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Role of Excited States of Li Ions in the Stopping Power of Molecular Hydrogen

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Abstract

We study the stopping power of H_2 for Li ions and atoms. We consider the charges and electronic states of Li for various densities of H_2. It is found that from the excited states of ions, the decay processes of radiative transition and electron loss of the projectile play an important role in the low density and high density, respectively. This leads to the fact that the stopping power depends on the density.

Keywords:

heavy particle, density effect, stopping power, charge number

1. Introduction

For stopping powers for ions, the charge number of the ions plays an important role [1]. When ions pass through matter, the charge number changes as a function of times. Therefore, the population of charge numbers gives a significant contribution to the stopping power.

When we treat protons as a projectile, the charge numbers are determined by processes of charge transfer ($A^{z+} + B \rightarrow A^{(z-1)+} + B^{+}$), and electron loss of the projectile ($A^{z+} + B \rightarrow A^{(z+1)+} + B + e^{-}$), where A^{z+}, B and e^{-} are a heavy particle, a target molecule, and an electron, respectively, and z is the charge number of the particle [2]. Suppose that the cross sections of the electron loss of the projectile and charge transfer are σ_{ELP} and σ_{CT}, respectively, then, the rates of the electron loss of the projectile and charge transfer become $n_t \sigma_{ELP} v_i$ and $n_t \sigma_{CT} v_i$, respectively, where n_t and v_i are density of the target and the velocity of the projectile, respectively. Then, by using a scaling parameter $r\,(= n_t v_i t)$, the rate equations [3,4], which solve the populations of protons (P_p) and hydrogen atoms (P_h), become $dP_p/dr = \sigma_{ELP} P_h - \sigma_{CT} P_p$ and $dP_h/dr = -\sigma_{ELP} P_h + \sigma_{CT} P_p$, where t is the time. Therefore, the populations become independent of n_t and can be expressed by analytical functions of σ_{CT} and σ_{ELP} [2]. The stopping power, which depends on the charge numbers [1], can also be given as a simple function of n_t. This comes from the fact that the charge transfer processes produce the ground state of hydrogen the most often.

For heavy particles, except for protons, charge transfer processes have often produced excited states of ions or atoms. Then, the excited states also revert to stable ones through not only electron loss of the projectile but also radiative transition and auto-ionization processes. After radiative transition processes occur, the ionization energy of the ions becomes larger, as a result, σ_{ELP} decreases (see Fig. 1, the details will be discussed later). Namely, after radiative transition processes, the electron loss of the projectile processes seldom occur, that is, radiative transition processes play the role of retaining the charge number. Radiative transition probabili-

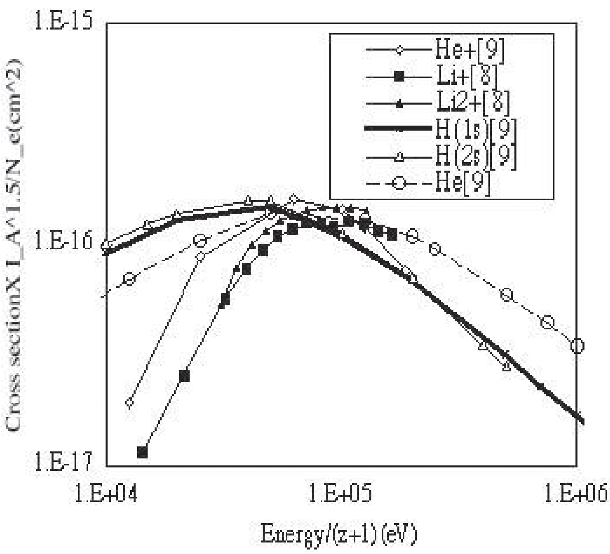

Fig. 1 Measured electron loss of the projectile cross sections [8, 9] scaled by $I_A^{1.5}/N_e$ vs. ion energy for various projectile and a target (H_2), where I_A and N_e are the ionization energy and total number of electrons of the projectile.

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ties are independent of n_t, on the other hand, the electron loss of the projectile processes, which increase the charge number, are in proportion to n_t as mentioned before. Therefore, it becomes more difficult to solve the rate equations. Resulting, the target density dependence of the stopping powers for the heavy particles becomes more complex.

In this paper, in order to study the effect of the excited states of ions on stopping powers, we treat the passing of Li ions through various densities of H_2. We consider the ground state and the excited states (principal quantum number $n = 1-3$) of the Li atom and $Li^{(1-3)+}$ ions. The rates of radiative transition processes from $n = 2$ to 1 (A_r^{2-1}) are about 10^{10}/s. On the other hand, σ_{ELP} of $Li^{2+}(n = 1)$ and v_i at E_i of ~ 100 keV are about $10^{-17}\,cm^2$ and 10^8 cm/s, respectively. Since the rate of electron loss is $r_{ELP} = n_t\sigma_{ELP}v_i \sim 10^{-9}n_t$, it is comparable to the rate of the radiative transition at $n_t \sim 10^{19}\,cm^{-3}$. The densities we employ are $10^{15}\,cm^{-3}(A_r^{2-1} \gg r_{ELP})$, $10^{19}\,cm^{-3}(A_r^{2-1} \sim r_{ELP})$, and $10^{22}\,cm^{-3}(A_r^{2-1} \ll r_{ELP})$.

