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Double K-shell-to-K-shell electron transfer in ion-atom collisions

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In this paper we present the first study of the role of double K-shell-to-K-shell electron transfer in heavy-ion–atom collisions. Consistent analysis procedures for obtaining total cross sections for both single and double K-shell-to-K-shell electron transfer are outlined based on the charge-state dependence of the total x-ray-production cross sections for K-shell satellite and hypersatellite x rays, respectively. Theoretical calculations for the single and double electron-transfer cross sections based on the two-state atomic expansion model and the independent-electron approximation are presented and are found to be in excellent agreement with experiment.

Double electron transfer has been investigated in some detail in the resonant $He^{2+} + He \rightarrow He + He^{2+}$ collision.[1-6] These measurements are performed by a charge-state analysis of the scattered beam. It is known that the two K-shell electrons of the target are transferred primarily to the K shell of the projectile, even though the final states of the projectile are not determined in these experiments. The theory of double K-shell-to-K-shell transfer has been discussed by Lichten,[7] and Fulton and Mittleman.[8]

In heavy-ion collisions double K-shell to K-shell transfer cannot be determined from charge-state analysis of the beam, but must be deduced from measurements of the deexcitation of the double K-shell vacancy state. However, mechanisms other than double K-shell-to-K-shell electron transfer can give rise to double K-vacancy states in the target. Considerable interest has been shown in the mechanisms for double K-vacancy production since the first observation by Richard *et al.*[9] of $K\alpha$ hypersatellites resulting from the deexcitation of double K-vacancy states. Olsen *et al.*[10] have studied the energy dependence of the ratio of double-to-single K-vacancy production for the case of Ca bombarded by oxygen and have found qualitative agreement between experiment and calculations based on the binary-encounter approximation (BEA). More recently, Kawatsura[11] and Awaya *et al.*[12] have investigated the projectile Z_1 dependence of double K-vacancy production, again in very asymmetric collision systems, and have proposed that the double K-vacancy production cross-section scales as Z_1^4 which is consistent with a Coulomb ionization mechanism. Double K-vacancy sharing in heavy, near-symmetric collision systems has been studied by various techniques.[13] Finally, an enhancement in double K-vacancy production for incident bare ions over that for one-electron ions in heavy, near-symmetric systems has been observed by Woods *et al.*[14] and attributed to the transfer of two electrons from the target K shell to the empty projectile K shell (double K-shell-to-K shell electron transfer). In this paper we present the first systematic study of the role of double K-shell-to-K-shell transfer in double K-vacancy production in ion-atom collisions. A consistent analysis is developed for obtaining total cross sections for both single and double K-shell-to-K-shell transfer based on the projectile charge-state dependence of the total x-ray-production cross sections. These deduced total cross sections for single and double K-shell-to-K-shell electron transfer are compared with theoretical calculations using the two-center two-state atomic expansion (TSAE)[15] model and with the one-center multistate expansion model[16] in the independent-electron approximation.

The experiment was performed with beams of N, F, Mg, Al, Si, and Cl in the 2.0–6.0 MeV/amu range obtained from the model MP tandem Van de Graaff accelerator at Brookhaven National Laboratory. These beams were focused onto thin (~1 $\mu g/cm^2$) transmission-mounted Ti foil targets oriented 45° with respect to the beam axis. Titanium K x rays were detected by a solid state Si(Li) detector (resolution ~175 eV at 5.9 keV) mounted in a vacuum at a laboratory angle of 90° with respect to the beam axis. Simultaneous with x-ray detection, projectile ions scattered by a thin layer of Au (~5 $\mu g/cm^2$) evaporated onto the backside of each target were detected by a surface barrier detector mounted in vacuum at a laboratory angle of 30° with respect to the beam axis. Assuming Rutherford scattering of the incident ions, the yield of target K x rays per scattered ion can be shown to be directly proportional to the total K x-ray-production cross section, σ_{Kx}, for a given projectile atomic number, energy, and incident-charge state. The constant of proportionality was determined by normalizing to a measured value of $\sigma_{Kx} = (6.63 \pm 0.99) \times 10^3 b$ for 1.7 MeV/amu F^{+5} + Ti due to Schmiedekamp *et al.*[17]

The energy resolution of the detector was sufficient to distinguish the hypersatellite x-ray peak due to the decay of double K-vacancy states from the satellite x rays due to the decay of the single K-vacancy states. A least-squares analysis of the low resolution Ti x-ray spectra thus allows σ_{Kx}, the total x-ray production cross section, to be broken down into satellite and hypersatellite components. The cross section for hypersatellite production, $\sigma_{Kx}(H)$ is obtained from a ratio of x-ray yields, $Y_{K\alpha^h}/Y_{K\alpha_{\text{total}}}$, according to $\sigma_{Kx}(H) = \sigma_{Kx}(Y_{K\alpha^h}/Y_{K\alpha_{\text{total}}})$ and is related to the double K-vacancy production cross section, σ_{DKV}, by the relation

$$\sigma_{\text{DKV}} = \frac{\sigma_{Kx}(H)}{\omega_K} . \tag{1}$$

The single K-vacancy production cross section, σ_{SKV}, is given by the relation

$$\sigma_{\text{SKV}} = \frac{\sigma_{Kx} - 2\sigma_{Kx}(H)}{\omega_K} . \tag{2}$$

