K-Vacancy Sharing in Near-Symmetric Heavy-Ion Collisions*

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Relative production cross sections for beam (Z_1) and target (Z_2) K vacancies in heavy-ion collisions are explained for situations where $Z_1 \simeq Z_2$. Electron promotion creates a vacancy in the $2p\sigma$ molecular orbital. As the collision partners retreat, the vacancy has a probability $w(v_1, Z_1, Z_2) \leq \frac{1}{2}$ to be transferred to the $1s$ level of the higher-Z collision partner. With a charge-transfer theory of Demkov, a universal form for w is obtained, which is in excellent agreement with all available data for Ni, Br, and I beams over extended target and energy ranges.

Various measurements of the production cross sections for beam (Z_1) and target (Z_2) K x rays in heavy-ion collisions have been made.[1-4] Close to symmetry ($Z_1 \simeq Z_2$), cross sections are enhanced 10^2 to 10^3 times over predictions of the Coulomb-excitation theory,[5] if Coulomb deflection of the projectile and electronic binding energy changes during the collision are taken into account.[6]

One theory for the large enhancement of near-symmetric collision cross sections is based on the electron-promotion model.[7,8] For K-vacancy production this model must assume[8] (1) that a vacancy exists in the $2p$ subshell of the higher-Z collision partner, (2) that a K electron of the lower-Z partner is promoted from the $2p\sigma$ molecular orbital (MO) to the $2p\pi$ MO by rotational coupling at small internuclear distances (see inset in Fig. 1 for schematic MO level arrangement), and (3) that this electron fills the original vacancy in the $2p$ subshell of the higher-Z partner, leaving a vacancy in the K shell of the lower-Z partner at the end of the collision. The main point of the present note is that in near-symmetric collisions electron promotion cannot directly enhance vacancy production in the $1s$ level of the *higher-Z* partner [$1s(H)$]; but experimentally, large enhancements are found even for that partner. A typical example[4] is shown in Fig. 2. I provide an explanation for this effect by suggesting that, after $2p\sigma$-$2p\pi$ electron promotion by rotational coupling[9] at small internuclear distances, vacancy transfer can take place by radial coupling[8] from the $2p\sigma$ to the $1s(H)$ state with a certain probability w.

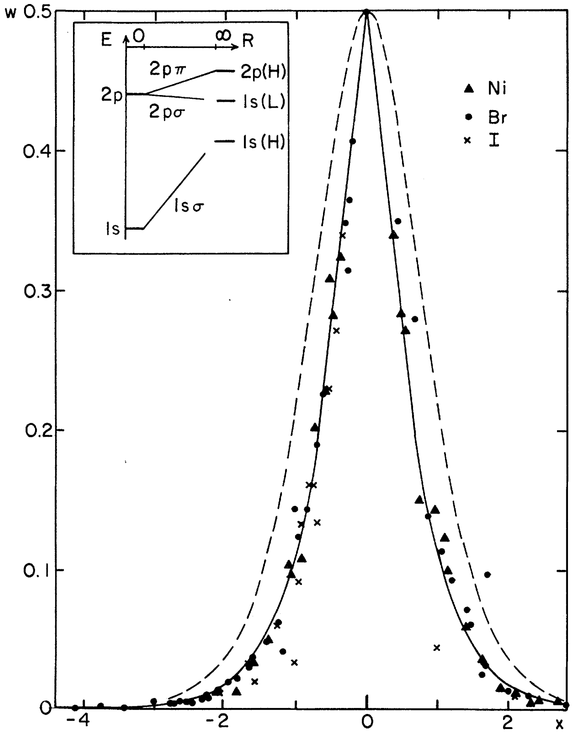

FIG. 1. K-vacancy transfer probability w for Ni, Br, and I beams for extended target and energy ranges (see text) versus universal parameter x [Eq. (6)]. Typical errors on w are ±25%. Solid line, Eq. (5); dashed line Eq. (7). In inset, gap in line between separated-atom and molecular levels indicates symbolically the assumed MO↔AO transition region.