The effect of target densities on charge transfer processes was already studied by Shevelko *et al.* [5]. They solved cross sections of the charge transfer of O^{7+}+ He as a function of densities. They considered excited states of O^{6+} produced through charge transfer processes and employed the processes of charge transfer and electron loss of the projectile as one successive process. On the other hand, we treat the two processes separately and solve rate equations [3,4], which estimate the populations of the electronic states of the Li ions or atom as a function of times. Further, we calculate the stopping power by using the populations.

2. Method of calculations

We assume Li^{3+} ions with the energy of 1 MeV/u as an initial projectile. Then, we calculate ion energies by using stopping powers and the populations of the electronic states of the Li ions or atoms from the rate equations as a function of times. The stopping powers are calculated by the same method given in Ref. [2].

Here the atomic data treated here and the production of the excited states of the Li ions and atom are shown. We have employed the measured cross sections of impact ionization [6], charge transfer [7], and electron loss of the projectile [8], respectively. No paper giving cross sections of Li + H_2 and of the excited states of Li ions has been found. Suppose that the total number of electrons and ionization energy are N_e and I_A, respectively, then, we derive the scaling for the electron loss of the projectile from the measured cross sections of H (1s) + H_2 [9], H (2s) + H_2 [9], He + H_2 [9], He^+ + H_2 [9], Li^++ H_2 [8], Li^{2+} + H_2 [8]. Namely, the cross section of the electron loss of the projection (σ_{ELP}) $\propto N_e/I_A^{1.5}$. Further, for ion energy (E_i) lower than 300 keV/u, $\sigma_{ELP} \propto E_i^{-0.6}$. Figure 1 shows the cross sections scaled by using these scaling from the experimental data [8,9]. For ion energies higher than 100 keV/u, the errors of the scaling are lower than 50 %. On the other hand, for energies lower than 100 keV/u, the cross sections of the projectile of ions show a trend different from those of neutral atoms. Therefore, we employ the cross sections of Li atoms and Li ions scaled from those of He atom and $Li^{+(or2+)}$ ions, respectively. For the radiative transition probabilities and auto-ionization rates, we use atomic data calculated by the Cowan code [10].

Suppose that ionization energies of the projectile of $A^{(z-1)+}$ and the target of B are I_A and I_B, respectively, then, energy loss by charge transfer processes is given by

$$\Delta E = \frac{1}{2}m_e v_i^2 + I_B - I_A \qquad (1)$$

where v_i and m_e are the velocity of the projectile and the mass of the electron, respectively. We assume that the charge transfer process occurs only where ΔE shows the minimum value. This comes from the following points. Janev *et al.* mentioned that the maximum of σ_{CT} appears at $v_i \sim (I_B - I_A)^{1/2}$for high energy ions ($v_i \sim 3$(a.u.)) [11]. On the other hand, Ryufuku *et al.* assumed for low energy ions ($v_i \ll 1$(a.u.)), where the term $(1/2m_e v_i^2)$ is ignored, that charge transfer processes often take place at $(I_B - I_A + (z-1)/R) \sim 0$ and $\sigma_{CT} \propto R^2$, where R is the nuclear distance between A^{z+} and B [12]. Namely, σ_{CT} increases as the value of $(I_B - I_A)$ becomes smaller. They also showed that σ_{CT} given by their assumption agrees well with some experimental results [12].

3. Results and discussions

Figures 2 (a)–(c) show the stopping power as a function of ion energies for n_t of 10^{15}, 10^{19}, and $10^{22}\,cm^{-3}$, respectively. It should be noted that the atomic and molecular data for Li atom treated here may not be valid at the density of $10^{22}\,cm^{-3}$ because the bound electrons of the Li atom overlap with those of hydrogen molecules. However, we judge that we can satisfactorily discuss the density effect. The reason will be discussed later. The contribution of processes of the impact ionization, charge transfer, and electron loss of the projectile to the stopping power is also shown. The charge transfer and electron loss of the projectile play an important role at the low energy region (less than a few 100 keV/u). Among Figs. 2 (a)–(c), we see five

