K-Vacancy Creation by High-*Z* Heavy-Ion Impact

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A competing process to direct *K*-shell ionization by heavy-ion impact is suggested to account for some recent data by Macdonald *et al.* It is found that the high-*Z* dependence of the x-ray yields can be accounted for by inclusion of *K* charge exchange into bound states of the fully stripped projectiles.

Considerable interest has been shown recently in the collision of heavy ions with atoms.[1] *K*-shell x-ray yields have been studied for a variety of target atoms, as well as a wide range of projectiles from protons to heavy ions in various charge (Z) states, and at various energies.[2-4] Disagreement with the Z^2-dependent cross section for inner-shell ionization as calculated in the Born approximation[5] has been reported in most of this range. Some of the discrepancies for the case of low-Z projectiles have been explained[2-4] using polarization and increased binding effects for $(v/u)^2 \ll 1$ and polarization effects for $(v/u)^2 \gtrsim 1$, where v is the projectile velocity and u the electron velocity in the K shell of the target.

More surprising difficulties have been reported recently by Macdonald *et al.*[6] who studied collisions of fully stripped projectiles H^+, C^{+6}, N^{+7}, O^{+8}, and F^{+9} with argon atoms at velocities v/u in the range 0.4–0.6. They found that the K-shell x-ray yields increase much more rapidly than the Z^2 dependence of the ionization cross section would indicate. They point out that various attempts to explain this appear inadequate. Polarization effects have not been estimated in this range. McGuire's suggestion of charge exchange to the continuum of the projectile, mentioned in Ref. 6, needs concrete calculations for justification.

We should like to suggest that K-shell electron charge exchange to a bound state of the projectile (K pickup) can explain the high Z dependence of the x-ray yields. While for proton projectiles the K pickup is negligible in comparison with the ionization, the high Z dependence of the pickup process makes it more competitive as Z increases, and indeed dominates for $Z \sim 8$ or 9 for the range of v/u considered.

Various attempts to calculate charge-exchange cross sections in atomic collisions have been made over the years[7,8] using single-particle models. The basic problem then reduces to that of a three-body rearrangement collision, with its well-known theoretical difficulties. The old Brinkman-Kramers[9] (BK) cross section σ_{BK} is known to overestimate considerably the experimental cross sections, while the Born approximation σ_{B} by Jackson and Schiff[10] seems to fit data for protons on hydrogen and helium much better over a reasonable range of energies. Mapleton[11] has shown that σ_{B} and σ_{BK} are related by a scaling factor $R = \sigma_{\mathrm{B}}/\sigma_{\mathrm{BK}}$ (for protons on H and He) that varies from 0.1 to 0.6 and generally increases with velocity. (The result for helium is somewhat more meaningful for our case because it is an asymmetric collision.) Nikolaev,[12] using an extended version of σ_{BK} and accounting for shielding, obtained total charge-exchange cross sections which scale to the experimental cross section by the same order of magnitude: $\sigma_E/\sigma_{\mathrm{BK}} \sim 0.1 - 0.3$. Calculations with the second Born approximation[7] and impulse approximation[7] indicate that for protons on hydrogen, $\sigma \sim 0.3\sigma_{\mathrm{BK}}$. No calculations of the relative size of Born, second Born, or impulse approximations to σ_{BK} for large Z have been made, and since all those calculations are on theoretically precarious ground, we felt it would be sufficient to use the BK approximation and attempt to fit the Macdonald data by using a scaling factor for each velocity.

The BK formula as given by Nikolaev[12] (without shielding) for K pickup to a given projectile state of principal quantum number n is

$$\sigma_{\mathrm{BK}} = \sum_n \frac{2^{19}}{5} \pi a_0^{\,2} \frac{Z^5}{n^3} Z_m^{\,5} \left(\frac{v}{v_0}\right)^8 \times \left\{ \left[\left(\frac{v}{v_0}\right)^2 + Z_m^{\,2} - \frac{Z^2}{n^2} \right]^2 + 4\left(\frac{v}{v_0}\right)^2 \left(\frac{Z^2}{n^2}\right) \right\}^{-5}.$$

a_0 is the Bohr radius; v is the projectile velocity; $v_0 = u/Z_m$; Z_m is the target nucleus charge, which for argon is 18; and Z is the projectile charge. We included $n = 1, 2, 3$ in calculating σ_{BK}. The $n = 1$ contribution dominates, while the $n = 2$ one is down by more than an order of magnitude. The

TABLE I. K-shell vacancy cross sections in argon. σ_{BK} is the Brinkman-Kramers K pickup cross section. σ_D is the Z^2 scaled cross section from H^+ scattering. σ_E is the experimental cross section from Ref. 6. The cross sections are in units of 10^{-20} cm^2. x is the scaling factor used at each velocity to give the curves in Fig. 1.

