude

$$a_{if} = -i\, 2^{1/2}\, Z_1 Z_2^4 \frac{B^2}{A^2 v} K_2(BA), \tag{3}$$

where $A=(\alpha^2+\beta^2)^{1/2}$, $\alpha=\Delta E/v$, $\beta=3Z_2/2$, v is the velocity of the projectile, B is the impact parameter, and $K_L(x)$ is the modified Bessel function of the third kind with the order of L.

Similarly for the $1s-2p_0$ transition we can obtain

$$\begin{aligned} a_{if}^{(0)} = \frac{2^{17/2} Z_1}{3^5 Z_2 v} \Big[& \alpha K_0(\alpha B) + \left\{ \frac{2\alpha}{AB} - \frac{9\alpha B Z_2^2}{8A} \right\} K_1(AB) \\ & - \left\{ \alpha + \frac{3^4 B^2 Z_2^2 \alpha}{2^7 A^2} \right\} K_2(AB) \Big], \end{aligned} \tag{4}$$

and for the $1s-2p_{\pm 1}$ transition

$$a_{if}^{(\pm 1)}=-i\frac{2^{17/2}Z_1}{3^5 Z_2 v}\Big[\alpha K_1(\alpha B)-\Big\{A+\frac{3^4 B^2 Z_2^4}{2^7 A}\Big\} \times K_1(AB)-\frac{9}{8}BZ_2^2 K_0(AB)\Big]. \tag{5}$$

For $Z_1=Z_2=1$, *i. e.* in the case of proton impact on hydrogen atom, Eqs. (3)—(5) reduce to the expressions obtained by Bates,[5] and Van den Bos and De Heer.[6]

The probability for the $1s-2s$ transition as a function of the impact parameter B is given by

$$P(1s,\ 2s,\ B)=|a_{if}|^2. \tag{6}$$

On the other hand, the probability for the $1s-2p$ transition is expressed as

$$P(1s\ ,2p,\ B)=\frac{1}{3}|a_{if}^{(0)}|^2+\frac{2}{3}|a_{if}^{(\pm 1)}|^2. \tag{7}$$

In order to estimate the collision-induced intershell transition probability, we use a concept of averge impact parameter. Lapicki and Losonsky[7] showed that the average impact parameter for i-shell ionization can be written by

$$\bar{B}_i=A_i/q_{0i}, \tag{8}$$

where q_{0i} is the minimum momentum transfer in the i-shell ionization process and A_i is the constant depending on the atomic shell. According to Lapicki and Losonsky,[7] this constant is taken to be 0.85 for K shell, 1. 5 for L_1 shell, and 2. 0 for $L_{2,3}$ shell. By the use of $\bar{B}_i$, the vacancy transition probability from the i shell to the j shell during$i$- shell ionization is expressed as

$$P(i,\ j)=P(i,\ j,\ \bar{B}_i). \tag{9}$$

At slow collisions ionization takes place mainly when the projectile goes close to the nucleus of the target atom. This means that intershell transitions are probable only along the outgoing path of the projectile. Then we can assume that this effect is taken into account by multiplying the correction factor of 1/2 to Eq. (9).

Considering this correction factor and the number of electrons in the atomic shells, the K-shell ionization cross section with inclusion of the collision-induced intershell transitions is given by

$$\begin{aligned}\sigma_K^{IS}=&\sigma_K[1-P(K,\ L_1)-P(K,\ L_2)-2P(K,\ L_3)]\\ &+\sigma_{L_1}P(L_1,\ K)+\sigma_{L_2}P(L_2,\ K)+\sigma_{L_3}P(L_3,\ K),\end{aligned} \tag{10}$$

where σ_i is the i-shell ionization cross section.

In general, $P(i,\ j,\ B)=P(j,\ i\ ,B)$, but $P(i,\ j)\neq P(j,\ i)$ because $\bar{B}_i$ is not equal to $\bar{B}_i$.

