Single electron loss in the collisions of C^{3+} and atomic hydrogen*

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This paper studies the projectile electron loss cross sections of C^{3+} colliding with atomic hydrogen in the frame work of extended over-barrier model at intermediate velocities (25 keV/u–600 keV/u). The electron loss is calculated in terms of the interaction between the screened target nucleus and the active projectile electron and of the interaction between projectile electron and target electron. Compared with the convergent close-coupling calculations, screening and anti-screening calculations, this model satisfactorily reproduces the experimentally obtained energy dependence of the electron-impact ionisation cross sections and the single electron loss cross sections over the energy range investigated here.

Keywords: single electron loss, over-barrier model
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1. Introduction

Projectile electron loss, also referred as projectile ionisation, is one of the events which may occur in a collision between clothed ion and a target atom over a wide range of energy. Their thorough understanding and experimental separation are important not only in themselves, but also for accurate predictions of target x-ray production in particle identification by x-ray emission. Electron loss from partially stripped ion colliding with atom at intermediate velocities is governed by two different and competing mechanisms: (a) the electron–nucleus interaction between the screened target nucleus and the active projectile electron (e–N interaction), (b) the electron–electron interaction between projectile electron and target electron (e–e interaction), in which the projectile electron is ionised and the interacting target electron is also simultaneously either excited or ionised. The e–N mechanism is generally the more important process and historically thoroughly studied. The e–e interaction allows the target electron to act as quasi-free electron and obey kinematical conditions with the projectile.

Projectile electron loss increases the charge state of the projectile and is often associated with simultaneous ionisation of the target. Because of its fundamental nature, the knowledge of the cross section for this process is essential in many applied areas, such as atomic physics, plasma physics, chemical physics, material science, radiotherapy and radiation research. For these reasons, a considerable effort has been spent to improve our understanding of this process during the last few decades. Experimentally, electron loss with lowly charged ions, especially hydrogen-like ions, as projectiles were investigated for several targets (atomic and molecular hydrogen, rare gases) at intermediate to high energy to obtain a detailed survey of the mechanisms which are responsible for it.[1−10] Shah *et al.*[1,2,4] measured the one-electron loss cross section in the collision of He^+, Li^+, Li^{2+} and H, H_2, He. The cross section for electron loss of He^+ and C^{3+} projectile ions on atomic and molecular hydrogen were measured in 0.5–3.5 MeV energy range by Sant' Anna, Melo and their team, the connection between anti-screening model and the electron impact ionisation of multi-charged ions was explored.[6] This team also measured the cross sections for the process of projectile electron loss of C^{3+} and O^{5+} ions impinging on rare gases in the energy range of 1.0–3.5 MeV,[7] and the measured cross sections present a strong saturation as the target atomic number increases. Montenegro *et al.*[8] separated the mechanisms leading to elec-

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tron loss experimentally through the measurement of the recoil ions and the emergent charge states in the collisions $He^+ + (H_2, He) \rightarrow He^{2+} + (H_2^+, He^+)$. The experimental investigations on projectile electron loss in collisions of partially stripped ions and atomic hydrogen were done earlier, only the total single loss cross sections are reported.

On the other side, since the quantum description of the electron-loss process for the projectile colliding with neutral target was established by Bates and Griffing[11] about 40 years ago, numerous theoretical studies have been performed. Montenegro and Meyerhof[12,13] performed calculations in terms of the screening effect and anti-screening effect in the projectile ionisation probability by using time-dependent semi-classical approximation. Non-perturbative theory was used in the calculation of projectile-electron loss.[14,15] Montanari *et al.*[16] calculated the projectile electron loss cross section due to the electron-electron interaction using atomic anti-screening theories. Olson *et al.* used a many-body classical trajectory Monte Carlo treatment to calculate single- and multiple-loss cross section.[17,18] Bohr,[19] basing his calculation on the free collision approximation and ignored the binding energy of the electron being removed, derived a simple formula to predict the stripping cross section.

In this paper, the single electron loss cross sections of C^{3+} impinging on atomic hydrogen are calculated by using the extended over-barrier model in terms of the interaction between the screened target nucleus and the active projectile electron and of the interaction between projectile electron and target electron at intermediate velocities (25 keV/u–600 keV/u). In Section 2, the extended over-barrier model and the expressions of the electron loss probabilities caused by screened target nucleus and target electron as well as the single electron loss probability are obtained. Section 3 contains a comparison of present results with those previously obtained, both experimentally and theoretically. Finally, in Section 4 the summary of this work is presented.

