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Single- and Double-Electron Removal from H^- in Energetic Collisions with Multiply-Charged Argon Ions.

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Abstract. – Absolute cross-sections have been measured and compared to CTMC-calculations for single- and double-electron removal from H^- in collisions with Ar^{q+} ions ($q \leq 8$) at $E_{c.m.} = 50$ keV. The single-electron removal cross-sections are found to scale with $q^{1.3}$, and for the $H^- + Ar^{4+}$ system, this cross-section is found to have a weak energy dependence from 3 keV to 100 keV. A major implication of our measurements is that plasma neutralizers based on multiply charged ions for high-efficiency conversion of intense H^- beams into H^0 gain little in expected reduced length due to the inapplicability of q^2-scaling in the H^- single-electron removal cross-section.

The injection of energetic neutral beams of $H^0(D^0)$ is a proven technique for auxiliary heating of magnetically confined fusion plasmas. Presently, the production of multi-megawatt neutral beams is based on the neutralization of intense H^+ ion beams for energies up to about 60 keV/u. However, future fusion devices call for injection energies at hundreds of keV where the neutralization efficiency of positive ions is very small ($< 1\%$) due to decreasing electron capture cross-sections. For the latter requirements, the only efficient method of generating intense beams of H^0 is via neutralization of an accelerated H^- beam. Collisional neutralization efficiencies of $H^- \rightarrow H^0$ in gas targets are on the order of 50% and are almost independent of energy above about 50 keV/u.

A novel idea has been proposed and shown to give even higher neutral beam efficiencies. It is to employ a plasma neutralizer consisting of free electrons and ions [1-4]. For such a neutralizer, the conversion efficiency of H^- to neutral H^0 is expected to be $\approx 85\%$. Further, the use of a plasma neutralizer based on multiply-charged ions is expected to benefit from a substantially reduced optimum line density due to the larger electron removal cross-sections. These studies [5, 6] assumed a q^2-dependence for the H^- single-electron removal cross-section, which advantageously leads to a reduced apparatus length for operation at similar electron densities. However, design and modelling studies for plasma neutralizers have suffered from the lack of experimental cross-sections for the single-electron removal

$$H^- + X^{q+} \rightarrow H^0 + \ldots \tag{1}$$

and the double-electron removal reactions

$$H^- + X^{q+} \rightarrow H^+ + \ldots . \tag{2}$$

Reaction (2) is especially important since it directly degrades the efficiency of a plasma neutralizer.

In this letter, we present the first experimental data for reactions (1) and (2) for multiply-charged ions. Absolute cross-sections for $H^- + Ar^{q+}$ ($q \leq 8$) collisions have been measured by means of the crossed-beams technique. Theoretical calculations based on a simple model for H^- qualitatively reproduce the measured cross-sections and lead to an easily understandable interpretation of the electron removal mechanisms.

The principle experimental arrangement [7] and the signal-recovery technique [8] used for the present measurements have been described previously. Briefly, two well-collimated (< 2 mm diam.) and charge-analysed ion beams of adjustable energies (H^- beam: $(8 \div 117)$ keV, $(4 \div 70)$ nA; Ar^{q+} beam: $(20 \div 80)$ keV, $(2 \div 200)$ nA) are arranged to intersect at an angle $\theta = 45°$ in an ultrahigh vacuum region. The collision products (H^0, H^+) formed in the H^- beam are separated immediately after the interaction region by electrostatic deflection and counted individually by a channeltron-based single-particle detector.

Some crucial apparatus improvements, however, have been necessary to achieve the present measurements. A newly designed [9] small 5 GHz ECR ion source has been utilized for the production of intense and stable beams of multiply-charged argon ions. The most serious experimental problem has been provided by background events due to H^0 and H^+ particles, respectively, which result from the interaction of H^- ions with the residual gas. In order to reduce this background the ultrahigh vacuum in the interaction region has been lowered to about $2 \cdot 10^{-11}$ mbar with both beams «on». Furthermore, the H^- beam has been cleaned, shortly before intersection, by electrostatic deflection. Even under these conditions, however, a beam modulation technique [8] had to be employed for signal recovery since the signal of 4 to 200 counts/s was masked by a background which was a factor 2000 to 50 higher, respectively. Typical measurement times were up to 4 hours for one cross-section.

