Electron-capture and impact-ionization cross sections for multiply charged ions colliding with helium

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The classical-trajectory Monte Carlo method has been used to calculate the single-electron capture and impact-ionization cross sections for collisions between fully stripped ions (H^+ to O^{+8}) and He at energies of 100–500 keV/amu. Except for the H^+ and He^{++} systems, electron capture dominates over impact ionization at the lower energies, whereas at higher energies impact ionization is the dominant mechanism for electron loss from He. The sum of the calculated electron-capture and impact-ionization cross sections is well represented by the expression $\sigma_{ec+ion} = 3.1\times10^{-16}q\{(52q/E)[1 - \exp(-E/52q)]\}$ cm^2, where q is the charge state of the incident ion and E is expressed in units of keV/amu. The calculated cross sections are in reasonable agreement with available experimental values.

INTRODUCTION

In a recent paper[1] we applied the classical-trajectory Monte Carlo method to collisions between multiply charged ions and atomic hydrogen. The classical-trajectory method was found to be extremely valuable because it is easy to apply for a wide range of incident ions, yields both the electron-capture and impact-ionization cross sections simultaneously, and produces cross sections for hydrogenic targets that are in reasonable agreement with experiment.[2-5] Moreover, this method, along with the Glauber method,[6] is applicable to the intermediate collision velocity region $v \gtrsim v_e$, where v_e is the orbital velocity of the electron being detached from the target. At lower velocities $v \lesssim v_e$, theoretical molecular treatments are valid,[7] whereas at high velocities $v \gg v_e$, theoretical methods such as the plane-wave Born approximation[8] (PWBA), binary-encounter approximation[9] (BEA), semiclassical approximation[10] (SCA), and Magnus approximation[11] become valid.

Since the three-body, three-dimensional classical-trajectory method has proved to be so effective for collisions between multiply charged ions and hydrogenic targets, we are investigating the possibility of using the method for other target species. In this paper we investigate the single-electron-loss reactions with He as the target:

$$A^{+q} + \mathrm{He} \begin{cases} A^{+q-1} + \mathrm{He}^+ \ \text{(electron capture)}, & \text{(1a)} \\ A^{+q} + \mathrm{He}^+ + e^- \ \text{(impact ionization)}. & \text{(1b)} \end{cases}$$

Calculations are performed for fully stripped incident ions with charge states $q = 1-8$ and for collision energies $E = 100-500$ keV/amu. As a reference, v_e for He is 2.93×10^8 cm/sec, which corresponds to a collision energy of 45 keV/amu.

THEORETICAL METHOD

The calculational procedure using the three-body, three-dimensional classical-trajectory Monte Carlo method is described in detail in Ref. 1. This theoretical method is based on solving Hamilton's equations of motion for the three-body system,[12] which includes the incident ion, the target nucleus, and an electron initially bound to the target nucleus. The equations are solved for a distribution of initial conditions that include varying the impact parameter and the position and momentum of the electron initially bound to the target nucleus.[13] Six random numbers are used to generate the distribution of initial conditions. For each distribution, the classical trajectories of the nuclei are calculated from a large internuclear separation (normally, $10q - a_0$) to the distance of closest approach, and out again to a large internuclear separation. The Coulomb forces between all three bodies are included in the calculation. If, at the end of an individual trajectory, the electron is still bound to the target nucleus, it is cataloged as no reaction. However, if the electron is found bound to the projectile ion, it is cataloged as electron capture, and if the electron is bound to neither nucleus, it is cataloged as impact ionization. The cross sections for the various processes are then directly related to the ratio of successful tries for that process to the total number of trajectories calculated. In the calculations presented here, 2000 trajectories at a given energy were normally adequate to determine the cross sections for reactions (1a) and (1b), with a statistical uncertainty of less than 10%.

The three-body classical-trajectory method can be directly applied to one-electron targets such as hydrogenic ions or atoms, or to systems where the scattering is determined by a valence electron such as in alkali-atom targets.[14] However,

it is of interest to extend this method to multielectron targets in a way that eliminates the necessity of solving Hamilton's equations of motion for each participating electron, incident ion, and target nucleus.

