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Publication Date
1978-06-01

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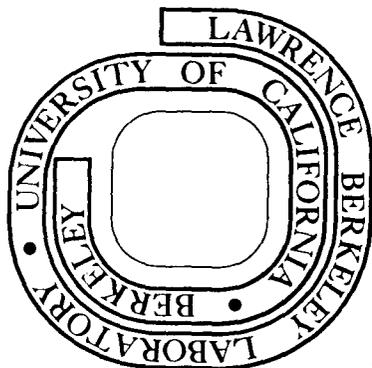A. S. Schlachter and J. W. Stearns

June 1978

DISCLAIMER

Charge-State Dependence of Electron Loss From H By Collisions with
Heavy Highly Stripped Ions

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June 1, 1978

ABSTRACT

Theoretical calculations, confirmed by experimental measurements, are used
to obtain a new scaling rule for electron loss from a hydrogen atom in collision
with a heavy highly stripped ion. The calculations cover the energy range
50 keV/amu to 5000 keV/amu and charge-states q from 1 to 50; the cross-section re-
sults for electron loss are very close to the Born-approximation scaling of $q^2(\ln E)/E$
at high velocities and yield a classical limit of $4.6 \times q \times 10^{-16}$ cm^2 at low
velocities. A simple analytic expression that describes the electron-loss cross
section for $1 \leq q \leq 50$ in the energy range 50 keV/amu to 5000 keV/amu is presented.
The experiments are in the range 108 keV/amu to 1140 keV/amu and charge-states
3 to 22.

In this Letter we present a new scaling rule for electron loss for heavy highly charged particles colliding with atomic hydrogen for energies from 50 keV/amu to 5000 keV/amu and for $1 \leq q \leq 50$. Electron loss from H resulting from a collision with an ion A^{+q} is the sum of charge exchange and ionization:

$$A^{+q} + H \Bigg\langle \begin{array}{lll} A^{+q-1} + H^+ & \text{(charge exchange)} \quad \sigma_{cx} & \text{(1a)} \\ \\ A^{+q} + H^+ + e^- & \text{(ionization)} \quad \sigma_i & \text{(1b)} \end{array}$$
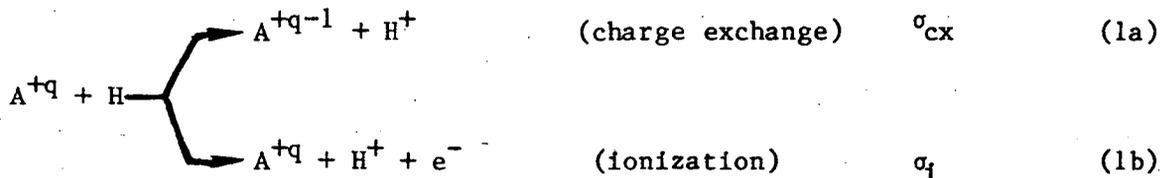
i.e., $$\sigma_{loss} = \sigma_{cx} + \sigma_i \;. \qquad\qquad\qquad \text{(1c)}$$

We find that, for this wide range of energies and charge states, electron-loss cross sections for collisions with any ion A^{+q} can be represented by a single curve when plotted with the reduced parameters $\sigma_{loss} \div q$ vs. (energy per amu) $\div q$.

At low collision energies charge exchange determines the H-atom electron-loss cross section, while at high energies ionization is the dominant reaction. These collisions are generally classified by whether the heavy-particle velocity is less than, or greater than, the orbital velocity of the electron being detached. For H-atom targets, this velocity is $v_e = 2.2 \times 10^8$ cm/sec, which corresponds to a collision energy of 25 keV/amu.

For collision velocities $v \ll v_e$, a molecular theoretical treatment of the scattering processes is generally applicable. At these velocities several the- ories [1-3] and a combination of theory and experiment [4] have been presented to describe the charge-state dependence of charge exchange, the dominant electron-loss process.

On the other hand, at very high velocities, generally characterized for a hydrogen-atom target by $v/v_e \gg q$, perturbation treatments such as the plane-wave Born approximation (PWBA) become valid. [5] Such treatments lead to the result that the electron-loss cross section (reaction 1) will scale as q^2 times the cross section for $H^+ + H$.