The theoretical calculations employed the three-body classical trajectory Monte Carlo (CTMC) method [10] and the independent particle model [11]. The principal difficulty in implementing any theoretical method is in the development of a suitable model for the H^- ion. Recalling the quantum-mechanical two-term spatial wave function approximation for the H^- ion

$$\Psi = N(\exp[-\alpha r_1] \exp[-\beta r_2] + \exp[-\alpha r_2] \exp[-\beta r_1]), \tag{3}$$

it is possible to relate classically the parameters α and β to the effective charge experienced by each electron. Using Slater's rules, $\alpha = \beta = 0.6875$, and the total electronic energy calculated for H^- is -0.4727 a.u. (*i.e.* not bound); the experimental value is -0.5277 a.u. Moreover, such values for α and β classically require each electron to be bound by 0.2363 a.u. ($\alpha^2/2$ and $\beta^2/2$), which is unacceptable since the first and second ionization potentials are 0.0277 a.u. and 0.5 a.u., respectively. Since within the independent particle model the electrons are distinguishable, it is possible to use effective charges of $\alpha = 0.2354$ and $\beta = 1.0$ for the two electrons. With these values the experimental ionization potentials are reproduced, and a quantum-mechanical configuration interaction calculation by us using the split shell wave function given by eq. (3) yields an electronic energy of -0.5125 a.u., which is 72% closer to the experimental value than the single parameter result.

During the course of our investigation, a particularly simple model for the mechanism of double-electron removal evolved. It is simply related to the product of the probability of removing the outer, loosely bound electron P_O times the probability of removing the more tightly bound inner electron P_I:

$$P_{\text{2-ion}} = P_\mathrm{O} P_\mathrm{I} . \tag{4}$$

The cross-section is

$$\sigma_{-+} = 2\pi \int P_\mathrm{O} P_\mathrm{I}\, b\, \mathrm{d}b . \tag{5}$$

However, since the limits of integration of (5) are restricted to small impact parameters by P_I, where P_O is approximately constant, we can rewrite (5) as

$$\sigma_{-+} = 2\pi P_\mathrm{O} \int P_\mathrm{I}\, b\, \mathrm{d}b . \tag{6}$$

One can immediately see that eq. (6) is simply

$$\sigma_{-+} = P_\mathrm{O}\, \sigma_{0+} , \tag{7}$$

where σ_{0+} is the well-known single-electron removal cross-section from neutral H^0

$$\mathrm{H}^0 + \mathrm{X}^{q+} \rightarrow \mathrm{H}^+ + \ldots . \tag{8}$$

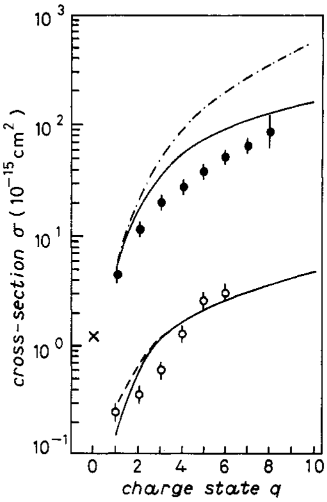

Fig. 1. – Experimental single (●) and double (○) electron removal cross-sections for $\mathrm{H}^- + \mathrm{Ar}^{q+}$ ($q \leq 8$) collisions at $E_\mathrm{c.m.} = 50$ keV. An experimental data point (×) for single-electron removal in $\mathrm{H}^- + \mathrm{Ar}^0$ collisions (ref. [12]) is shown for comparison. The solid lines are CTMC calculations for the respective processes. The dot-dashed line is the Bethe-Born calculation of ref. [13]. The dashed line is the electron removal cross-section for neutral H^0 (ref. [14]).

The experimental and theoretical cross-sections for single-electron removal are compared to one another in fig. 1 at a centre-of-mass energy of 50 keV ($v = 3.1 \cdot 10^6$ m/s). Both the Bethe-Born [13] and the CTMC methods reproduce the $q = 1$ experimental result. However, as the charge state of the ion increases, the q^2 scaling predicted by the first-order Born approximation becomes increasingly invalid even though the collision energy of 50 keV/u is well above the projectile-electron velocity-matching region of ≈ 1.4 keV/u. In fact, the experimental cross-sections scale, within error bars, with a $q^{1.3}$ dependence on the ionic charge (fig. 2).

