Stopping power for hydrogenlike and heliumlike particles: Bethe theory

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An analytical formula for the electronic stopping power S of atoms with atomic number Z_2 and mean excitation energy I can be obtained, on the basis of Bethe theory, for fast hydrogenlike ($Z_p=Z_1$, $N_e=1$) and heliumlike ($Z_p=Z_1-\frac{5}{16}$, $N_e=2$) projectiles with atomic number Z_1 and velocity v. The resultant expression is $S=(4\pi e^4/mv^2)NZ_2L(Z_1,Z_2,v)$, where $L(Z_1,Z_2,v)=(Z_1-N_e)^2\ln(2mv^2/I)+(2Z_1N_e-N_e^2)\ln(v/Z_pv_0)+Z_1N_e-\frac{11}{12}N_e^2$.

Recently, it became possible to measure the energy loss of fast hydrogenlike ions in a preequilibrium charge state passing through very thin foils in the field of atomic collisions in solids. Especially, one is much concerned with focusing on a projectile with atomic number Z_1 in the velocity region where two charge components, i.e., fully stripped and hydrogenlike ions, are allowed to be dominant inside materials.[1] On the other hand, in the field of plasma-wall interaction, hydrogen penetration through a first wall became a problem. These circumstances seem to need a basic expression for the energy-loss formula of hydrogenlike (H-like) ions.

So far, the electronic stopping power of atoms for fast and fully ionized projectiles with velocities v has been investigated by means of the Bethe-Bloch theory[2,3] including the correction terms. The standard formula for the electronic stopping power $S=-dE/dx$ is described[4] by

$$S=\frac{4\pi e^4}{mv^2}NZ_2L(Z_1,Z_2,v)\ , \tag{1}$$

$$L(Z_1,Z_2,v)=Z_1^2L_0(Z_2,v)+Z_1^3L_1(Z_2,v)+Z_1^4L_2(Z_2,v)\ . \tag{2}$$

In the above, m, e, and N are the electron rest mass, the elementary charge, and the number density of the target with atomic number Z_2, respectively. $L_0(Z_2,v)$ is known to have the form $L_0(Z_2,v)=\ln(2mv^2/I)$, where I is the mean excitation energy of a material Z_2. As for partially stripped ions, a basic treatment was given by Kim and Cheng.[5] However, an analytical formula has not been given yet.

The aim of this paper is to present an explicit analytical formula for the electronic energy loss for fast H-like and He-like projectiles in a frozen charge state during the passage. The case is considered where v is larger than both the average orbital velocity of the target electrons, i.e., $v>Z_2^{2/3}v_0$ ($v_0=2.18\times10^8$cm/s), and the 1s orbital velocity, i.e., $v>Z_1v_0$. Our procedure is based on the first-order perturbation treatment so that the formula derived later is corresponding to the first term of the RHS of Eq. (2). Other correction terms are all neglected. In addition the projectile excitation process is also ignored. In the final expression one will find that the power expression like Eq. (2) is not valid for hydrogenlike and heliumlike projectiles, and that the formula derived later should be employed instead of Eq. (2) especially for light H-like and He-like projectiles.

Let us begin with a general expression of the electronic stopping power S in the Born approximation as follows:[5–7]

$$S=\sum_n(E_n-E_0)\int_{q_{\min}}^{q_{\max}}(dq/q^3)8\pi(e^2/\hbar v)^2\times|F_{00}^p(-\mathbf{q})|^2|F_{n0}^t(\mathbf{q})|^2\ . \tag{3}$$

In the above, E_n and E_0 denote the eigenenergies of the target states n and 0, respectively, and $\hbar$ denotes the Planck constant divided by 2π. The momentum transferred to the target electrons ranges from $\hbar q_{\min}=(E_n-E_0)/v$ to $\hbar q_{\max}=2mv$. The form factor of the projectile $F_{00}^p(-\mathbf{q})$ and inelastic-scattering amplitude of the target atom $F_{n0}^t(\mathbf{q})$ are given by $F_{00}^p(-\mathbf{q})=Z_1-\langle 0|\exp(-i\mathbf{q}\cdot\mathbf{r})|0\rangle$, and

$$F_{n0}^t(\mathbf{q})=\left\langle n\left|\sum_j\exp(i\mathbf{q}\cdot\mathbf{r}_j)\right|0\right\rangle\ .$$