Until now there has been no scaling rule available for electron loss from H in collision with heavy highly charged ions at the intermediate collision-velocity range $1 \lesssim v/v_e \lesssim q$, nor has there been available a simple criterion for defining the region of applicability of the Born approximation. However, an empirical scaling relationship for charge exchange[6] has previously been presented.

In order to determine a scaling rule for electron loss for collisions of heavy highly charged ions colliding with H, we have calculated this cross section for the energy range 50 keV/amu to 5000 keV/amu ($1.4 < v/v_e < 14$) and for q in the range 1 - 50. The theoretical calculations employ the classical trajectory Monte Carlo method which has been described previously.[7] The energy range for these calculations is determined by two limits: At low energies ($v/v_e \lesssim 1$ or $E \lesssim 25$ keV/amu) molecular effects become important and we do not expect a classical-trajectory method to be valid, while at high reduced energies ($\gtrsim 5000$ keV/amu $\div q$) we were unable to employ the classical-trajectory method because the transition probabilities become so small that it is difficult to obtain reasonable statistics on the cross sections. It is important to note that the calculated electron-loss cross section at a given relative velocity for an H-atom target is determined only by the charge-state q; our calculations show no dependence on the reduced mass of the colliding pair. Since the H electron-loss cross section is determined by large impact parameter collisions, up to b = 25 Bohr radii for q = 50, the collision may be described as between point charges. (If we wish to examine the individual components of the electron-loss cross section, i.e., electron capture or ionization, it is sometimes necessary to employ an effective charge for the incident ion that reflects its electronic shell structure.[8]) Thus, the electron-loss cross sections calculated for this Letter are appropriate for a wide range of collision systems involving heavy highly stripped ions and atomic hydrogen. Our theoretical results for H^+ + H are within ± 20% of the experimental results for energies 50 - 200 keV/amu[7,9] and agree within ± 25% at the higher energies

with the Born-approximation calculations of Bates and Griffing.[10] We estimate the uncertainty in all of the calculated cross sections to be $\pm$ 25%.

We have previously reported[11] experimental measurements of σ_{cx}, σ_i and σ_{loss} for Fe ions in collision with H_2 for the energies 274 keV/amu and 1140 keV/amu and for q in the range 9 - 22; our apparatus and experimental method also are described in this publication. We have extended these measurements to q = 10 - 15 at 290 keV/amu, q = 3 at 110 keV/amu, and q = 7-11 at 108 keV/amu; these results will be described in detail in another publication.[12] The experimental cross-section results for an H_2 target have an uncertainty of $\pm$ 10%

To compare our experimental measurements in an H_2 target with calculations for an H target we have used the results of Kim et al.[13] Their results show that at 108 keV/amu the ratio of σ_{cx} for Fe^{+q} in H_2 and H ranges from 1.7 for q = 7 to 1.5 for q = 11; for high energies and low q's the ratio is approximately 2. This latter ratio is consistent with the measurements of Gilbody et al., which show that the ratio of cross sections for H_2 and H targets for both charge exchange[14] and ionization[15,16] is 2.0 $\pm$ 0.4 for an H^+ projectile with an energy above ~110 keV/amu (charge exchange) or ~200 keV/amu (ionization). We have thus divided our experimental results by 2 to obtain an estimate of the atomic-H cross sections, except for the experimental results at 108 keV/amu, which were divided by the ratios obtained from Kim et al.[13] We estimate the uncertainty in the ratio for comparing H_2 measurements with H calculations to be $\pm$ 25%; the overall uncertainty in our experimental cross section results for comparison with the calculations is thus $\pm$ 30%. It should be noted that the ratio of σ_{cx} for H_2 and H targets[13,17,18] has been observed for a wide variety of incident ions to be independent of ion species and to be determined by the velocity (or energy per amu) and the charge state of the ion.

It is possible to present all our theoretical calculations, our experimental measurements and the experimental results of others[15,16,19-23] on a single curve

parameterized by $\sigma_{loss}(cm^2) \div q$ as the ordinate and $E(keV/amu) \div q$ as the abscissa. At high velocities the classical calculation yields σ_{loss} proportional to q^2/E. Therefore, at high velocities, the classical-trajectory results should have a slope of -1 on a log-log plot. At low velocities, for which the collision time becomes comparable to the time for the target electron to orbit about the H^+ nucleus, a simple classical argument by Bohr and Lindhard,[24] based on determining the inter-nuclear separation where the force on the electron from the incident projectile A^{+q} is equal to that from the H^+ nucleus, is valid. In this model it is assumed that the electron will be removed from the target atom for all impact parameters smaller than this separation. Within this simple approximation it can be shown that $\sigma_{loss} \simeq (2-4) \times q \times 10^{-16}$ cm^2. Note the absence of energy dependence and the linear dependence on incident charge-state q. We thus expect the same parameter-ization that applies at high velocities to yield a constant in the low-velocity, high-q regime.