The first requirement for such an extension is to determine the effective charge Z_{eff} of the target nucleus as seen by the active electron. Several methods exist for determining Z_{eff}, such as using Slater rules[15] or the single-zeta Hartree-Fock wave functions calculated by Clementi and Roetti.[16] For a He-atom target, the above methods yield a Z_{eff} of 1.70 and 1.69, respectively. We have used the Hartree-Fock value of 1.69 in the calculations presented here.

The other extension required to handle multielectron targets is the manner in which the number of active electrons enters the cross-section formulas. In many formulations (PWBA and BEA), the cross sections are calculated assuming one active electron and then multiplied by the number of electrons in the electronic shell being considered. This method is valid if the transition probabilities are small, but is invalid for large transition probabilities, because in many cases a direct multiplication of the one-electron transition probability by the number of active electrons violates the "unitarity" of the S matrix.

Since the classical-trajectory calculations yield the one-electron detachment transition probabilities $p(b)$ as a function of impact parameter, we have chosen to use an exponential approximation[17] to obtain an estimate of the transition probability $P(b)$ for the multielectron target system. The quantity $\delta(b)$ is first determined by

$$\delta(b) = -\ln[1 - p(b)]. \tag{2}$$

Then the detachment transition probability for the electronic shell being considered is obtained from

$$P(b) = 1 - \exp[-n\delta(b)], \tag{3}$$

where n is the number of electrons in the electronic shell. The use of Eqs. (2) and (3) thus preserves the unitarity of the S matrix and becomes equivalent to multiplying the one-electron target cross section by n to obtain the multielectron target cross section when the transition probability is small. For all systems studied here, the one-electron target transition probabilities exceeded 50% for small impact parameters and low collision energies; the higher charge states possessed this characteristic to higher energies.

One additional uncertainty in our calculations is the manner in which the multielectron-target electron capture and impact-ionization transition probabilities are determined from the calculated one-electron target quantities. We have simply used the ratio of the electron-capture and impact-ionization cross sections obtained from the one-electron target calculations to scale the total electron-detachment cross section obtained from Eqs. (2) and (3) into its individual components. We fully expect this approximation and the extension to a multielectron target system to add an additional uncertainty to our calculations of at least ± 25%. For hydrogenic targets, we have generally found by comparison with experiment that the classical-trajectory cross sections have uncertainties of ± 25%–40%; hence, we expect that the He target calculations presented here will be uncertain by ± 50%.

RESULTS AND DISCUSSION

The cross sections calculated using the classical-trajectory method are presented in Figs. 1–3. General characteristics are that the electron-cap-

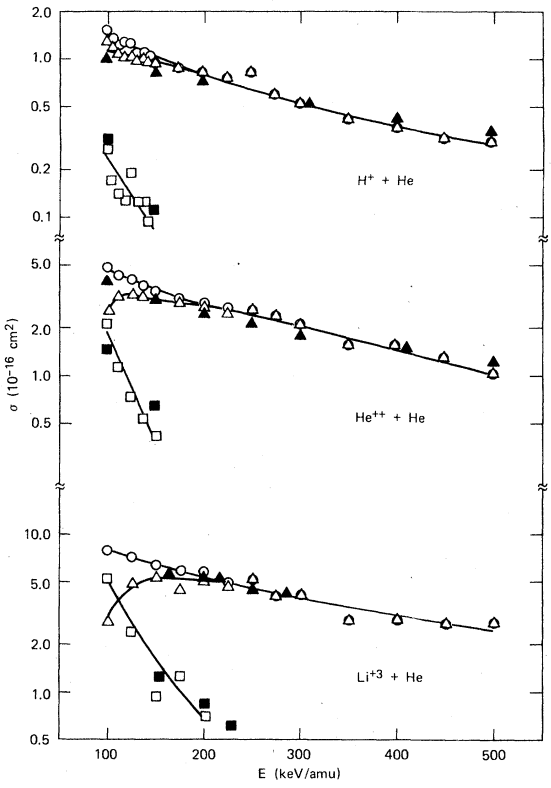

FIG. 1. Classical-trajectory cross sections for H^+, He^{++}, Li^{+3} + He collisions for single-electron capture (open squares), impact ionization (open triangles), and the sum of electron capture and impact ionization (open circles). Lines have been drawn through the theoretical points as a visual aid. Experimental data are denoted by solid symbols and were obtained from Barnett *et al.* for H^+ (Ref. 18), Puckett *et al.* for He^{++} (Ref. 21), and Pivovar *et al.* for Li^{+3} (Ref. 23).