I sketch a derivation of w based on the charge-transfer model of Demkov[10] who considers a two-state system of one electron (or one vacancy) in the neighborhood of two ions separated by a distance R, with a wave function

$$\Psi(r,t) = a(t)\,\psi_1(r,R) + b(t)\,\psi_2(r,R). \qquad (1)$$

He chooses ψ_1 and ψ_2 such that for $R \to \infty$ they become the atomic orbitals (AO) for the electron in the neighborhood of each separate ion, respectively. He assumes that as R decreases, Ψ changes from the AO form ψ_1 (or ψ_2) to the MO form $(1/\sqrt{2})(\psi_1 \pm \psi_2)$ under the influence of a perturbation $H_{12} = \beta\exp(-\kappa R) = \beta\exp(-\gamma t)$. He shows that the change takes place in a relatively narrow range of R. For the present purpose we need to com-

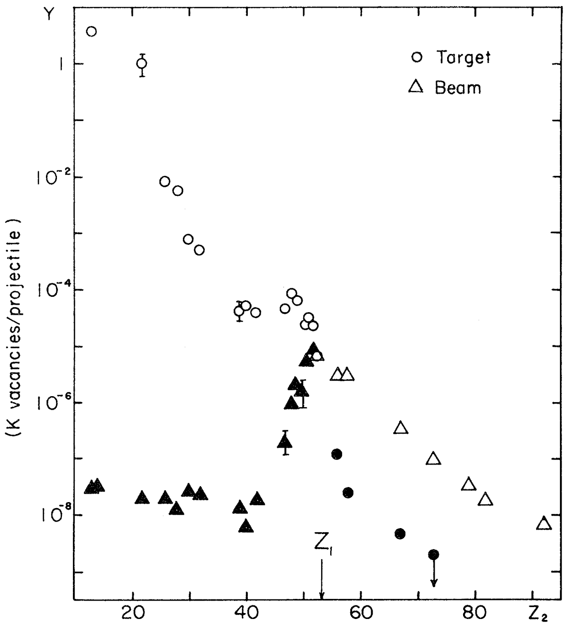

FIG. 2. K-vacancy yields from thick targets bombarded with 47-MeV I versus target atomic number. Target and beam yields are shown. Yield of the higher-Z collision partner is shown with a closed symbol. The enhanced yield of the higher-Z partner near $Z_2 = Z_1$ is apparent.

pute the transition probability from the initial state $(1/\sqrt{2})(\psi_1 - \psi_2)$, representing the $2p\sigma$ MO, to the final state ψ_1, representing the $1s(H)$ AO. The transition probability w is then given by $|a(\infty)|^2$.

After a simple phase transformation, the time evolution of a and b in Eq. (1) is given by[10] ($\hbar = 1$)

$$\begin{aligned} i\dot{a} &= a\alpha + b\beta \exp(-\gamma t), \\ i\mathring{b} &= -b\alpha + a\beta \exp(-\gamma t), \end{aligned} \tag{2}$$

where it has been assumed that the matrix elements $H_{11} = \alpha$ and $H_{22} = -\alpha$ do not vary with time in the important time interval in which Ψ changes its form. By the substitution $\tau \equiv \exp(-\gamma t)$ one can show that a and b obey Bessel-type equations and have the solutions

$$a = \tau^{1/2}[AJ_s(y) + BJ_{-s}(y)], \tag{3}$$

$$b = -i\tau^{1/2}[AJ_{s-1}(y) - BJ_{-s+1}(y)], \tag{4}$$

where $s \equiv \frac{1}{2} - i\alpha/\gamma$ and $y \equiv \beta\tau/\gamma$. The constants A and B are determined from the initial ($\tau = 1$) conditions $a = 1/\sqrt{2}$, $b = -1/\sqrt{2}$. Assuming $\beta/\gamma \gg 1$, which is physically reasonable [$\beta/\gamma \simeq (I/2mv_1^2)^{1/2}$, with I the ionization energy of $2p\sigma$ MO, m the electron mass, and v_1 the projectile velocity], it is possible to show after considerable algebra that