In the above equations, it is assumed that the hypersatellite fluorescence yield is equal to the average K-shell fluorescence yield, ω_K, determined from the intensity distribution of the $K\alpha$ satellite peaks observed in high resolution.[18] Fluorescence yields determined in this way mirror the L-shell ionization probability and tend to decrease monotonically for Ti from $\omega_K \simeq 0.25$ at 2 MeV/amu to $\omega_K \simeq 0.23$ at 6 MeV/amu. The second term in the numerator of Eq. (2) corrects for the hypersatellite x rays and the cascading from the double K-vacancy states through the satellite x rays. The two terms contribute equally to give the factor in Eq. (2).[19]

The projectile charge-state dependence of single K-vacancy production, σ_{SKV}, and double K-vacancy production, σ_{SKV}, using Eqs. (1) and (2) are given in Fig. 1 for 5 MeV/amu Si^{q+} + Ti. The single K-vacancy production cross section for the one-electron-ion beam, σ^1_{SKV}, shows an increase over that for the many-electron-ion beam, σ^0_{SKV} due to single K-shell-to-K-shell charge transfer. A similar increase occurs for K-vacancy production by a bare-ion beam σ^2_{SKV}. The single K-shell-to-K-shell electron-transfer cross section is taken as

$$\sigma^{K-K} = \sigma^2_{\text{SKV}} - \sigma^0_{\text{SKV}} . \tag{3}$$

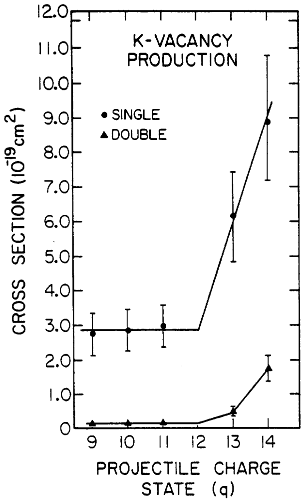

FIG. 1. The charge-state dependences of single K-vacancy production, σ_{SKV}, and double K-vacancy production, σ_{DKV} in Ti for 5 MeV/amu Si^{q+} + Ti collisions obtained using Eqs. (2) and (1), respectively, are presented. The error bars indicate the absolute errors in the cross sections. The relative errors are at least a factor of 2 smaller. The cross sections for the two-electron-ion beam are omitted due to the metastable $1s2s\ ^3S$ component in the beam. The solid lines are eye guides.

To obtain Eq. (3) it is assumed that the average K-shell fluorescence yield and the contributions to σ^i_{SKV} due to processes other than K-shell to K-shell transfer are independent of the incident-charge state. This procedure has been used in several previous publications.[20] The present analysis differs from the previous work in that σ^i_{SKV} is corrected for double K-vacancy production according to Eq. (2). The projectile charge-state dependence of double K-vacancy production (see Fig. 1) also shows a small enhancement for the case of one-electron-ion beams. This enhancement is due to the opening of the single K-shell-to-K-shell channel (i.e., double K-vacancy production due to K-shell-to-K-shell transfer simultaneous with target K-shell to projectile L-shell transfer, K-shell ionization, or K-shell excitation). The larger enchancement observed for the bare-ion beam is attributed to double K-shell-to-K-shell electron transfer plus the additional increase in the K-shell-to-K-shell transfer exhibited in σ^2_{SKV}. Using the same assumptions leading to Eq. (3), we can show[19] that the double K-shell-to-K-shell cross section, σ^{2K-2K}, is given by

$$\sigma^{2K-2K} = \sigma^2_{\text{DKV}} - 2\sigma^1_{\text{DKV}} + \sigma^0_{\text{DKV}} . \tag{4}$$

To study single as well as double K-shell-to-K-shell electron-transfer processes, we have adopted a theoretical model modified from the earlier work of Lin.[21] By considering the two K-shell electrons only and using an independent electron approximation, we assume that the time evolution of the two-electron wave function can be expanded in terms of three *atomic* eigenstates: (1) the initial two-electron state centered around the target; (2) the final double electron-transfer state centered around the projectile; and (3) the intermediate state in which only one electron is transferred. This close-coupling expansion allows us to derive a set of time dependent coupled equations which can be solved to obtain single and double K-shell-to-K-shell charge transfer probabilities. However, unlike the work in Ref. 21, if the intermediate state is properly symmetrized with respect to the interchange of two electrons, one can show that the double electron-capture probability at each impact parameter is given by $P_2 = P^2$ and the single electron-transfer probability is given by $P_1 = 2P(1-P)$, where P is the electron-transfer probability calculated in the *one-electron* two-center, two-state atomic model.[15] Thus a single calculation allows us to obtain single as well as double K-shell-to-K-shell electron-transfer cross sections. By comparing experimental single and double electron-transfer cross sections with this simple model, we test the basic assumptions of both the independent electron model and the TSAE model.