2. Theory

2.1. The theoretical model

We consider the Coulomb potential barrier formed by the superposition of the Coulomb field of the projectile and the target core. This has a saddle structure along the inter-nuclear axis. The potential maximum lies at the distance $\sqrt{Z_t}R/(\sqrt{Z_t} + \sqrt{Z_p})$ from the target core, where R is the inter-nuclear distance, Z_p and Z_t are the effective charges of the projectile and of the target seen by the electron in consideration, respectively. An electron moving around the core in one dimension has a turning point at Z_t/E_n, where E_n is the binding energy of the target electron. We assume that the electron can overcome the binding energy and escape from the target when the turning point is equal to the saddle point. Thus the released distance satisfies (atomic units will be used unless otherwise stated)

$$R_r = \frac{Z_t + \sqrt{Z_t Z_p}}{E_n}. \tag{1}$$

In Bohr–Lindhard's over-barrier model,[20] the capture takes place where the potential energy of the electron in the ionic field is numerically larger than its kinetic energy in the ion frame, i.e., the limiting condition for capture is given by $Z_p/R_c = V^2/2$, where V is the ion velocity, and hence capture is possible when the ion–atom distance is smaller than

$$R_c = \frac{2Z_p}{V^2}. \tag{2}$$

In this model, we assume that the Coulomb deflection is neglected. Thus, the projectile moves along a straight-line trajectory with the impact parameter b and the impact velocity V. When $R_r \leq R_c$ at low velocities, the ion is close enough for capture to take place, the condition is automatically fulfilled. In this region, the released electron will be captured. When $R_r > R_c$ at higher velocities, only the electron released within the distance of R_c will be captured. The electron released between R_c and R_r can be ionised or back to the target core. Consequently a criterion for ionisation has been introduced.

Let us consider that an electron escapes from the target core in the saddle point. The released electron will be accelerated by the approaching ion. The total kinetic energy of the electron obtained equals the sum of kinetic energy transferred by the ion during the collision and the difference of the ionisation energy of the quasi-molecular states. At some distance R_i, the electron itself will have enough kinetic energy to be ionised. The ionisation distance is given by

$$\frac{2Z_p^2}{V^2 R_i^2} + \frac{Z_p + Z_t}{R_i} - \frac{Z_p}{R_r} = E_n. \tag{3}$$

In the case of the projectile ionisation caused by the e–e interaction, the electrons are considered as free electrons, loss will happen when the energy transferred to the electron in the projectile frame is high enough

to ionise it, i.e., $\Delta E = 2/V^2 R_e^2 > E_n^p$ where E_n^p is the binding energy of the projectile electron. The projectile ionisation distance R_e resulted from the e–e interaction is expressed as

$$R_e = \sqrt{\frac{2}{E_n^p}} \cdot \frac{1}{V}. \quad (4)$$

The maximum energy transferred by the target electron is $V^2/2$, namely, $\Delta E = 2/V^2 R_e^2 \leq V^2/2$. So, R_e should not be smaller than $R_{em} = 2/V^2$. When $R_e \leq R_{em}$, the maximum energy transferred is less than E_n^p, the projectile electron can not be ionised. The projectile electron loss caused by e–e interaction takes place between R_e and R_{em}.

2.2. Evaluation of cross sections

In our model, when $R_r \leq R_c$ at low velocities, the released electron will be captured. Therefore, the capture cross section equals the released electron cross section. When $R_r > R_c$, the electron released within the distance of R_c can be captured. The released electron between R_c and R_i can be ionised. Release is a gradual process, which takes place with a probability per unit time of the order of $1/T$, where T is the period of the electron moving along its orbit. On the part of the projectile electron loss caused by e–N interaction, C^{3+} is ionised by H^+. Here, we still call C^{3+} ion the projectile and H^+ the target for the convenience of understanding. Before calculations, we hypothesize that the trajectory of the projectile is straight line, and the orbital period of the electron is not influenced by the ion.

When a projectile with charge state Z_p, and velocity V moves on a straight line trajectory with impact parameter b, the release starts at the time $t_i = -\sqrt{R_r^2 - b^2}/V$ and ends at $t_f = \sqrt{R_r^2 - b^2}/V$, the interacting time $t = 2\sqrt{R_r^2 - b^2}/V$. Then, the release probability is

$$p_r(b) = 1 - \exp(-2\ln 2\sqrt{R_r^2 - b^2}/VT_{1/2}), \quad (0 \leq b \leq R_r), \quad (5)$$

where $T_{1/2}$ is the half period of the electron moving round its core. When $t = -\sqrt{R_c^2 - b^2}$, the capture starts. The single electron capture probability is expressed as

$$p_c(b) = 1 - \exp(-2\ln 2\sqrt{R_c^2 - b^2}/VT_{1/2}), \quad (0 \leq b \leq R_c). \quad (6)$$