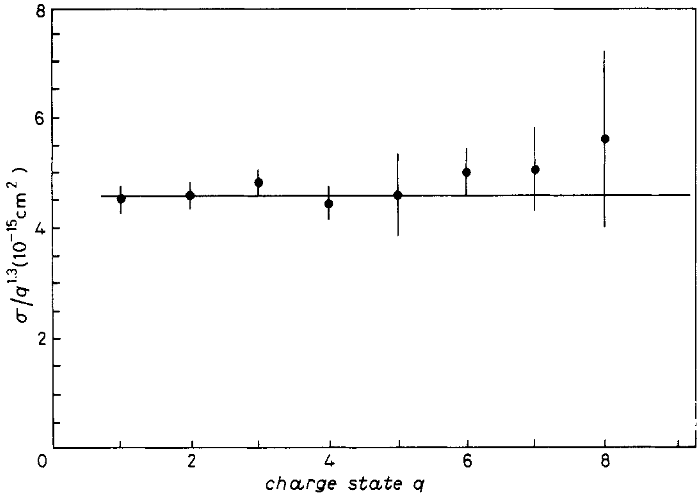

Fig. 2. – Experimental single-electron removal cross-sections of fig. 1 scaled by $q^{1.3}$.

The reason for the lack of q^2 scaling is realized by examining calculated transition probabilities for removing the weakly bound electron on H^- (dashed lines in fig. 3). One can readily see that the transition probabilities saturate close to unity for all charge states so

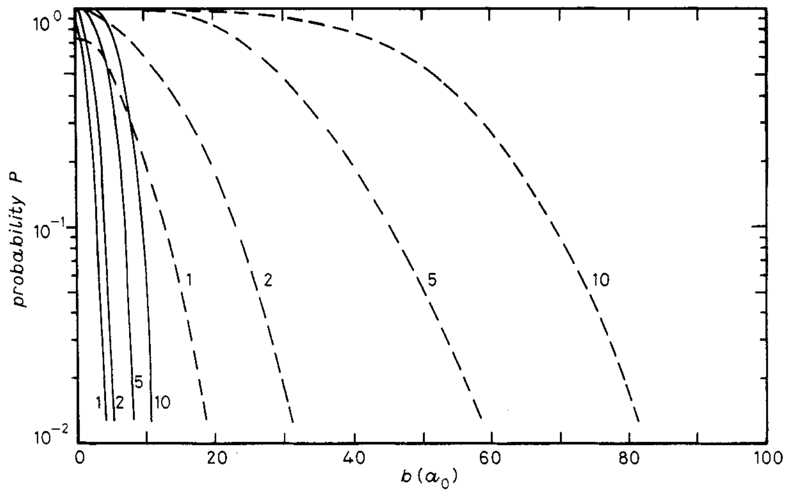

Fig. 3. – Transition probabilities calculated by the CTMC-method for electron removal (ionization + + capture) for the loosely bound 1s′ electron (dashed lines) and the tightly bound 1s electron (solid lines) at $E_{\text{c.m.}} = 50$ keV for ion charge states $q = 1, 2, 5, 10$ vs. impact parameter.

that a q^2-dependence on the cross-section cannot be realized. Furthermore, the range of single-electron removal is quite large and on the order of several tens of a_0 for even the low-charge state ions. Therefore, we are lead to predict that the single-electron removal cross-section will be independent of the ion species of the multiply-charged ion and simply be a function of its charge state. The CTMC calculations reveal that $> 95\%$ of the single-electron removal for charge states $1 \leq q \leq 10$ is due to impact ionization rather than electron capture.

In fig. 4 are shown the velocity dependence of the $H^- + Ar^{4+}$ single-electron removal cross-section along with that for $H^- + H^+$. When scaled by $q^{1.3}$, the results are nearly identical, thus displaying the lack of dependence on ion species. The behaviour of the cross-sections in velocity is far removed from the $\sim 1/v^2$ scaling predicted by asymptotic theories. The CTMC results for $H^- + Ar^{4+}$ are also shown in fig. 4. The calculated energy dependence is similar to that observed, however, the absolute magnitude is $\approx 50\%$ too large. The probable reason for this discrepancy is that the simple hydrogenic model employed here yields too high of a density of the low momenta electrons when compared to accurate *ab initio* results [16]. Thus, the impact parameter range of the single-electron removal is over-estimated.

