Charge- and Angle-Correlated Inelasticities in Collisions of Bare Fast Carbon Ions with Neon

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We have studied the detailed energy balance in collisions of 10-MeV C^{6+} ions with Ne. In these collisions, the Ne is multiply ionized and the C ion may emerge as either C^{6+} or C^{5+} . Projectile energy loss and scattering angle for a given carbon-ion charge state were determined in a high-resolution magnetic spectrograph and were measured in coincidence with the formation of a given Ne recoil-ion charge state. The amount of energy transferred to the continuum electrons exceeds, by far, the sum of the values of the ionization potentials.

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The understanding of multielectron ionization and transfer processes in single ion-atom collisions is still not far advanced because of the complexity of this *n*-body problem. In some cases, the features of multiple ionization in energetic collisions can be described in terms of an independent-electron model which results in a binomial distribution of charge states.¹⁻³ Another theoretical procedure is to employ an energy disposition model⁴ which has been found to work well in some systems.⁵ Both of the above models are unable to describe the dynamics of the collisions in terms of physical parameters such as the angular scattering and energy changes of the projectile or recoil ions. In order to lend further insight into the collision mechanisms, we report in this study experimental measurements and a newly developed theoretical model that yields the first information on projectile energy loss and angular scattering correlated with the target multiple ionization state for megaelectronvolt/ nucleon collisions.

In general, for collisions of this type, much of the inelasticity is carried off by electrons either by direct ionization or by autoionization following inner-shell excitation or ionization. However, the total amount of energy transferred to the continuum electrons, during a multielectron process, has not been reported in previous experiments. For single-electron (and some double) charge transfer processes at lower energies, translational energy spectroscopy has been shown to be a very useful tool. When the projectile velocity, v_p , is much less than the electron orbital velocity, v_e , only a small number of reaction channels are open, and it has been possible to isolate certain reaction channels, even with moderate energy resolution.⁶⁻⁹ At higher collision energies $(v_p \gtrsim v_e)$, corresponding to megaelectronvolt/nucleon ion energies, the number of reaction channels and active electrons in a multielectron-target collision increases strongly, and the measurements of inelasticities on an atomic scale require much higher energy resolution.

In order to obtain this information, we determined the degree of target multiple ionization (recoil-ion charge state Q) by a time-of-flight technique. The inelasticity. the projectile charge state q, and the angular distribution were measured simultaneously with a high-resolution magnetic spectrograph. Here, we give only a brief account of the experimental procedure; a more detailed description will be given elsewhere.¹⁰ A 10-MeV C³⁺ beam was post stripped after passing through a 90° magnet; a second 90° magnet selected the desired charge state and, coupled with two sets of slits, acted to define the beam energy. The angular divergence was determined by a third slit in front of the gas cell. The gas target was isolated by three stages of differential pumping. With a gas-cell pressure of 1 mTorr, a pressure of 10^{-7} Torr could be maintained in the beam line. The gas cell could be raised to a potential of 5 kV for energy calibration of the magnetic spectrograph.¹⁰

About 50 cm after the gas target, the projectile ions entered the field of the Elbek magnetic spectrograph.¹¹ For optimum resolution and unit magnification, a maximum bending radius of about 1.2 m was chosen and a two-dimensional position-sensitive channel-plate detector was placed in the focal plane. The two-dimensional position-sensitive channel-plate detector had an active sensitive length of 30 mm, and resolution of 0.1 mm. Because of the large dispersion of the magnet, only one exit charge state of the projectile, e.g., q-1, could be detected for a given setting of the magnetic field. Since the Elbek magnet is only single focusing, the displacement of the particle perpendicular to the magnetic analyzing plane is a measure of the scattering angle. The flight path of the ions through the magnet of 320 cm and the beam width of 0.3 mm at the detector gave a range of measurable scattering angles of 0.005° to 0.27°.