In the same way, the single electron ionisation probability is expressed as

$$p_i(b) = 1 - \exp(-2\ln 2\sqrt{R_i^2 - b^2}/VT_{1/2}), \quad (R_c \leq b \leq R_i). \quad (7)$$

During the process of the release, the electron is co-owned by the ion and the target core. Note that the derivation above does not account for the possible return of the electron from the other potential well. In order to take into account the factor that the electron released back to the target, an over-barrier factor f is introduced here. It is defined as

$$f = E_p^b/(E_n + E_p^b), \quad (8)$$

where E_p^b is the ground state energy of the projectile. For the symmetric case, $f = 1/2$.[21–23] Note that C^{3+} is considered as hydrogen-like ion here, the two electrons on shell K do not take part in the reaction. Then the probability is given as

$$P_{r,i,c}(b) = f \cdot p_{r,i,c}(b). \quad (9)$$

The projectile electron loss cross section caused by the e–N interaction is

$$\sigma_{e-N} = 2\pi \int p_i(b) b \mathrm{d}b. \quad (10)$$

On the part of the projectile ionisation caused e–e interaction, the projectile electron loss probability P_e is given as

$$P_e = 1 - e^{-b/R_e}, \quad (R_{em} \leq b \leq R_e). \quad (11)$$

So far as the projectile ionisation resulted from the e–e interaction is concerned, the electron on hydrogen interacts with the electron on projectiles.

The projectile electron loss cross section caused by the e–e interaction is

$$\sigma_{e-e} = 2\pi \int p_e(b) b \mathrm{d}b. \quad (12)$$

Because the electron loss by the e–e interaction results mostly in the simultaneous ionisation of the projectile

active electron and the target electron, the only possibility for electron capture to occur concomitantly with electron loss is through the loss by the e–N interaction. Thus the probability for single electron loss is given as

$$P_{\rm sl} = (1 - P_{\rm c}^{\rm p})P_{\rm i} + P_{\rm e}, \tag{13}$$

where $P_{\rm c}^{\rm p}$ is the projectile electron capture probability, which can be calculated in the same way as $P_{\rm c}$. The projectile single electron loss cross section in the collision of C^{3+} and atomic hydrogen can be calculated by using

$$\begin{aligned}\sigma_{\rm sl} &= 2\pi \int (1 - P_{\rm c}^{\rm p})P_{\rm i}(b)b{\rm d}b + 2\pi \int P_{\rm e}(b)b{\rm d}b \\ &= (1 - P_{\rm c}^{P})\sigma_{\rm e-N} + \sigma_{\rm e-e}. \end{aligned} \tag{14}$$

3. Results and discussion

As mentioned above, the projectile electron loss results from the e–N interaction and the e–e interaction. Present calculated projectile electron loss cross sections of C^{3+} caused by the e–N interaction are shown in Fig. 1, those caused by the e–e interaction are shown in Fig. 2, the projectile single electron loss cross sections by our model are shown in Fig. 3.

Figure 1 shows our calculated electron loss cross sections for C^{3+} induced by the e–N interaction, together with those of Sant' Anna *et al.*[6] for screening. By comparison, we can see clearly that present results agree well with the calculations of Sant' Anna *et al.* in the tendency, but overestimate the calculations of Sant' Anna *et al.* by a factor of about 1.6 in the high energy region.

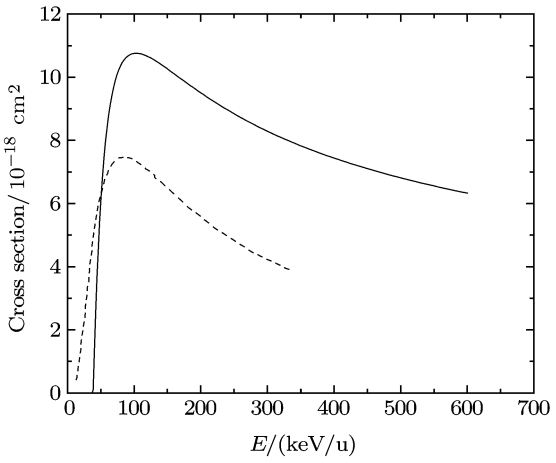


Fig. 1. Electron loss cross sections of C^{3+} projectile on atomic hydrogen by the e–N interaction. Solid curve: this work; dashed curve, screening, Ref. [6].