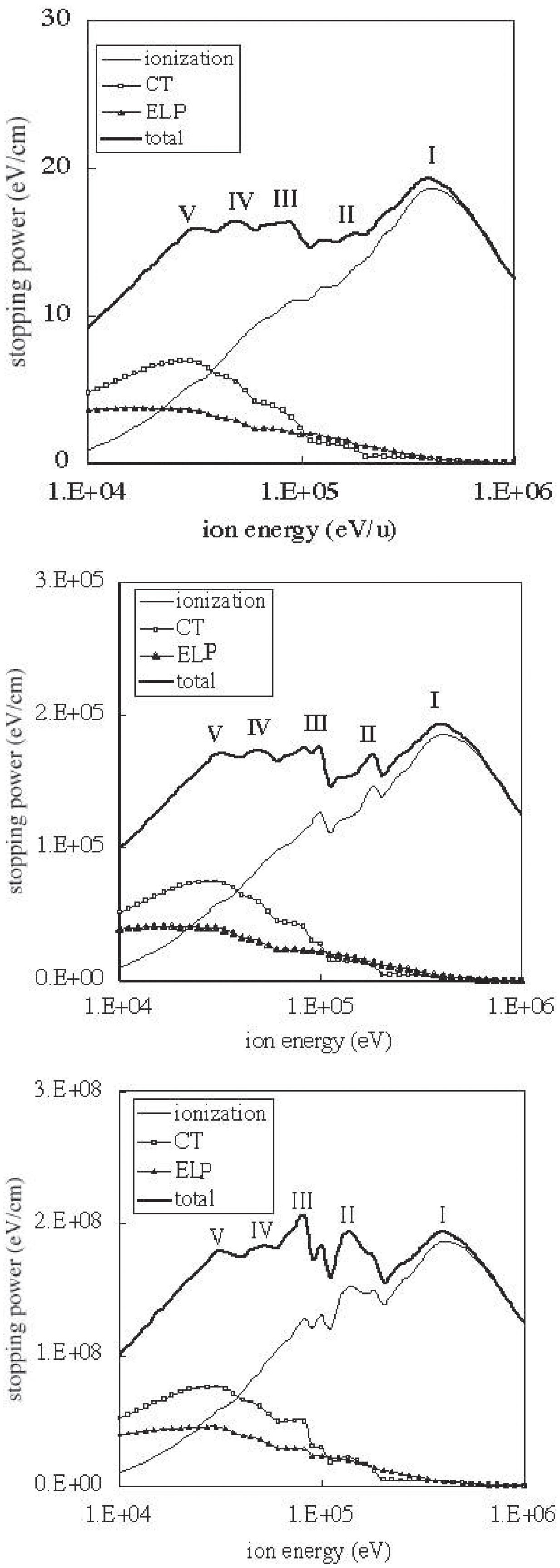

Fig. 2 Stopping powers vs. ion energies for target densities of (a) 10^{15} cm^{-3}, (b) 10^{19} cm^{-3}, and (c) 10^{22} cm^{-3}. The contribution of processes of the impact ionization, charge transfer, and electron loss of the projectile to the stopping power is also shown.

peaks, which we call them Peak I to V (shown in Figs. 2), respectively. Peak IV comes from the relationship between ionization and charge transfer. Namely, the stopping powers of charge transfer and impact ionization increase and decrease, respectively. Peak V corresponds to the maximum value of charge transfer process. The heights of Peak II and III depend on the density, where the peaks become higher as the density increases.

Firstly, we will show that the production of Peak II and III is caused from the peaks shown in Fig.3. Figure 3 shows the averaged ion charge number (Z_{av}) as a function of ion energies for n_t of 10^{15}, 10^{19}, and 10^{22} cm^{-3}. In this figure, we mark the corresponding energy to Peak II and III whose average charge numbers are also on the top of the peaks. As seen in Ref. [6], the impact ionization cross sections increase as the charge number becomes larger. The increase of Z_{av} corresponds to the increase of impact ionization cross sections, furthermore, to the increase of the stopping powers. Namely, the peaks in Fig. 3 bring about Peak II and III. As mentioned before, the atomic and molecular data for Li atoms may not be valid for the density of 10^{22} cm^{-3}. However, the Peaks II and III appear at $Z_{av} \sim 1.5$ and $Z_{av} \sim 1$, respectively. Namely, the atomic and molecular data for Li atoms have a little effect on the production of these peaks. This is the reason why it is judged that we could satisfactory discuss the density effect here.