In order to help understand the collision dynamics, an *n*-body classical-trajectory Monte Carlo method (nCTMC) was developed which explicitly incorporates all the electrons in the collision. The nCTMC method includes all the forces between the projectile ion and the target nucleus, and its electrons. The forces between the target nucleus and its electrons are also included and the electron-electron interactions are approximated with effective charges between the electrons and target nucleus. Hamilton's equations of motion are numerically solved (72 coupled first-order differential equations) for a microcanonical distribution of the electrons about the



FIG. 1. Counts in the focal plane of the Elbek magnet for single capture of C^{6+} ion in coincidence with different Ne recoil-ion charge states as marked in this figure. The displacement from the vertical line is a measure of the inelasticity. Each shade of grey corresponds to a factor of 2 in intensity.

target nucleus. Such a procedure allows us, for the first time, to determine not only the various total cross sections, but the angular and energy spectra of the recoil and projectile ions without the need of choosing some arbitrary central potential for the collision.

Figure 1 shows the distributions of C^{5+} ions in the two-dimensional position-sensitive channel-plate detector for three examples of recoil-ion charge states, Ne^{2+} , Ne^{4+} , and Ne^{6+} from 10-MeV C^{6+} incident ions. The x axis represents the momentum of transmitted C^{5+} ions; the y axis, their angular distribution. Two things can be seen immediately: With increasing target ionization, the angular (y) distribution gets wider and the x displacement increases corresponding to lower momentum of the projectile ions. The dashed line marks the value of constant momentum. An, at first sight, surprising result is that for any given recoil-ion charge state, the inelasticity is independent of the scattering angle.

Since the angular distribution and inelasticity are not strongly correlated, we project the two dependences separately out of the two-dimensional spectra. The projection on the y axis, perpendicular to the dispersion plan, gives the angular differential cross section $d\sigma/d\theta_y$ and some examples are shown in Fig. 2. Here, we show some



FIG. 2. Angular differential cross section as a function of the projectile scattering angle for Ne¹⁺ and Ne⁴⁺ recoil ions produced by pure ionization (q=6) and by electron capture (q=5) of 10-MeV C⁶⁺. Statistical errors in the CTMC calculation range from $\simeq \pm 15\%$ at small angles to $\simeq \pm 30\%$ at large angles.

 θ_{ν} distributions for single capture producing Ne¹⁺ and Ne^{4+} , and for pure ionization to produce Ne^{1+} and Ne^{4+} . Differential cross sections calculated with the nCTMC method are also shown in Fig. 2 for the Ne⁴⁺ case. The theoretical values have been convoluted to reflect the apparatus geometry and are in reasonable agreement with the experiment. Although the total cross sections for ionization to produce $C^{6+} + Ne^{4+}$ and transfer to yield $C^{5+} + Ne^{4+}$ are similar ($\sigma \approx 10^{-17}$ cm^2), there is a noticeable difference in the shapes of the differential cross sections. With direct ionization, the products are produced at larger impact parameters than in the transfer reaction and are more sharply peaked at small angles. The impact-parameter range probed by Ne⁴⁺ production is $\simeq 0.6a_0$ with a half width of $\simeq 0.4a_0$. The Ne L-shell electrons dominate this reaction since collisions that remove K-shell electrons give rise to much higher stages of Ne^{q+} ionization, and would show a minimum inelasticity of ≈ 1 keV. The $d\sigma/d\theta_{v}$ values are very different for the production of Ne^{1+} by charge capture vis-à-vis by direct ionization; this is due to the ionization total cross section being approximately 2 orders of magnitude larger than that for capture, with ionization dominating the Ne⁺ production at large impact parameters.

The projections on the x axis yield the inelasticities for a given degree of multiple ionization. As the absolute beam energy cannot be measured with the necessary accuracy, we measure the change of inelasticity relative to that for producing Ne¹⁺. These energy differences, i.e., $(\Delta E_Q - \Delta E_Q - 1)$ are plotted in Fig. 3 (right-hand scale) versus the degree of multiple ionization Q. Theoretical inelasticity values for the production of Ne^{Q+} via direct ionization are also shown; the slope with respect to Qtends to be somewhat larger than the experimental value.