Z	σ_{BK}	σ_D	σ_E
	$v/u=0.424$, $x=0.12$		
1	3×10^{-4}	0.16	0.16
6	4.8	5.8	4.9
7	13.0	7.8	6.5
8	32.7	10.2	12.0
9	78.0	13.0	25.0
	$v/u=0.507$, $x=0.24$		
1	7×10^{-4}	0.25	0.25
6	9.4	9.0	13.0
7	23.9	12.3	18.0
8	56.1	16.0	31.0
9	123.6	20.3	51.0
	$v/u=0.568$, $x=0.33$		
1	10^{-3}	0.33	0.33
6	12.7	11.9	17.0
7	31.4	16.2	29.0
8	70.7	21.1	44.0
9	148.2	26.7	70.0

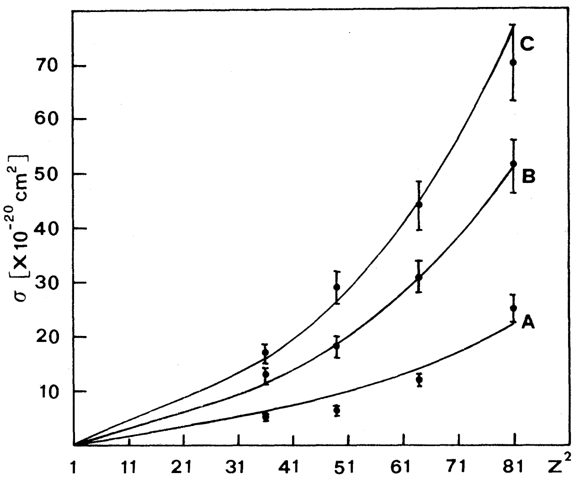

FIG. 1. Plot of total cross section for K-shell vacancy production versus the square of projectile charge. Dots (with error bars, see text), Macdonald *et al.*'s (Ref. 6) data; curves are theoretical: $\sigma_D+x\sigma_{\text{BK}}$. A, $v/u=0.424$, $x=0.12$; B, $v/u=0.507$, $x=0.24$; C, $v/u=0.568$, $x=0.33$.

$n=3$ contribution is negligible for all but the highest Z.

The contribution due to ionization, σ_D, was obtained by scaling Macdonald *et al.*'s data for H^+ by the usual Z^2 factor. (This is legitimate since K pickup by H^+ on argon is negligible.) In Table I we list the cross sections for K pickup (σ_{BK}), for ionization (σ_D), and from experiment (σ_E) for all various charges Z and velocities. In addition, the scale factor x, used to obtain the fits in Fig. 1, is listed for each velocity. The curves in Fig. 1 are given by $\sigma_D+x\sigma_{\text{BK}}$. The data points of Ref. 6 have been given a lower absolute error of 10% as a guide, although a higher figure is indicated. It should be noted that the scale factors x are within the ranges discussed above and increase with velocity as expected from Mapleton's data. The uncertainties in the data are sufficiently large that the values of x could well be varied somewhat. We have not shown a fit to Macdonald *et al.*'s earlier data on scattering of different charge states of fluorine on argon[13] at $v/u\sim0.585$, because of the complications associated with the incompletely stripped projectile. We can match the $Z=9$ data with $x\sim0.4$. It is also interesting to note the sharp rise in the cross sections as the fluorine charge state goes from 7 to 8 and 8 to 9 (which corresponds, respectively, to one and two vacancies in the projectile ground state). This is consistent with the large pickup rate into the projectile ground state which can occur for these cases. We should also point out that although in both the earlier and more recent experiments of Macdonald *et al.*, less than 5% of the beam undergoes charge exchange, a rough estimate indicates that for their targets, this is fully consistent with our K-shell pickup cross section if we assume the ratio of total charge exchange to K pickup given by the BK formalism of Nikolaev[12] to be approximately correct.

We feel that the fits in Fig. 1 indicate that K-shell electron pickup into bound states of the projectile is the most likely cause of the high Z dependence of the cross-section data of Macdonald *et al.* It also indicates that the theoretical situation on charge exchange needs further clarification so that the velocity dependence of the scale parameter x can be quantitatively justified.

The dominance of K pickup for high-Z projectiles indicates the possible use of K x-ray yields as a direct measure of the K-shell charge-exchange process itself, by subtraction of the ionization cross section. This would be particularly useful in helping to unravel the theoretical difficulties associated with the various charge-exchange approximation schemes. To do this, even higher-Z projectiles should be studied, and somewhat better calculations of the direct ionization cross section need be made, taking into account polarization and distortion of the incoming projectile wave function. The authors have made rough estimates of the latter effect, using an eikonal approximation, which indicate that although such distortion could not account for the high Z dependence in the data, it could possibly contribute towards the deviation from a Z^2 dependence of the cross section.

We note that although we have restricted our considerations to K-vacancy formation, the same arguments will also hold for L-vacancy formation. Although the data from Ref. 13 on L x-ray yields indicate the effect, no data on fully stripped ions of high Z exist where the effects should be most clear. As L-ionization calculations exist,[5] we urge further experimental investigations for L x-ray yields by fully stripped ions.

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