Dynamics Of Multiply Charged Ion-atom Collisions: U^{32+}+Ne

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LETTER TO THE EDITOR

Dynamics of multiply charged ion–atom collisions: $U^{32+}+Ne$

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Abstract. Measurements and calculations are presented for the mean recoil-ion energies of Ne^{i+} produced in 1.4 MeV u^{-1} (0.33 GeV) collisions of U^{32+} with Ne. Recoil-ion charge states $i=1$–8 have been observed; the mean recoil energies are low and do not exceed 1 eV until $i>6$. Calculations employing a newly developed *n*-body classical trajectory Monte Carlo method are found to yield results in qualitative agreement with the recoil-ion experiment. Calculations also are presented for the ionisation and charge exchange cross sections, the projectile energy loss and the ejected-electron energy and angular spectra. The importance of fast ejected electrons in the dynamics of energetic multiply charged ion–atom collisions is noted.

It is well established that in fast, heavy-ion–atom collisions multiple ionisation plays an important role even at large impact parameters. In these ionisation processes up to several keV of energy can be transferred from the projectile kinetic energy to the ejected electrons, whereas the recoil ion produced in the collision will be nearly at rest in the laboratory frame. This phenomenon can be qualitatively explained by the laboratory kinematics of the two-body ion–atom collision system. The large energy loss (Q value approximately greater than 1 keV) of the ionisation process changes the centre-of-mass kinetic energies (greater than 10 MeV) of both collision partners by a small fraction. Therefore, the resulting laboratory system recoil ion is negligibly influenced by the large Q value. For the two-body collision system, the recoil-ion energy (or projectile scattering angle) is thus a sensitive function of the impact parameter. In such a multiple ionisation process, moreover, the total momentum of the ejected electrons can easily exceed that of the recoil ion. Therefore, the resulting electron momenta can strongly influence the kinematics of the scattering of the heavy nuclei.

The mean recoil ion energy $\bar{E}_R(i)$ as a function of the recoil-ion charge state i depends on the multiple ionisation transition probability as a function of the impact parameter with corrections due to anisotropic electron ejection. $\bar{E}_R(i)$ is thus a stringent test of collision theory, much more so than the usual comparison of total cross sections. In this letter we provide the first measurements and calculations of the recoil-ion charge-state dependence of $\bar{E}_R(i)$ for a collision involving a highly charged, energetic projectile ion:

$$U^{32+}+Ne \rightarrow U^{(32-j)+}+Ne^{i+}+(i-j)e. \tag{1}$$

One other work has presented the case for low charge state I^{5+} projectile ions (Levin *et al* 1987). Further, we present calculations indicating the importance of fast ejected electrons in energetic multiply charged ion–atom collisions.

The experimental data have been obtained at GSI Darmstadt (Stripperhalle). By performing a recoil-ion–projectile-ion coincidence, the recoil-ion time-of-flight distributions (see figure 1) have been determined. The time-of-flight spectrometer allows the separation of the final recoil-ion charge state. A detailed description of this spectrometer will be given in a more complete paper. The observed charge-state-dependent time-of-flight distributions are obtained from measurements made transverse to the projectile beam. These measurements allow the mean recoil-ion energies $\bar{E}_R(i)$ to be precisely determined. In figure 2 the $\bar{E}_R(i)$ are presented as a function of the recoil-ion charge state (experimental data: full circles). The bars represent the measured half widths. The error bars for $\bar{E}_R(i)$ are smaller than the size of the data points, except for $i = 8$. The open circles represent calculations made using a newly developed n-body classical trajectory Monte Carlo (nCTMC) method which explicitly incorporates all the electrons in the collision.

The nCTMC method includes all the forces between the projectile ion (assumed to be completely stripped) and the target nucleus and its electrons. The forces between the target nucleus and the electrons are also included. Excluded are the electron-electron interactions, which are approximated by using effective charges between the electrons and their parent nucleus as a means of representing the average field experienced by each electron.

The classical Hamiltonian for the system used in this study is given by

$$H = \frac{p_a^2}{2m_a} + \frac{p_b^2}{2m_b} + \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N} \frac{z_a z_i}{R_{ai}} + \sum_{i=1}^{N} \frac{z_b z_i}{R_{bi}} + \frac{z_a z_b}{R_{ab}} \tag{2}$$

where N is the number of electrons ($N = 10$ for the Ne target) and the indices a and b represent the projectile ion and target nucleus, respectively. It is necessary to numerically solve $6(N+2)$ coupled, first-order differential equations arising from the

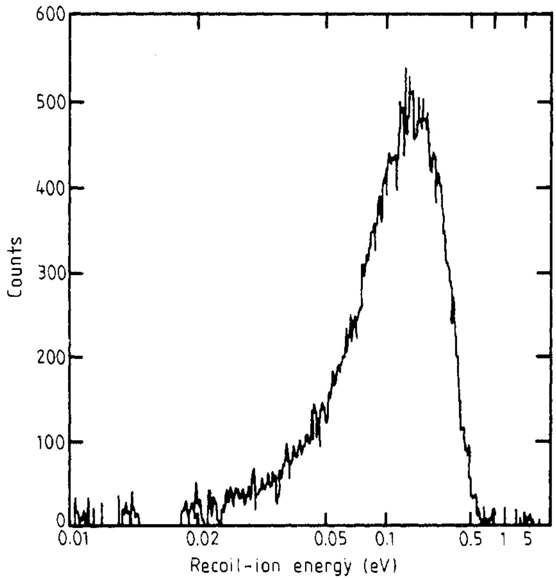

Figure 1. Representative spectrum for the transverse recoil energy of Ne^{3+} produced in 1.4 MeV u^{-1} U^{32+} + Ne collisions.