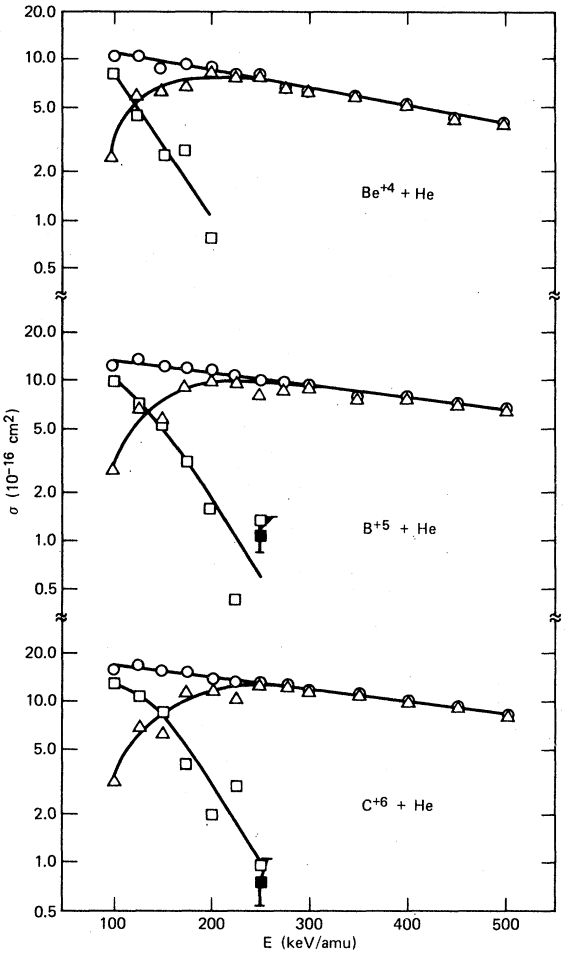

FIG. 2. Classical-trajectory cross sections for Be^{+4}, B^{+5}, and C^{+6}+He collisions. The same notation is used as in Fig. 1 except the data points for B^{+5} and C^{+6} are from Guffey *et al.* (Ref. 24).

ture cross sections decrease rapidly with increasing energy, with impact ionization dominating the electron detachment at the higher energies. The one difficulty with using the classical-trajectory method is that it requires considerable computer time to obtain reasonable statistics for a cross section when the transition probabilities are low, or when one cross section dominates over the other. Hence it is difficult to compute an accurate electron-capture cross section when it is a factor of 10–20 smaller than an impact-ionization cross section or vice versa.

For the H^++He system we have obtained reasonable agreement between our calculated results and experimental data[18] for electron capture and impact ionization that have estimated uncertainties of only ± 25% (Fig. 1). The Born and the Glauber methods have also been applied to impact ionization of He by H^+. The classical-trajectory

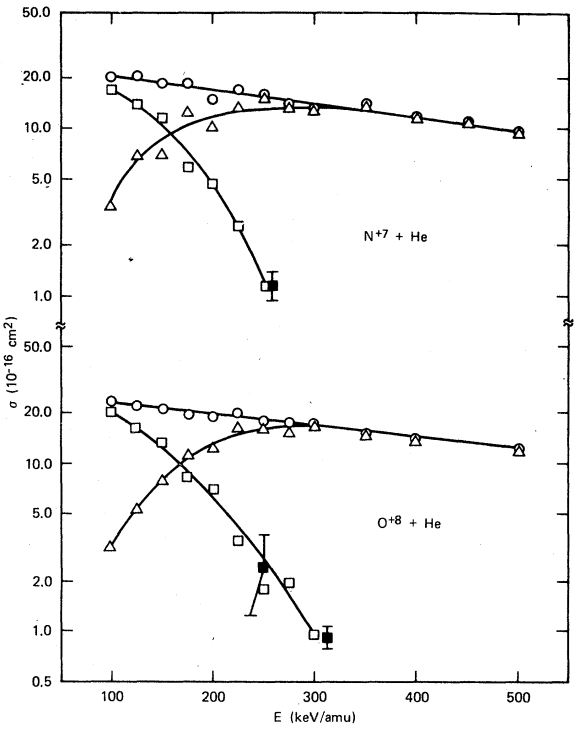

FIG. 3. Classical-trajectory cross sections for N^{+7} and O^{+8}+He collisions. The same notation is used as in Fig. 1., with the data points for N^{+7} and O^{+8} from Guffey *et al.* (Ref. 24).

