Statistical Interpretation of Transfer Ionization in Slow Collisions of Multiply Charged Ions with Atoms

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A statistical approach to transfer ionization is used to calculate multiple-ionization probabilities for target ions produced in slow multielectron-capture collisions of multiply charged ions and atoms.

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Recent coincidence experiments[1-5] have demonstrated that in electron-capture collisions between slow multiply charged ions and atoms the target may lose a larger number of electrons than found attached to the projectile when detected long after the collision. This process, termed transfer ionization (TI), can proceed via many different individual reaction channels. Although the most relevant mechanisms contributing to TI have been discussed[6,7] for the special case of one-electron capture with additional ionization of a single (further) target electron, the attempt of a rigorous quantum theoretical treatment would be extremely difficult because of the inherent complexity of the multichannel problem. This is even more true for TI processes in multielectron-capture reactions where even the contributing mechanisms are still unexplored.

In this Letter we present a statistical interpretation of TI processes in atomic collisions at kiloelectronvolt energies,

$$A^{q+} + B \rightarrow A^{(q-k)+} + B^{i+} + (i-k)e + \Delta E\ , \qquad (1)$$

where a multiply charged ion A^{q+} captures $k=2$ or 3 electrons from an atom B which is left in charge state $i \geq k$. Calculated multiple-ionization probabilities are found in striking agreement with measured charge-state fractions of target ions B^{i+} obtained in a systematic experimental study[5] with projectiles A = C, N, Ne, Ar, Kr, and Xe in charge states up to $q=15$ (for Xe) and target atoms B = Ne, Ar, Kr, and Xe. Furthermore, the statistical model used provides a scaling which allows quantitative predictions for any given collision system (1).

In our experiment the target ions B^{i+} were charge-state analyzed and detected in correlation with charge-transferred projectiles $A^{(q-k)+}$ by using a time-of-flight coincidence technique. These measurements yield directly the probabilities for pure capture as well as for additional single or multiple target ionization in electron-capture collisions. A detailed analysis of the experimental results for the various collision systems shows that in exoergic reactions the potential energy available in the collision system is the dominant parameter which determines the degree of additional target ionization; the observed charge-state fractions are independent of the kinetic impact energy in the kiloelectronvolt energy range studied.

Since the potential energy can be dissipated for additional target ionization via very many different reaction channels a statistical treatment seems an adequate approach to the problem. We simply assume that the energy is statistically distributed among electrons which initially belong to the target and may evaporate.

The maximum potential energy ΔE_m available when k electrons are captured by an ion A^{q+} from an atom B is easily obtained from tabulated ionization energies[8] $I_A^{(j)}$ and $I_B^{(j)}$ for the respective particles A^{j+} and B^{j+}:

$$\Delta E_m = \sum_{j=q-k}^{q-1} I_A^{(j)} - \sum_{j=0}^{k-1} I_B^{(j)}\ . \qquad (2)$$

The mathematical procedure is based on a statistical distribution of infinitely small units of energy, the sum of which is ΔE_m, among N outer-shell electrons of the target ion B^{k+} which already has lost k electrons to the projectile. An averaged ionization potential $\langle I_B \rangle$ is introduced for the electrons "boiling off" the ions B^{k+}. One can then calculate the probability $P_n(N, \Delta E_m)$ that n electrons gain enough energy to overcome $\langle I_B \rangle$ and escape from B^{k+}. The mathematical derivation of this probability leads to

$$P_n(N, \Delta E_m) = \binom{N}{n} \sum_{j=0}^{l} (-1)^j \binom{N-n}{j} \times \left(1 - \frac{n+j}{\Delta E_m / \langle I_B \rangle}\right)^{N-1} \qquad (3)$$

with l defined by $n + l \leq \Delta E_m / \langle I_B \rangle \leq n + l + 1$. This equation has also been derived by Russek and Meli[9] in their theory for ionization processes in violent ion-atom large-angle scattering.

The number of electrons N among which the energy ΔE_m is distributed can be assumed to be the number of electrons in the outermost shell of the ion B^{k+}. Since we used rare-gas targets with B = Ne, Ar, Kr, and Xe we chose $N = 8 - k$.