In Fig. 1 we present both the theoretical and experimental data. The agreement between theory and experiment is excellent. Both the theory and experiment are absolute, independent, and each covers a wide range of energies and charge states. This result is notable in that cross sections for ions in charge states from 1 to 50 and for energies ranging over two orders of magnitude coalesce into a single curve. At low reduced energies, both the classical-trajectory and the experimental data in-dicate that the cross sections approach the classical limit, which is $\sim 4.6 \times q \times 10^{-16}$ cm^2. This is consistent with low-velocity ($v \ll v_e$, high q) theories[2-3] and data,[4] below the energy range of our present calculations, which show charge-exchange cross sections generally invariant with energy and depending linearly on the charge of the incident ion.

The curve shown in Fig. 1, which represents the results of the classical trajectory Monte-Carlo calculations, can be approximated by an analytic expression of the form,

$$\sigma_{loss} = 4.6 \times q \times 10^{-16} \quad \left[(32q/E)(1 - \exp(-E/32q))\right] \tag{2}$$

where σ_{loss} is the H-atom electron-loss cross section in cm^2, q is the ion charge state, and E is the energy in keV/amu. It should be reemphasized that Eq. 2 is only valid for $1 \leq q \leq 50$ and for energies in the range 50 keV/amu to 5000 keV/amu.

For comparison we also present the PWBA ionization cross section[10,25] for H$^+$ + H collisions in Fig. 1. This quantum-mechanical perturbation approach yields σ_{loss} proportional to $q^2(\ln E)/E$ at high velocities. Above 50 keV/amu ÷ q there is reasonable agreement between the classical-trajectory and the PWBA cross sections, with the PWBA results being larger at the highest energies studied. This difference is due to the classical vs. the quantum-mechanical description of the electron distribution about the target nucleus and indicates that electron transitions from the classically forbidden region ($r_e > 2$ Bohr radii) become important at high energies and low transition probabilities. We thus expect that the classical-trajectory method will underestimate the true results at the highest energies; this trend is confirmed by comparison with experimental data for reduced energies above 1000 keV/amu ÷ q. For low velocities the PWBA ionization cross section lies much below the electron-loss cross section calculated using the classical-trajectory method because (1) the Born approximation is not expected to be valid at low velocities, and (2) charge exchange makes an increasingly large contribution to σ_{loss} at low velocities.

We are presently extending our experimental measurements to higher charge-state ions in hydrogen targets. We are also extending our experiments and calculations to non-hydrogenic targets in order to study the application of our reduced

curve to a broader range of systems. Preliminary calculations on helium targets indicate that the scaling parameters presented here will yield a similar curve for this system.

ACKNOWLEDGEMENTS

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Figure Caption

FIG 1.   Solid line: Calculated cross section σ_{loss} for electron loss by atomic

hydrogen in collision with an ion in charge-state q; this curve is valid

for $1 \leq q \leq 50$ and for energies in the range 50 keV/amu to 5000 keV/amu.