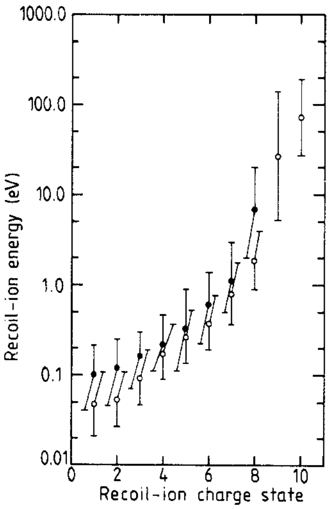

Figure 2. Mean recoil-ion energies of the Ne^{i+} ions produced in 1.4 MeV u^{-1} U^{32+} + Ne collisions. The full circles are experimental data and the open circles are theoretical calculations based on the *n*CTMC method. The bars represent the halfwidths of the energy spread except for the experimental point for $i=8$ and the theoretical values at $i=9$ and 10 which have broadened widths due to statistical uncertainties.

xyz Cartesian coordinates of each particle:

$$\mathrm{d}c_j/\mathrm{d}t = \partial H/\partial p_j \tag{3}$$

and the *xyz* momenta of each particle

$$\mathrm{d}p_j/\mathrm{d}t = -\partial H/\partial c_j. \tag{4}$$

The electrons are initially started in a microcanonical distribution about the target nucleus with an effective Z determined by the sequential binding energies of the Ne atom. Such a procedure ensures that the total electronic energy of the target atom is correct. The eccentricities of the individual electron orbits are determined from phase space arguments based on the quantum mechanical angular momentum distributions (Olson 1981). The sensitivity of the cross sections to the initial relative orientation of the electron orbits to one another (such as the p electrons) was tested and changes outside the statistical error bars were not noted. We attribute this result to the relative long-range nature of the collision and to the polarisation of the electrons by the large electric field of the projectile ion.

It should be noted that the numerical solution of equation (2) provides, for the first time, a method for determining angular distributions and energies of the recoil ion, the projectile ion and the ejected electrons. Theoretical procedures based on the independent-electron model (Hansteen and Mosebekk 1972, Olson 1979, Horbatsch and Dreizler 1985) fail to provide this information unless an arbitrary central potential is chosen for the collision system.

As shown in figure 2, the calculations are in reasonable agreement with the experimental data for neon recoil charge states $4 \leqslant i \leqslant 7$, indicating that the impact parameter dependence of the multiple ionisation process is well described by the *n*CTMC approach. For low Ne charge states ($i \leqslant 3$), i.e. very low $\bar{E}_R(i)$, the experimental data are somewhat higher than the calculated values. This deviation is expected and

is due to the intrinsic temperature of the Ne gas target (approximately 0.03 eV), which is not included in the theoretical model. Also not included is broadening of the recoil energies due to Auger events. This effect could be particularly important for $i=8$ ions where helium-like metastables are known to be produced. In fact, the experimental data point at $i=8$ shows a broadened energy distribution. However, the experimental point at $i=8$ suffers from poor statistics due to the small cross section, so it is not unequivocal that metastable ions affect the energy widths. The calculated values of $\bar{E}_R$ for producing hydrogenic Ne^{9+} or fully stripped Ne^{10+} show sharp rises to 26 or 71 eV, respectively. This effect is due to the enhanced recoil energy produced by the very small impact parameter collisions ($b \leqslant 0.7\, a_0$) needed to remove the K-shell electrons from Ne.

To provide a more complete description of the scattering process, calculated values for the ionisation and charge exchange cross sections are given in figure 3. Significantly, single charge exchange is a true n-body process, with the maximum cross section realised when there is an additional ionisation of five electrons. The magnitude of the cross sections (greater than 10^{-18} cm^2) further indicates the long-range nature of these collisions.

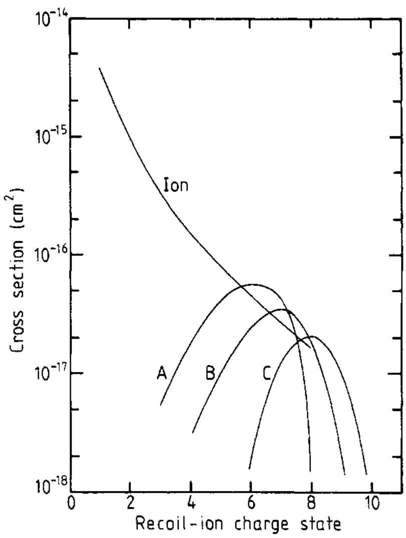

Figure 3. Calculated values for the ionisation and charge exchange cross sections for the U^{32+} + Ne collision system at 1.4 MeV u^{-1}. Curve A, single charge exchange; curve B, double charge exchange; curve C, triple charge exchange.