Figure 2 shows the electron impact ionisation cross sections of C^{3+} by present model. These results are also shown in this figure: the open circles are the measurements of Crandall *et al.*,[24] the dashed line is the anti-screening calculation of Ref. [6] and the dotted line is the convergent close-coupling calculation of Ref. [25]. It is clear that our calculations satisfactorily reproduce the energy dependence of the electron loss cross section for C^{3+} ionised by electron impact, particularly in the low energy region. By comparison, we found that present calculations are agree better with the measurements of Crandall *et al.*[24] than the convergent close-coupling calculations[25] and the anti-screening calculations based on the plane-wave Born approximation.[6]

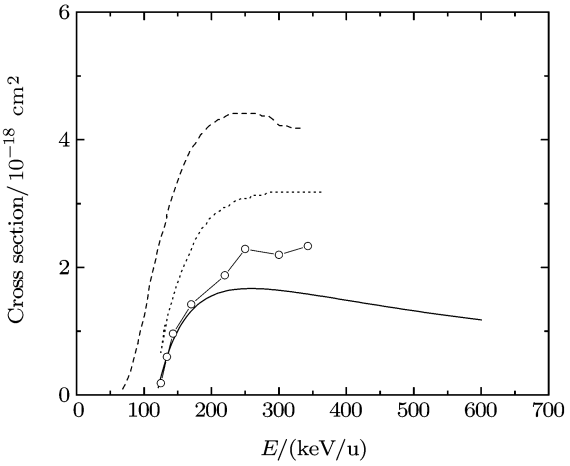


Fig. 2. Electron loss cross sections of C^{3+} induced by the e–e interaction. Experiment: open circles, Ref. [24]. Theory: solid curve, present model; dashed curve, anti-screening calculations, Ref. [6]; dotted curve, the convergent close-coupling calculations, Ref. [25].

Figure 3 shows our calculations for the single electron loss cross section of C^{3+} on atomic hydrogen, together with the measurements of Goffe *et al.*[26] and Sant'Anna *et al.* [6] for C^{3+} projectile. The sum of the two contributions is also shown in Fig. 3 by the dash-dotted curve. It is found that the projectile electron capture affects the single electron loss much more at low energies than at high energies. We can see that, over the energy range investigated here, the e–N mechanism dominates over the e–e interaction. Our calculation for single electron loss shows a broad maximum for projectile energy around 170 keV/u, which is essentially due to the onset of the e–e contribution. This behaviour was already indicated by the early calculations of Bell and Kingston[27] for the loss cross sections of He^+ on atomic hydrogen. Present calculations give a good description of the trend of the experimental

data but overestimate it by about 25% around the cross section maximum.

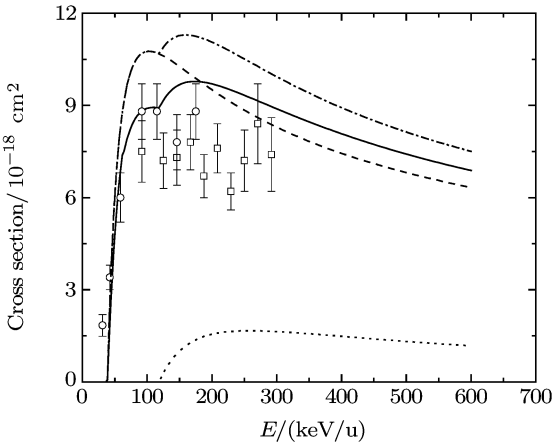


Fig. 3. Single electron loss cross sections of C^{3+} on atomic hydrogen. Experiment: open squares, Ref. [6]; open triangles, Ref. [26]. Theory: dashed curve, the e–N interaction; dotted curve, the e–e interaction; dash-dotted curve, the e–N interaction plus the e–e interaction; solid curve, single electron loss cross section of C^{3+} on atomic hydrogen.

From the above figures, it is found that this model slightly underestimates the projectile single electron loss cross section at low energy, and appears to overestimate it at higher energy. As we know, at low energies, a quasi-molecular is formed by the projectile, target core and the electron under consideration, while at high energies the projectile interacts directly with the target electron on the part of projectile ionisation caused by the e–N mechanism. The released distance defined in this model does not account to the transformation of the mechanism. It is less than normal at low energy and is bigger at high energy. This leads to the difference in the agreement between this model and the experimental data at different velocity.

4. Conclusion

In this paper, the projectile electron loss cross sections are calculated by using the extended over-barrier model in the field of classical mechanics in terms of the e–N mechanism and the e–e mechanism. Present calculations for the ionisation cross section of $C^{3+}$by the e–e interaction agree well with the measurements of electron-impact ionisation of C^{3+}. Our model slightly underestimates the projectile electron loss caused by the e–N interaction at low energy, and appears to overestimate it at high energy. In general, present calculations for single electron loss give a good description of the trend of the experimental data and satisfactorily reproduced the energy dependence obtained experimentally.

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