The range of E/q values for which the curve is valid is indicated by the

bars drawn in the lower portion of the figure. The uncertainty in the
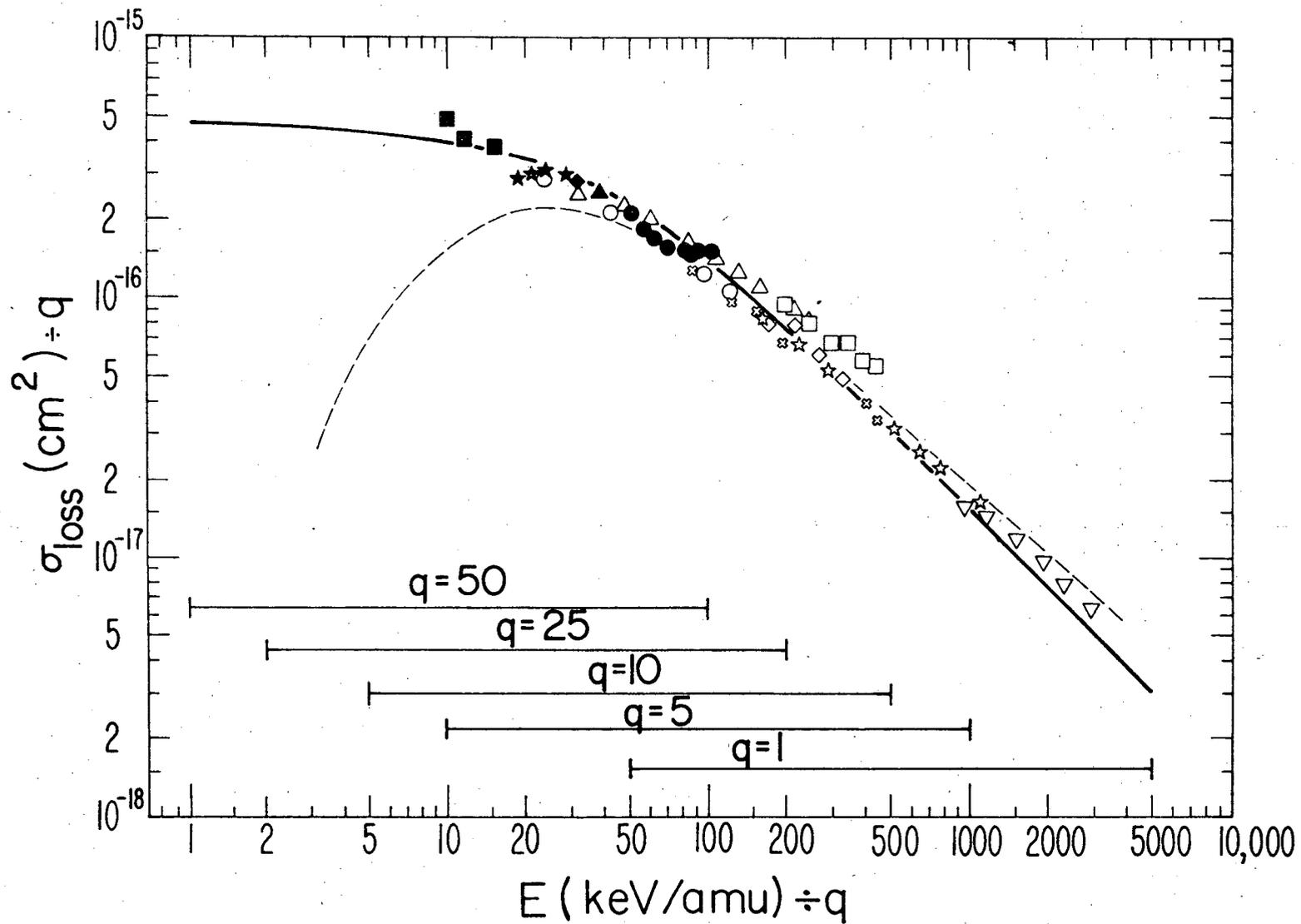
calculated cross sections is $\pm$ 25%.

Dashed line: Plane-wave Born-approximation cross section for ionization

only.[10,25]

Closed symbols: Present experimental results for Fe^{+q} + H_2 divided by

a number between 1.5 and 2.0 to allow comparison with the calculations

(see text). The uncertainty is $\pm$ 30%.

■   108 keV/amu   q = 7-11

▲   110 keV/amu   q = 3

◆   282 keV/amu   q = 9

★   290 keV/amu   q = 10-15

●   1140 keV/amu   q = 11-22.

Open symbols: Published results for H^+, He^+ and He^{++} + H, H_2 (repre-

sentative points only). All results for an H_2 target are divided by 2

to allow comparison with the calculations.

◇ H^+ + H   Gilbody and Ireland[16]

☆ H^+ + H_2 Hooper et al.[19]

▫ H^+ + H_2 Gilbody and Lee[15]

▽ H^+ + H_2 Pivovar and Levchenko[20]

△ He^+ + H_2 Langley et al.[21]

▢ He^+ + H_2 Pivovar et al.[22]

○ He^{++} + H_2 Puckett et al.[23]

Figure axes: σ_{loss} (cm^2) $\div$ q (vertical) versus E (keV/amu) $\div$ q (horizontal)

q = 50
q = 25
q = 10
q = 5
q = 1

XBL 783-2458A