III. RESULTS AND DISCUSSION

The calculated probabilities for K-L_1 and K-L_2 transitions for 5-MeV and 20-MeV

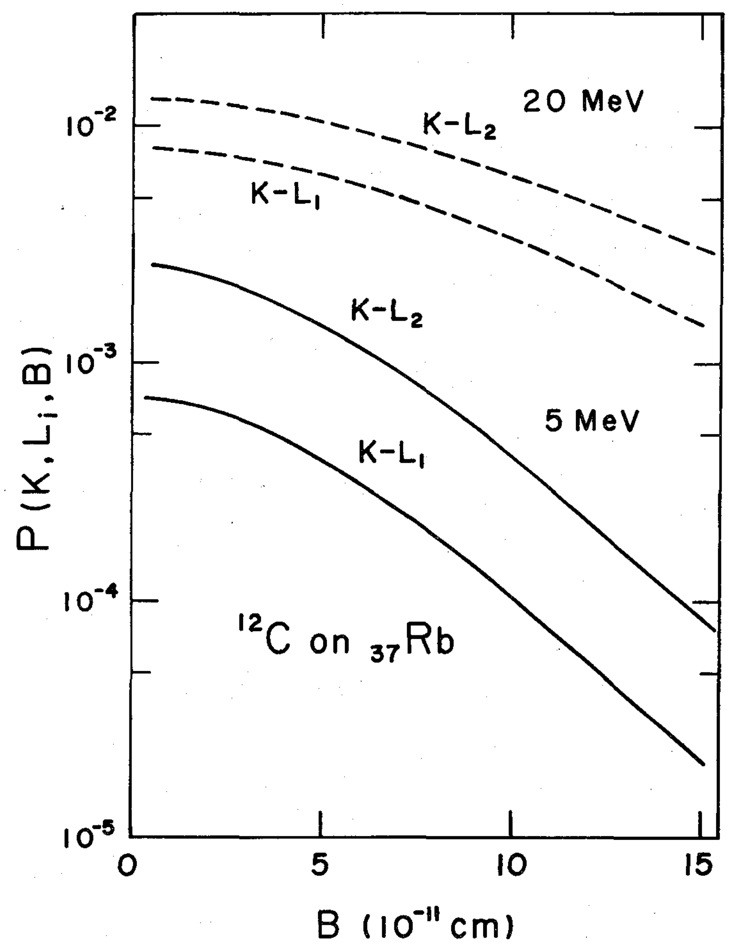

Fig. 1. The collision-induced intershell transition probability for ${}^{12}C$ ions on Rb as a function of impact parameter. The solid curves indicate the $K-L_1$ and $K-L_2$ transition probabilities for 5-*MeV* ${}^{12}C$-ion impact, while the dashed curves represent those for 20-*MeV* ${}^{12}C$ ions.

${}^{12}C$ ions on Rb ($Z=37$) are shown in Fig. 1 as a function of the impact parameter B. The K-L_3 transition probability is almost same as the K-L_2 transition. All the transition probabilities decrease rapidly with increasing B. This fact suggests that in Eq. (10) the contributions from the primary L-shell ionization are small becasue $\bar{B}_{L_i}(i=1, 2, 3)$ is considerably larger than $\bar{B}_K$.

The K-shell ionization cross sections including the collision-induced intershell transition between K and L shells have been calculated by the use of Eq. (10). For the K-shell ionization cross section σ_K, we used the relativistic plane-wave Born-approximation cross section corrected for the binding-energy and Coulomb-deflection effects (RPWBA-BC).[8,9] On the other hand, the L-shell ionization cross sections were obtained by the plane-wave Born approximation corrected for the binding-energy, Coulomb-deflection, polarization, and relativistic effects (PWBA-BCPR).[7] The PWBA-BCPR calculations were made by the use of computer code DEKY3.[10] All the calculations have been performed on the FACOM M-200 computer in the Data Processing Center of Kyoto University.

The calculated results for ^{12}C ions on $Y(Z=39)$ are shown in Table I and compared with σ_K and the experimental data of Wheeler *et al.*[11] The σ_K values were obtained by the RPWBA-BC theory.[8,9]

The contributions from the L-shell ionization are negligibly small due to the small intershell transition probabilities at the average impact parameters for L-shell ionization. This means that the collision-induced intershell transition reduces the K-shell ionization cross section and σ_K^{IS} becomes smaller than σ_K. The difference between σ_K and σ_K^{IS} increases with increasing projectile energy in the energy region considered here. However, the difference is only a few percent and introduction of the collision-induced intershell transition does not change the general behaviour of the K-shell ionization cross sections by heavy-ion bombardments.