$$|a(\infty)|^2 \equiv w = 1/(1 + \exp|2x|), \tag{5}$$

$$x \equiv \pi\alpha/\gamma = \pi(I_1 - I_2)/[(8mI)^{1/2}v_1]. \tag{6}$$

In Eq. (6) we have substituted $2\alpha \equiv H_{11} - H_{22} = I_1 - I_2$ and $\gamma \equiv \kappa\nu_1 = (2mI)^{1/2}\nu_1$ ($\hbar = 1!$), where in the present case I_1 and I_2 are the κ binding energies of the colliding atoms. Following a proposal by Olson,[11] we set $I^{1/2}$ equal to $1/2(I_1^{1/2} + I_2)^{1/2}$. Expression (5) had been given by Andukinov, Bobashev, and Perel,[12] but the factor 2 is missing in their exponent, and had been deduced semi-empirically by Barat and Lichten[8] with x similar to Eq. (6). Expression (5) leads correctly to the "two-passage" transfer probability[13] computed by Demkov,[10]

$$w_D = 2w(1 - w) = \tfrac{1}{2}\operatorname{sech}^2 x, \tag{7}$$

except for an interference term which is obtained only with the initial conditions appropriate to the two-passage problem.

According to our present ideas, then, the cross sections $\sigma_K(H)$ and $\sigma_K(L)$ for K-vacancy production in the higher-and lower-Z collision partners, respectively, are related by

$$\sigma_K(H) = w[\sigma_K(H) + \sigma_K(L)], \tag{8}$$

where the bracketed quantity is the total $2p\sigma$ vacancy production cross section due to electron promotion. Equation (8) assumes that, in the region of interest, Coulomb excitation makes a negligible contribution to the cross sections. To extract the experimental values of w [Eq. (8)] we use all available K-vacancy production cross sections for Ni beams[3] on $Z_2 = 20$ to 38 at 45, 61, and 94 MeV; Br beams[3,4] on $Z_2 = 22$ to 45 at 30, 45, 60, 85, and 110 MeV; and K-vacancy yields for 47-MeV I beams[4] (see Fig. 2) on $Z_2 = 47$ to 58, with some isolated measurements at energies between 12.5 and 80 MeV. Typical experimental errors are ± 25%, although in some cases they are as high as a factor of 2. All experimental x-ray–production data have been corrected with neutral-atom fluorescence yields.[14] According to Eq. (5), if the values of w are plotted against the parameter x given by Eq. (6), they should fall on a universal curve given by Eq. (5). For the K binding energies we have used tabulated values[15] for separated atoms. The success of this prescription can be seen in Fig. 1. All the diverse experimental data indeed fall on a universal curve (solid line), even in the wings of the curve. This indicates that Eqs. (5) and (6) contain the correct Z and v_1 dependence of w. For comparison we also show Eq. (7) (dashed line). The good fit with Eq. (5) but not with Eq. (7) supports the assertion that at least the major portion of the K-vacancy transfer from the $2p\sigma$ MO to the $1s(H)$ AO takes place in a single transition region, i.e., on the outgoing part of the trajectory.

Several comments are in order. (1) Use of the unperturbed K binding energies in Eq. (6) implies that the transition region must lie well outside of the mean K Bohr radius a_K. Indeed, because of mutual atomic polarization the $2p\sigma$ and $1s\sigma$ adiabatic MO levels in an asymmetric system "pull together" near $R \simeq 5a_K$ [see, e.g., Müller, Rafelski, and Greiner[16]] so that it would be reasonable to assume that vacancy transfer takes place near there. (2) The use of K x-ray cross sections and yields from solid targets might be questioned (see discussion in Kessel and Fastrup[17] and Garcia, Fortner, and Kavanagh[18]). In particular, the recoil of the target atom through the lattice produces additional, electron-promotion–enhanced, yield through secondary collisions. Indeed, from a detailed examination[4] of Fig. 2 in the "Coulomb-excitation region" ($Z_2 \simeq 26$ to 42), one finds that the target yield could be enhanced through recoil effects by as much as an order of magnitude. But, extrapolating the trend of these points to the "electron-promotion region" ($Z_2 \simeq 47$-56), we note that the recoil effect cannot affect the target yield there by more than a few percent. The beam yield must be much less affected in any case, since the secondary processes in the Coulomb-excitation region are not enhanced by electron promotion. (3) One may question the use of neutral-atom fluorescence yields. It appears, though, that for K fluorescence yields, the effect of electron stripping at the energies of interest here (~ 1 MeV/amu) is at most of the order of 10%[19] (see also discussion in Ref. 18). (4) One feature in the proposed K-vacancy transfer mechanism is the need to provide a $2p$ vacancy in the higher-Z partner before the collision, or early enough in the collision, so that the suggested electron promotion between the $2p\sigma$ and $2p\pi$ MO can take place. Possible mechanisms for this vacancy formation are discussed in Refs. 17 and 18.