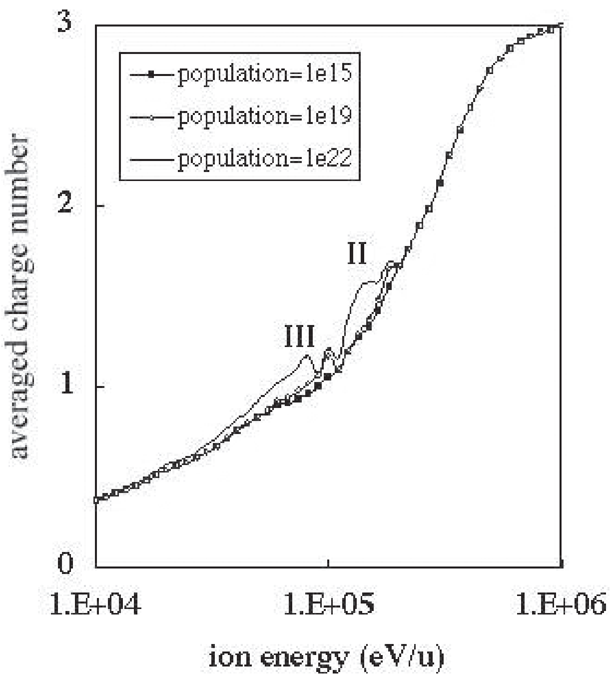

Fig. 3 Averaged charge number vs. ion energies for target densities of 10^{15} cm^{-3}, 10^{19} cm^{-3}, and 10^{22} cm^{-3}.

Next we show the reason why the peaks exist in Fig. 3 only at high densities. In the energy region higher than that Peak II, the charge transfer processes produce the ground state of the projectile ion. However, near Peak II and III, the excitation states of $n = 2$ and 3, are formed, respectively because the energy of the term of $1/2 m_e v_{ion}$ in eq. (1) becomes comparable to the bound energies of $n = 2$ and 3. As mentioned before, the rates of the electron loss of the projectile for $n = 2$ and 3 become much larger than those for $n = 1$. At high density, the processes of the electron loss of the projectile occur just after charge transfer processes. Namely, it looks as if charge transfer processes seldom occurred and for the existing electrons in the projectile ions, processes of the electron loss of the projectile continue to occur. This gives rise to the increase of the charge number and the peaks in Fig. 3. On the other hand, in the lower density region, the decay of the excited state to the ground state is faster than the processes of the electron loss of the projectile. Namely, only processes of the electron loss of the projectile from $n = 1$ appear. As a result, no peaks are seen in Fig. 3 for low density.

In this paper, we show the reason why the density effect appears. The effect comes from the fact that the charge number of the projectile ions becomes larger as the density increases. This result is consistent with that given in Ref. [5], where the charge transfer cross sections becomes smaller as the target density increases. Our model given may not be sufficient in the intermediate ion energy region. However, in this region, we show that the electronic states must be treated in the calculation of the stopping power because some excited states of ions are definitely produced.

4. Conclusion

We study the effect of the density of the target for the stopping power of H_2 for Li ions. We have found that the stopping power increases as the density becomes larger when charge transfer processes produce the excited states of the projectile ions. The electron loss of the projectile ions and the decay processes of radiative transition occur more often in the higher and lower energy region, respectively. As a result, in the higher density, the charge number becomes larger. This gives rise to larger stopping power because impact ionization cross sections increase according to charge number. For projectile ions with larger atomic number, the ion energy, which produces the excited states of ions, increases because the ionization energy of the ground state becomes larger. Namely, the electronic states may be more important even in the higher energy region.

We expect that the density effect and the peaks such as Peak I-V in Fig. 2 (c) shown here can be measured. This measurement may give us some new information such as the density of targets and ion energy there. The information of the density may be also useful for plasma diagnosis.

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References

[1] P. Sigmund, Phys. Rev. A, **56**, 3781 (1997).

[2] S. Uehara, *et al.*, Radiat. Phys. Chem., **59**, 1 (2000).

[3] K. Moribayashi, T. Kagawa and D.E. Kim, J. Phys. B, **37**, 4119 (2004).

[4] K. Moribayashi, A. Sasaki and T. Tajima, Phys. Rev. A, **58**, 2007 (1998).

[5] V.P. Shevelko, O. Rosmej, H. Tawara and I.Y. Tolstikhina, J. Phys. B, **37**, 201 (2004).

[6] M.B. Shah and H.B. Gilbody, J. Phys. B, **15**, 3441 (1982).

[7] M.B. Shah , T.V. Goffe and H.B. Gilbody, J. Phys. B, **11**, L233 (1978).

[8] M.B. Shah and H.B. Gilbody, J. Phys. B, **24**, 977 (1991).

[9] C.F. Barnett, J.A. Ray, E. Ricci *et al.*, *Atomic Data for Controlled Fusion Research*, (Oak Ridge National Laboratory, 1977).

[10] R.D. Cowan, J. Opt. Soc. Am., **58**, 808 (1968).

[11] R.K. Janev, L.P. Presnyakov and V.P. Shevelko, *Physics of highly charged ions*, (SPRINGER SERIES IN ELECTROPHYSICS, V.13, 1985) p.180.

[12] H. Ryufuk, K. Sasaki and T. Watanabe, Phys. Rev. A, **21**, 745 (1980).