As has been pointed out in our previous work,[12] in the heavy-ion impact the measured K-shell ionization cross sections are larger than the theoretical predictions at low projectile energies, but agree with the calculated values in the interwediate energy region. For higher energies, the measured values again become larger than the calculated ones.

It should be noted that the collision-induced intershell transition probability in the present work increases with increasing projectile energy, as can be seen from Fig. 1 and Table I. This fact seems to be in contrast to the collision-induced intrashell transition, which decreases with increasing energy.[2,3] However, if we consider broader energy range than that in the present work, the intershell transition probability increases with energy, reaches a maximum, and then decreases with increasing energy. This trend can be seen also in the $1s-2s$ and $1s-2p$ transitions in proton-hydrogen collision.[5,6]

In conclusion, we have calculated the collision-induced intershell transition probabilities during K-shell ionization by heavy-ion bombardments. The K-shell ionization cross sections by heavy-ion impact have been modified by taking into account the collision-induced K-L transition process. It is found that the collision-induced intershell transition slightly reduces the K-shell ionization cross section by heavy-ion impact, but the general

Table I. Comparison of K-shell ionization cross sections for ^{12}C on Y (barns). The experimental data are taken from Wheeler *et al.* (Ref. 11).

E_1 (Mev)	σ_K	σ_K^{IS}	σ_K^{exp}
8	1.21	1.20	1.69 ± 0.17
11	4.21	4.14	4.93 ± 0.49
12	5.84	5.75	6.48 ± 0.65
14	10.3	10.1	10.6 ± 1.1
17	20.8	20.3	21.1 ± 2.1
20	36.4	35.4	35.2 ± 3.5
24	66.8	64.7	69.0 ± 6.9
26	86.4	83.6	91.5 ± 9.2
29	122	117	155 ± 16
32	164	158	211 ± 21
36	232	223	268 ± 27

behaviour of the cross sections as a function of projectile energy does not change. However we have used in the present work the model based on the average-impact-parameter method. This model may be too crude because $P(K, L_i, B)$ is dependent on B in contrast to the case of intrashell transition probability. Finally the present work is based on the two-step model, but more realistic models for treating the multi-step processes, such as coupled-channel calculations,(13) would give better results. It is hoped to perform such clculations for K-shell ionization process by heavy-ion impact.

REFERENCES

(1) T. Mukoyama, L. Sarkadi, D. Berényi, and E. Koltay, *J. Phys. B: Atom. Molec. Phys.*, **13**, 2773 (1980).
(2) J. H. McGuire, D. J. Land, J. G. Brennan, and G. Basbas, *Phys. Rev. A*, **19**, 2180 (1979).
(3) L. Sarkadi and T. Mukoyama, *J. Phys. B: Atom. Molec. Phys.*, **14**, L255 (1981).
(4) L. Sarkadi and T. Mukoyama, *J. Phys. B: Atom. Molec. Phys.*, **13**, 2255 (1980).
(5) D. R. Bates, *Proc. Roy. Soc. A*, **245**, 299 (1950).
(6) J. Van den Bos and F. J. De Heer, *Physica*, **33**, 333 (1967).
(7) G. Lapicki and W. Losonsky, *Phys. Rev. A*, **20**, 481 (1979).
(8) T. Mukoyama and L. Sarkadi, *Bull. Inst. Chem. Res., Kyoto Univ.*, **57**, 33 (1979).
(9) T. Mukoyama and L. Sarkadi, *Phys. Rev. A*, **23**, 375 (1981).
(10) T. Mukoyama and L. Sarkadi, *Bull. Inst. Chem. Res., Kyoto Univ.*, **60**, 67 (1982).
(11) R. M. Wheeler, R. P. Chaturvedi, J. L. Duggan, J. Tricomi, and P. D. Miller, *Phys. Rev. A*, **13**, 958 (1976).
(12) T. Mukoyama and L. Sarkadi, *Nucl. Instr. and Meth.*, **186**, 641 (1981).
(13) R. L. Becker, A. L. Ford, and J. F. Reading, *J. Phys. B: Atom. Molec. Phys.*, **13**, 4059 (1980).