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Nonmonotonic Target Dependence of Cl *K* X-Ray-Production Cross Sections in Single Heavy-Ion–Atom Collisions*

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Chlorine *K* x-ray-production cross sections have been measured in single collisions of chlorine ions in low incident charge states with gas targets at MeV energies. The cross sections are nonmonotonic as a function of target atomic number, but they approach monotonicity with increasing projectile energy. To explain these results in terms of $2p\sigma$-$2p\pi$ transitions in nearly symmetric collisions effectively requires $2p$ vacancy production simultaneous with the promotion of Cl $1s$ electrons.

The production of Cl *K* x rays has been observed in single collisions of chlorine projectiles of low incident charge states with a variety of thin, gas targets at 0.1 to 1.5 MeV/amu. The experimental Cl *K* x-ray-production cross sections are plotted in Fig. 1 as a function of target atomic number Z_2 for projectile energies of 5 to 52 MeV. The cross sections exhibit a nonmonotonic dependence on Z_2 in contrast to the Z_2^2 dependence given by a one-electron Coulomb ionization process.[1,2] An enhancement of the cross sections observed at argon is greatest at the lowest energy and becomes less pronounced as the projectile energy increases. At the highest energy, the cross sections are monotonic as a function of Z_2. The careful monitoring of single-collision conditions and incident charge-state selection in this experiment allows one to obtain more information concerning the collision process than previous observations of nonmonotonic dependences of projectile *K* x-ray production on the atomic number of solid targets[3,4] have provided. The $2p\sigma$-$2p\pi$ transition suggested to explain the observations for solid targets is inadequate to account for the data presented in Fig. 1 for which the experimental restriction was imposed that no $2p$ vacancies be carried into the collisions that produced *K*-shell vacancies. Any promotion mechanism that attempts to account for these data by a coupling

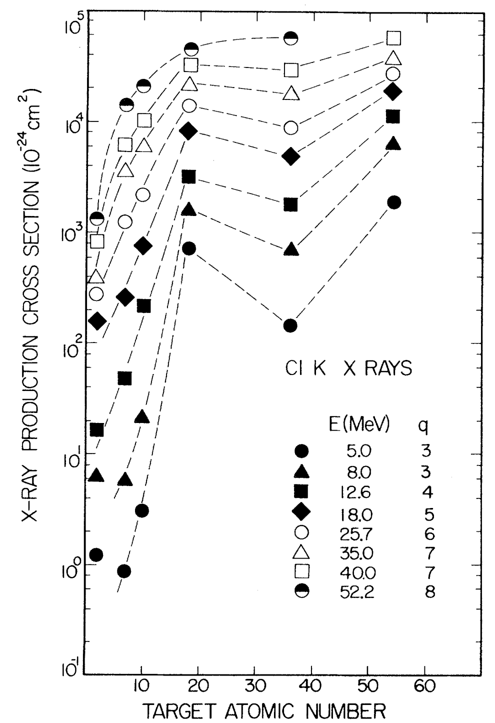

FIG. 1. Chlorine *K* x-ray-production cross section as a function of target atomic number for chlorine projectiles of incident energy *E* and charge state *q*. The dashed lines are drawn to guide the eye through the data points with constant energy.