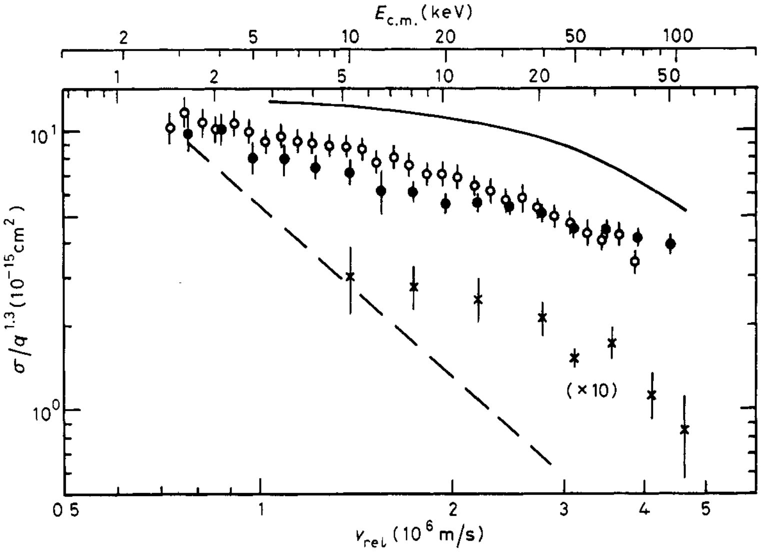

Fig. 4. – Scaled experimental single-electron removal cross-sections for $H^- + Ar^{4+}$ (●) and $H^- + H^+$ (○, ref. [15]). Scaled double-electron removal cross-sections (multiplied by a factor 10) for $H^- + Ar^{3+}$ are shown by crosses. The dashed line indicates a $1/E$ dependence for $H^- + Ar^{q+}$ collisions. The solid line is the CTMC result for the $H^- + Ar^{4+}$ system. The upper x-axis scales show the centre-of-mass energies for the systems $H^- + Ar^{4+}$ (above) and $H^- + H^+$ (below), respectively.

The double-electron removal cross-sections for reaction (2) are shown in fig. 1 for incident ion charge states of $q = 1$ to 6 at $E_{c.m.} = 50$ keV. There is qualitative agreement between experiment and the CTMC calculations. Referring to the transition probabilities for removing both the inner and outer electron (fig. 3), we find the overlap is concentrated at small impact parameters where the outer electron is ionized with an $\approx 100\%$ probability. This leads to the expectation that the double-electron removal cross-section from H^-, σ_{-+}, is approximately equal to single-electron removal from neutral H^0, σ_{0+}. The dashed line in fig. 1 displays the parameterized cross-section σ_{0+} for neutral H^0 [14].

The CTMC calculations indicate that the double-electron removal cross-sections shown in fig. 1 are primarily composed of both a double ionization component

$$H^- + X^{q+} \rightarrow H^+ + X^{q+} + 2e \tag{9}$$

and a transfer-ionization component

$$H^- + X^{q+} \rightarrow H^+ + X^{(q-1)+} + e\,. \tag{10}$$

For singly-charged projectiles, the above two reactions contribute approximately equally to the double-electron removal. However, the transfer-ionization component becomes increasingly important with higher charge states and is calculated to be approximately 70%, 90% and 97% of the double-electron removal cross-section for charge states $q = 2$, 5, and 10, respectively.

The charge state and velocity dependence of the double-electron removal is quite similar to that for single-electron removal. It is apparent that one should not expect an $\sim q^4/E^2$ behaviour, as predicted by perturbation theory and the independent particle model, to be valid in the intermediate energy regime for double-electron removal.

In summary, H^- single- and double-electron removal cross-sections for collisions with multiply-charged ions have been observed, for the first time, using a crossed-beams technique. The cross-sections for charge states from $q = 1$ to $q = 8$ and energies from 3 to 100 keV/u do not follow expected scaling rules. A simple model for the H^- ion has been applied to double-electron removal where we find $\sigma_{-+}(H^-) \approx \sigma_{0+}(H^0)$. We note from our cross-section measurements that the ratio of double to single ionization is approximately $(4.7 \pm 1.2)\%$.

Calculations based on the present data show that at 50 keV/u H^- neutralization efficiencies of 82 to 89% are realizable. Extrapolation of the data using the experimental energy dependence given in fig. 4 shows that at 300 keV/u the neutralization efficiencies decrease by only about 2%. The above results are consistent with previous predictions [5, 6]. However, our measurements do not bear out the expectation that plasma neutralizers can be made significantly more compact by employment of multiply-charged ions compared to singly-charged ions which are much easier to produce. This is the result of our observed $q^{1.3}$ scaling of the single-electron removal cross-section which is in contrast to the expected q^2 scaling. Our modelling calculations indicate a reduction of 3 in the target ion line density compared to 15 for using a $q = 5$ ion rather than a $q = 1$ ion. Moreover, our measurements and calculations indicate that the species of ions does not relevantly change the efficiency of H^- neutralization. Therefore, a plasma based on hydrogen or low Z alkali ions appears to be most advantageous.

* * *

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