The averaged ionization potential has to be determined for each ion B^{k+} separately. With increasing ΔE_m an increasing number of electrons can be released from B^{k+}. When ΔE_m facilitates the ejection of n electrons but not of $n+1$, i.e., for

$$\sum_{j=0}^{n-1} I_B^{(k+j)} \leq \Delta E_m < \sum_{j=0}^{n} I_B^{(k+j)}, \tag{4}$$

we set

$$\langle I_B \rangle = \frac{1}{n} \sum_{j=0}^{n-1} I_B^{(k+j)}. \tag{5}$$

The resulting step function for $\langle I_B \rangle$ is approximated by a smooth curve to obtain a physically more meaningful shape and to facilitate subsequent computations (see, for example, caption of Fig. 1). Probabilities $P_n(8-k, \Delta E_m)$ for n-fold ionization in Reaction (1) can now be calculated and compared to the corresponding experimental charge-state fractions F_i with $i = n + k$.

Figure 1 shows measured and calculated charge-state fractions of Xe^{i+} target ions produced in two-electron-capture collisions $Xe^{q+} + Xe \rightarrow Xe^{(q-2)+} + Xe^{i+} + (i-2)e$ with $q = 3, 4, \ldots, 15$. Noting the fact that there is not a single fit parameter in the model the overall agreement with the experiment is certainly remarkable.

A most important consequence of the statistical model is the prediction of a scaling behavior of TI: the target-ion charge-state fractions F_i for any given collision system $A^{q+} + B$ should fall on common curves when plotted as a function of $\Delta E_m / \langle I_B \rangle$ as long as the number k of captured electrons is fixed.

Figure 2 contains all our measurements for two-electron-capture reactions. It can be seen that the data indeed scale as expected and moreover, the striking quantitative agreement with the theoretical predictions, which is also found for the three-electron-capture reactions, strongly supports the statistical concept on which the model for transfer ionization is based.

The model also predicts the mean charge states $\langle i \rangle = \sum_i i F_i$ of target ions B^{i+} produced in Reactions (1). For any projectile-target combination the values of $\langle i \rangle$ should fall on common

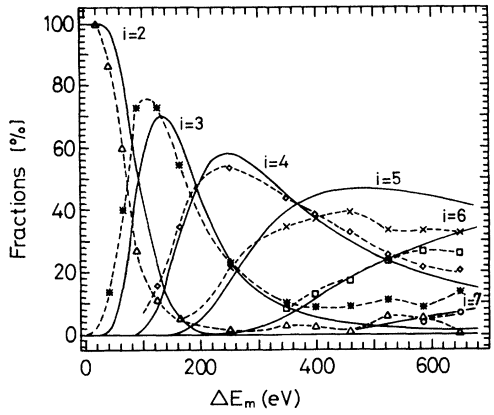

FIG. 1. Charge-state fractions of Xe^{i+} target ions produced in two-electron-capture collisions of Xe^{q+} ions with Xe atoms. The experimental points for a given target-ion charge state i are connected by dashed lines: $i=2$ (triangles), $i=3$ (asterisks), $i=4$ (diamonds), $i=5$ (crosses), $i=6$ (squares), $i=7$ (circles); the solid lines are calculated from Eq. (3). The step function obtained from Eqs. (4) and (5) is approximated by $\langle I_B \rangle = 13.3\ \text{eV} + (2.4\ \text{eV})[\Delta E_m/(1\ \text{eV})]^{1/2}$.