The step function in Fig. 3 shows the sum of the ionization potentials required to obtain a given Q. The difference between the measured inelasticities and this sum could appear as (1) recoil-ion energy, (2) targetatom excitation leading to radiation, (3) in the case of capture, a balance between energy gain due to an increase in binding energy on the projectile and the energy loss due to the captured electron's translational energy, and (4) energy transferred to electrons to the continuum electrons.

The first two of these arguments can be discarded on the following bases: (1) We have calculated the recoilion energies and they are less than 10 eV, even for the production of Ne⁸⁺; the Ne⁴⁺ value is 1.2 eV. Both values are consistent with the observations of Levin *et al.*¹² (2) The energy due to excitation cannot exceed the ionization energy of the last electron. As for (3), an energy loss of \approx 450 eV is expected because of the increased kinetic energy (lab) of the captured electron. This could be balanced by the increased binding on the C⁶⁺ core, the maximum being 480 eV for capture into



FIG. 3. Measured and calculated projectile inelastic energy loss as a function of the degree of multiple ionization. Experimental results shown are the differences in energy loss for single-projectile ionization and multiple-projectile ionization. Statistical errors in the CTMC calculation are $\pm 25\%$.

n=1. However, capture to n=1 should be rather improbable; we calculate it to be only about 16% of the total single-capture cross section ($\sigma_c \simeq 3 \times 10^{-17} \text{ cm}^2$). The dominant capture channel is predicted to be to C^{5+} (n=2) with 44% of the flux. Insofar as the *n* distribution for capture is independent of the recoil-ion charge state, this factor will appear as a constant offset. Auger events in our case would be due to K-shell capture or ionization. These events, although present, proceed with a cross section of about 3×10^{-18} cm², which is small compared to the other electron removal processes (L shell) except for high $(Q \ge 6+)$ recoil-ion charge-state production. Contributions from these events would appear at large scattering angles and would have appreciably larger energy losses. The minimum loss for just the removal of the K electron in direct ionization would be 870 eV. In the case of coincidence with capture, the minimum loss would be about the same (i.e., 870 eV for Ne K ionization, minus 490 eV for capture into carbon K plus 455 eV for acceleration up to C ion speed). This loss difference is resolvable in this experiment and is not observed.

We attribute the bulk of the excess energy loss to translational energy of the electrons in the continuum. Since we measure only energy differences, we do not know the absolute energy loss associated with Q=1 recoils. To get the average energy per emitted electron,

we take the energy differences for Q > 1 and divide them by the number of *additional* electrons emitted in the collision. These values range from about 100 eV up to about 200 eV per electron.

A remaining difficulty is the apparent independence of the inelasticity on scattering angle. This can be qualitatively understood from a calculation of the average energy deposited in a binary collision, $(\Delta E_e) = \int |\psi_L|^2 \times \Delta E_e d^3 r$. We obtain values for $\langle \Delta E_e \rangle$ which vary from 235 to 200 eV for b = 0.1 a.u. up to 0.8 a.u. This simple model would explain both the magnitude and the lack of impact-parameter dependence of the inelastic loss. It is, however, too simple to explain many of the details seen in these measurements (e.g., the angular dependence of the differential cross section and the differences in slope between $\langle \Delta E_e \rangle$ for capture and pure ionization).

In conclusion, we have been able to measure and calculate, for the first time, the complete set of physical parameters for fast ion-atom single collisions. These parameters are the projectile inelastic energy loss, the projectile scattering angle, and the incoming and outgoing projectile- and target-charge states. In these collisions, we see for a given recoil-ion charge state no direct correlation between inelasticity and scattering angle, but we see a strong correlation of both of them with the degree of multiple ionization. Also, a large difference in the angular dependence of the differential cross sections and in the inelasticity for multiple ionization accompanied by single-electron capture were found when compared to direct ionization. This research was sponsored by the U.S. Department of Energy, Division of Chemical Sciences under Contract No. DE-AC05-840R21400 with Martin Marietta Energy Systems, Inc. One of us (R.E.O.) acknowledges the support of the Office of Fusion Energy.

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