In order to further explore the collision dynamics, we show in figure 4 calculated values for the average kinetic energy lost by the projectile ion. For high recoil-ion charge-state production, $i > 4$, the projectile-ion energy loss is of the order of several keV. Since the target recoil ion is shown to gain only a few eV (figure 2), conservation of energy requires that the difference between the projectile-ion's energy loss and the target recoil-ion's energy gain must reside in electronic excitation of the recoil ion and/or the translational energy of the ejected electrons.

Figure 5 shows a representative differential energy loss cross section for the electrons ionised in the reaction

$$U^{32+} + Ne \rightarrow U^{32+} + Ne^{6+} + 6e. \qquad (5)$$

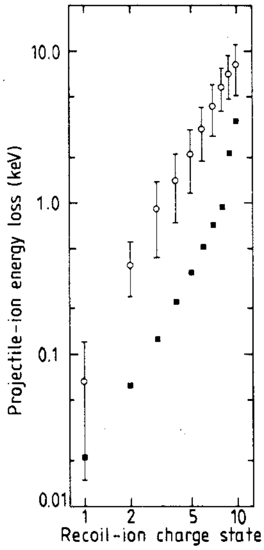

Figure 4. Average projectile-ion energy loss calculated for 1.4 MeV u^{-1} U^{32+} + Ne collisions using the *n*CTMC method (open circles). The error bars given are at the single standard deviation level. The full squares are the sum of the sequential ionisation potentials needed to remove *i* electrons from Ne.

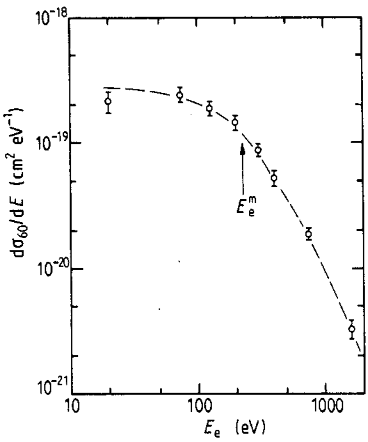

Figure 5. Representative electron differential energy loss cross section for the $U^{32+} + Ne \rightarrow U^{32+} + Ne^{6+} + 6e$ reaction at 1.4 MeV u^{-1}. The median electron-ejection energy is calculated to be about 210 eV. The error bars are at the single standard deviation level.

The median value for the ejected-electron energy is about 210 eV, while the average value is about 315 eV. The calculations clearly indicate the importance of fast ejected electrons.

One might question to what angular region the electrons are ejected. Figure 6 displays the angular differential cross section for reaction (5), which has been multiplied by $2\pi \sin\theta$ in order to obtain its relative contribution to the total cross section. Interestingly, we find that the electrons scattered to wide angles dominate the cross section. Such a prediction implies that the sum of the transverse momenta of the

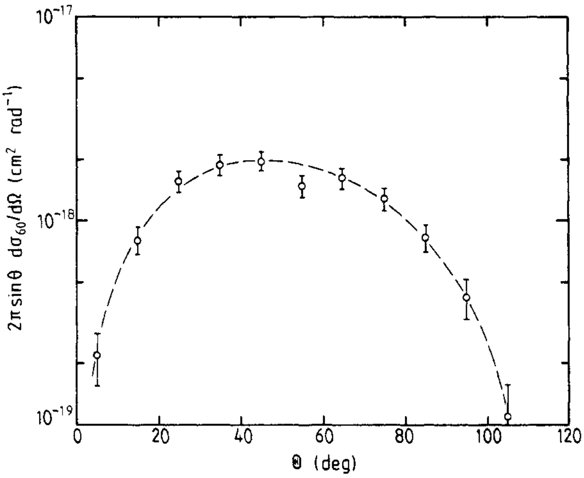

Figure 6. Angular differential cross section for the electrons ejected in reaction (5) at 1.4 MeV u^{-1}. The error bars are at the single standard deviation level.

ejected electrons can be comparable to that of the projectile and target recoil ion if there is an asymmetry in the electron-ejection angles relative to the deflection of the projectile ion. Although the electron spectra are based on classical calculations, it should be noted that the CTMC method has been found to qualitatively reproduce such spectra for the $H^+ + He$ ionisation reaction (Olson *et al* 1987). Note, the error bars shown in figure 6 are at the single standard deviation level. Hence, the dip displayed at 55° can only be attributed to statistical fluctuations in the calculations.

In summary, we have shown conclusive evidence that the recoil ions produced in energetic, multiply charged ion-atom collisions have very low translational energies. Our calculations also predict the importance of fast ejected electrons in these collisions and demonstrate the necessity of knowing the electrons' angular distributions in order to understand the dynamics of multiple ionisation collisions.

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