results are within ± 30% of the Born cross sections[19] over the energy range shown. They are a factor of 2 larger than the Glauber calculations[20] at the lowest energy calculated, but are within ± 30% of these calculations above 250 keV/amu. It was discussed in Ref. 20 that the possible reason why the Glauber method underestimates the impact-ionization cross section at the lower energies is the difficulty in accounting for the "charge-transfer-to-the-continuum" within this approximation. The classical-trajectory method correctly accounts for this phenomenon, but the charge-transfer-to-the-continuum process requires extensive computer time at the lower collision energies. This is because Hamilton's equations of motion must be integrated to larger than normal internuclear separations before a positive test of electron capture or impact ionization can be made.

The He^{++}+He calculations are presented in Fig. 1, and compared to the electron-capture and ionization data of Puckett *et al.*[21] Their data for electron capture agree well with the data of Pivovar *et al.*[22] As in the H^+ system, the calculated values are in reasonable agreement with experiment except at the lowest energies, where the He^{++} +He calculations overestimate the electron capture and underestimate the impact-ionization cross

sections.

In the Li^{+3} + He system, experimental data exist for both electron capture and impact ionization.[23] Over the limited energy range where the experimental and the theoretical values overlap, there is very good agreement (Fig. 1).

For the Be^{+4} system (Fig. 2) we could find no experimental data with which to compare our calculations. However, for the B^{+5}, C^{+6}, N^{+7}, and O^{+8} systems (Figs. 2 and 3), we can compare our electron-capture cross sections with the experiments of Guffey *et al.*[24] These authors measured the electron-capture cross sections for capture into excited states of the incident ion by monitoring the x-ray photon emissions. A direct comparison between theory and experiment is valid here since we have classically analyzed the electronic state populations of the ion after electron capture, and find the population of excited states maximizing at the $n \approx \frac{1}{2}q$ electronic level and shifting slightly to lower n with increasing collision energy. At 250 keV/amu, 90% of the ions, after electron capture, are found in excited states for the B^{+5} + He system with an increase to 96% found for the O^{+8} + He system. Thus a direct comparison with the experimental measurements is valid, and introduces, at most, an additional uncertainty of only 10%. Referring to Figs. 2 and 3, we find that, except for the B^{+5} system where our statistics are poor, our calculations agree well with the experimental results.

As shown in a previous paper,[25] a convenient way to reduce the single-electron-loss cross sections (sum of electron capture and impact ionization) for a wide range of ions colliding with a given target is to plot the cross section divided by charge state versus the collision energy in keV/amu divided by charge state. Figure 4 shows such a plot of our calculated values. The line drawn through the data may be represented analytically by

$$\sigma_{\text{loss}} = 3.1\times 10^{-16} q\{(52q/E)[1-\exp(-E/52q)]\}\ \text{cm}^2 . \tag{4}$$

For high collision energies where impact ionization is the dominant electron-loss mechanism, Eq. (4) yields

$$\sigma_{\text{loss}} = 1.62\times 10^{-14} q^2/E\ (\text{keV/amu})\ \text{cm}^2 , \tag{5}$$

a result that agrees well with both BEA and PWBA predictions[8,9] for collision energies 100–500 (keV/amu) $\div q$. At higher reduced energies the classical description becomes increasingly invalid because quantum-mechanical tunneling is neglected. The classical ionization cross sections then underestimate the true values whose analytical form is