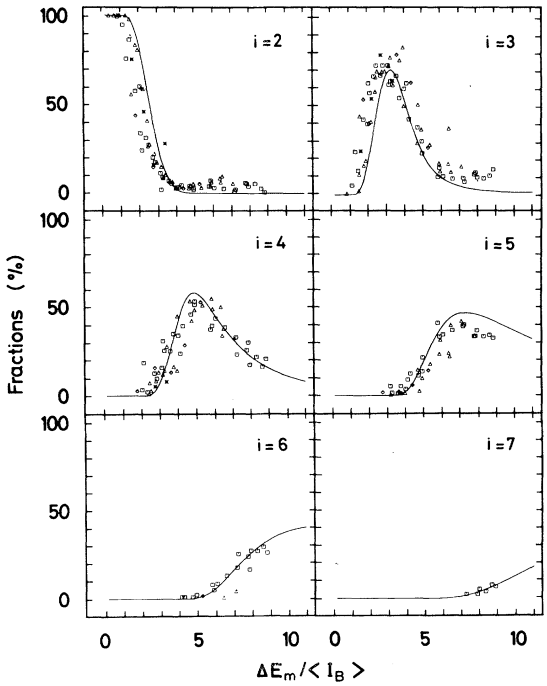

FIG. 2. Charge-state fractions of target ions B^{i+} produced in Reactions (1) with $k=2$ as a function of the reduced energy $\Delta E_m / \langle I_B \rangle$. The figure contains all experimental results for the different collision systems investigated. Symbols for the targets are the following: Ne (asterisks), Ar (triangles), Kr (diamonds), and Xe (squares). The solid lines represent the results of the statistical model.

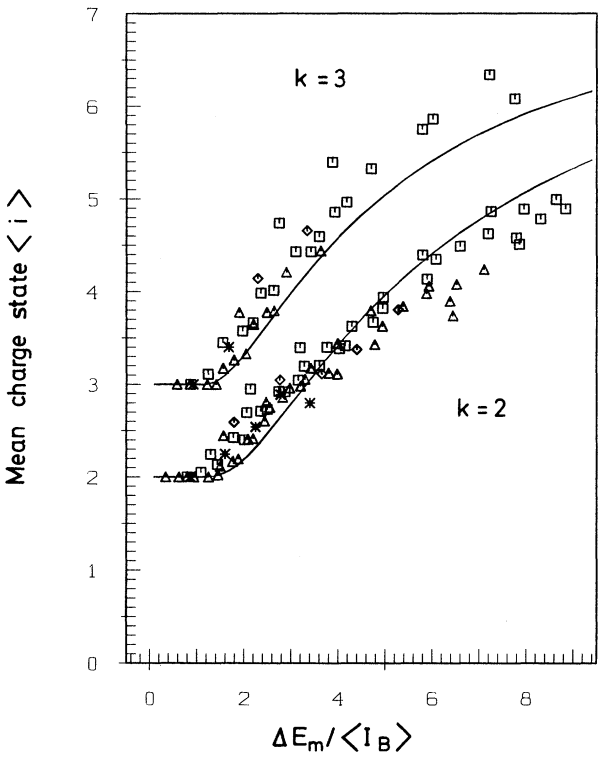

FIG. 3. Mean charge states $\langle i\rangle = \Sigma_i i F_i$ of target ions B^{i+} produced in Reactions (1) with $k = 2$ and $k = 3$ as a function of $\Delta E_m / \langle I_B \rangle$. Symbols for the targets are the following: Ne (asterisks), Ar (triangles), Kr (diamonds), and Xe (squares). The solid lines represent the results of the statistical model.

curves characterized only by the number of captured electrons when plotted as a function of $\Delta E_m / \langle I_B \rangle$ again. The results are shown in Fig. 3 where all our experimental data for $k = 2$ and $k = 3$ are included.

We point out that we have not assumed a specific TI mechanism in which initially k electrons are transferred from the target to the projectile and subsequently the available recombination energy ΔE_m is transferred back from the projectile to the target which then relaxes long after the collision. It is rather the vast number of interaction channels by which electrons, initially bound to the target, may be released that leads to the picture of statistical energy dissipation.

In the model described we introduced only such physical quantities which are directly accessible like the available recombination energy ΔE_m and the average ionization potential $\langle I_B \rangle$. Therefore we did not apply the model to TI processes in one-electron–capture collisions since it is well known that in these reactions predominantly excited projectile states which relax by radiative decay are populated. Additional assumptions would be necessary to account for the resulting reduction of the energy available for additional target ionization. In the case of multielectron capture, however, the k electrons found attached to the projectile may not have much excitation energy because otherwise autoionization in the projectile would have occurred already during the passage from the target to the detector system resulting in a noncoincident event. (The flight times are of order 1 μs which is long compared to autoionization life times.) This justifies the use of the maximum potential energy ΔE_m defined by Eq. (2) for our calculations instead of a slightly smaller quantity which is unknown for the investigated processes.

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