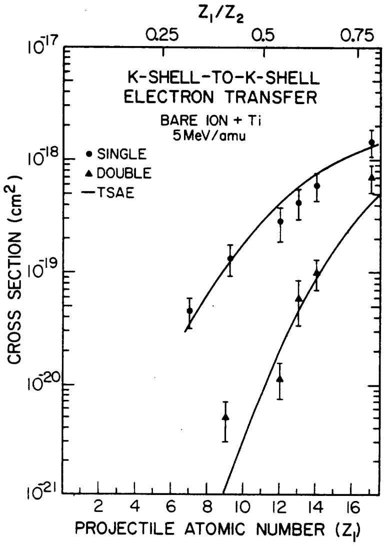

FIG. 2. The projectile Z dependences of single and double K-shell-to-K-shell electron transfer for bare ions on Ti obtained using Eqs. (3) and (4) are presented. The solid curves are the TSAE calculations for single and double K-shell-to-K-shell electron transfer as outlined in the text.

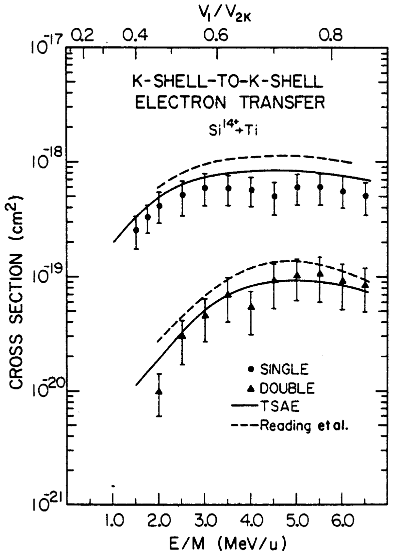

FIG. 3. The projectile energy dependences of single and double K-shell-to-K-shell electron transfer for bare Si ions on Ti obtained using Eqs. (3) and (4) are presented. The solid curves are the TSAE calculations for single and double K-shell-to-K-shell electron transfer as outlined in the text. The dashed curves are the one-center, multistate calculations of Reading *et al.*

The systematics of single and double K-shell-to-K-shell electron transfer are shown in Figs. 2 and 3 for a typical case. The theoretical curves represent the two-center, two-state atomic expansion (TSAE) calculations presented here (Figs. 2 and 3) and the one-center multistate calculation of Reading *et al.*[16] (Fig. 3). Both calculations assume the independent electron approximation. The whole of our data indicates that, for projectile scaled velocities $V_1/V_{2K} \gtrsim 0.04$ and $Z_1/Z_2 \gtrsim 0.50$, TSAE calculations are in excellent agreement with observed σ^{K-K} and σ^{2K-2K} energy and Z_1 dependences and the general magnitude of the experimental data. The electron-transfer component of the multistate calculation of Reading *et al.*,[16] available only for the case of Si + Ti, is also in good agreement with experiment.

It is significant to note that the observed cross-section ratio $\sigma^{2K-2K}/\sigma^{K-K}$ increases from ~4% at $Z_1 = 12$ to ~50% at $Z_1 = 17$ for 5 MeV/amu collisions (scaled velocity $V_1/V_{2K} \simeq 0.4$, see Fig. 2). At the higher Z_1 this translates to the observation that 48% of the total Ti K x-ray intensity for bare-ion beams of Cl is due to the production of double K-vacancy states during the collision. The ratio $\sigma^{2K-2K}/\sigma^{K-K}$ has a slow variation with energy as shown in Fig. 3. The ratio is ~2% at a scaled velocity of 0.4 and increases to $\sim 17\%$ at a scaled velocity of 0.75 where the cross sections appear to peak.

In conclusion, we have shown that double *K*-to-*K* electron transfer plays an important role in double *K*-vacancy production and may make a significant contribution to total *K*-vacancy production in near-symmetric collision systems as matched projectile velocity is approached. We have demonstrated that double *K*-shell-to-*K*-shell transfer is well represented by existing theoretical models for $V_1/V_{2K} \gtrsim 0.04$ and $Z_1/Z_2 \gtrsim 0.05$. A complete discussion of single and double *K*-vacancy production mechanisms along with tabulated data over a broad range of projectile energy will be presented in a forthcoming paper.

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[20] For a review see, Tom J. Gray, in *Methods of Experimental Physics,Vol. 17,* edited by P. Richard (Academic, New York, 1980), Chap. 5, pp. 193–278.

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