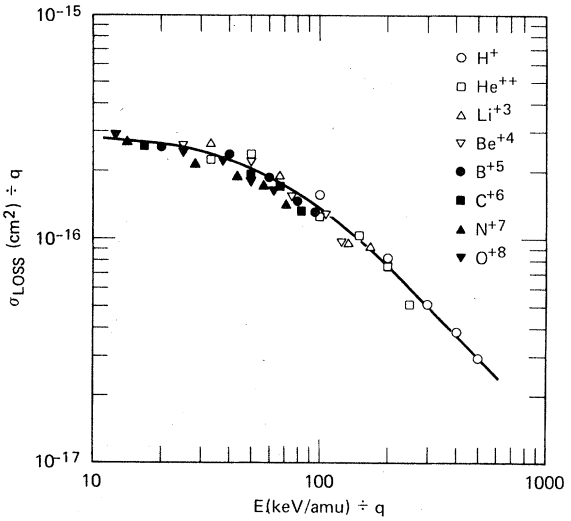

FIG. 4. Reduced plot of the classical-trajectory cross sections for single-electron loss (electron capture plus impact ionization) divided by the charge state of the incident ion vs the collisions energy in keV/amu divided by charge state.

proportional to $q^2(\ln E)/E$.

At low energies, where electron capture is the dominant electron-loss mechanism, our calculations approach the limit

$$\sigma_{\text{loss}} = 3.1\times 10^{-16} q\ \text{cm}^2 . \tag{6}$$

This linear dependence on charge state with no dependence on collision energy is in agreement with several theories[26–28] for electron capture by heavy, highly charged ions for low collision velocities $v \ll v_e$. Equation (6) is also in good agreement with the measurements reported by Müller and Salzborn,[29] who find a charge-state scaling for one-electron capture from He to be

$$\sigma_{ec} = 2.1\times 10^{-16} q^{1.17}\ \text{cm}^2 . \tag{7}$$

Their measurements include charge states between 2 and 8 for a wide range of incident ions and for laboratory collision energies from a few keV to 100 keV. For charge states between 2 and 8, Eqs. (6) and (7) yield cross sections that differ by less than 25%. We should caution that both Eqs. (6) and (7) are valid only for *heavy* ions where the number of product channels approaches a continuum.

The functional form of Eq. (6) can be rationalized simply by using the concept introduced by Bohr and Lindhard[30] for slow collisions between multiply charged ions and atom targets. These authors computed the internuclear separation R_d where the force felt by the active electron from both its parent nucleus and the incident ion is

equal. For smaller internuclear separations, it is assumed that the force from the ion will exceed that of the nucleus, and the electron will be detached. Thus the cross section is given by

$$\sigma_{\text{loss}} \approx \pi R_d^2 . \tag{8}$$

Classically, the largest distance from its nucleus at which a bound electron can be found is given by Z_{eff}/IP, where IP is the ionization potential in a.u. of the electron (for He, this distance is 1.87 a_0). Thus for slow collisions and charge states $q > Z_{\text{eff}}$, we find that

$$\sigma_{\text{loss}} \approx 0.88 \times 10^{-16} q Z_{\text{eff}}/(IP)^2 \text{ cm}^2 . \tag{9}$$

Note that Eq. (9) does not depend on the number of electrons in the shell being considered in this model because the transition probability is already assumed to be unity for impact parameters $b \leq R_d$. Applying Eq. (9) to a He target, we find $\sigma_{\text{loss}} \approx 1.8 \times 10^{-16} q$ cm^2, which is within a factor of two of the exact classical calculations given by Eq. (6).

CONCLUDING REMARKS

In our calculations we have assumed that single-electron detachment dominates over double-electron detachment. McGuire and Weaver[31] have presented formulas to estimate both the single- and double-electron ionization from the transition probabilities calculated in a one-electron formalism such as presented here. Their model assumes a sudden approximation, with the electrons frozen during the collision.

We have used this model to estimate the double-electron-ionization cross sections and find them an order of magnitude smaller than the single-electron-ionization cross sections for the low charge states, but for the high charge states and at the higher collision energies we find the double-electron ionization may reach 30% of the cross sections shown in Figs. 2 and 3. These results are very interesting but must be considered questionable since the sudden approximation of the model may not be fulfilled at the low collision energies considered here. However, the sum of the single- and double-ionization cross sections calculated using the sudden approximation and those presented here using the exponential approximation are identical at energies where impact ionization dominates over electron capture. Thus at the higher energies, our calculations may also be a very good estimate of the sum of single- and double-electron-ionization cross sections. Experimental data or more exact theoretical calculations that correctly include the two-electron character of the He-atom target are needed to assess the single- versus the double-electron-ionization processes.

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