It is convenient to divide the integration section $[q_{\min},q_{\max}]$ by two sections, i.e., $A=[q_{\min},q_0]$ and $B=[q_0,q_{\max}]$, where q_0 is a parameter appropriate enough to apply the dipole approximation to $F_{n0}^t(\mathbf{q})$. Using the dipole approximation, we have $\exp(i\mathbf{q}\cdot\mathbf{r}_j)=1-i\mathbf{q}\cdot\mathbf{r}_j$ and the contribution S_A from the section A is then reduced to

$$S_A=\sum_n(E_n-E_0)8\pi(e^2/\hbar v)^2|\mathbf{d}_{n0}|^2\times\int_{q_{\min}}^{q_0}(dq/q)|F_{00}^p(-\mathbf{q})|^2\ , \tag{4}$$

where $\mathbf{d}_{n0}$ is the dipole matrix element. On the other hand, the contribution S_B from the section B is expressed as

$$S_B=(\hbar^2/2m)Z_28\pi(e^2/\hbar v)^2\int_{q_0}^{q_{\max}}(dq/q)|F_{00}p(-\mathbf{q})|^2\ . \tag{5}$$

Here one can interchange the order of the summation over n and the integration over q since $q_{\max}$ and q_0 are independent of the target states. In addition, the sum rule

$$\sum_n (E_n - E_0)|F^t_{n0}(\mathbf{q})|^2 = (\hbar^2 q^2/2m)Z_2$$

is employed. The $1s$-state wave function of hydrogenlike and heliumlike projectiles is described by $|0\rangle = (\pi a^3)^{-1/2}\exp(-r/a)$, with $a = a_0/Zp$ ($a_0 = 0.529\times 10^{-8}$ cm). Here, one takes $Z_p = Z_1$ for H-like projectiles and $Z_p = Z_1 - \frac{5}{16}$ for He-like ones.[6] Then the form factor is found to have the form

$$F^p_{00}(-\mathbf{q}) = Z_1 - N_e/(1+a^2q^2/4)^{-2} ,$$

where N_e denotes the number of electrons bound on the projectile. The definite integrals in S_A and S_B are straightforwardly estimated if one uses the following result of the indefinite integral:

$$\begin{aligned}\int (dq/q)|F^p_{00}(-\mathbf{q})|^2 = (Z_1 - N_e)^2 \ln(q) \\ + (Z_1 N_e - \tfrac{1}{2}N_e^2) Y_1(q) \\ + \tfrac{1}{2}N_e^2 Y_2(q) .\end{aligned}$$

Here the functions $Y_1(q)$ and $Y_2(q)$ are defined by

$$Y_1(q) = \ln(q^2 + C) - (1 + q^2/C)^{-1}$$

and

$$Y_2(q) = \tfrac{1}{2}(1+q^2/C)^{-2} + \tfrac{1}{3}(1+q^2/C)^{-3} ,$$

with $C = 4/a^2$. Here we can assume that $q^2_{\min} \ll C$ holds valid in the velocity range considered. Then S_B is expanded in the Taylor series of $q^2_{\min}/C$. As a result, the total stopping power $S(=S_A + S_B)$ is expressed in the form of Eq. (1), where

$$\begin{aligned}L(Z_1,Z_2,v) = (Z_1 - N_e)^2 \ln(2mv^2/I) + (Z_1 N_2 - \tfrac{1}{2}N_e^2)[Y_1(2mv) - Y_1(0)] \\ + \tfrac{1}{2}N_e^2[Y_2(2mv) - Y_2(0)] + \alpha_{-2}(Z_p v_0/v)^2 + \alpha_{-4}(Z_p v_0/v)^4 + O(v^{-6}) ,\end{aligned} \tag{6}$$

where

$$\alpha_{-2} = -\frac{(Z_1 N_e - N_e^2)a_0^2}{2(Z_p e)^4}\frac{2m}{\hbar^2 Z_2} G_3 , \tag{7}$$

$$\alpha_{-4} = \frac{(3Z_1 N_e - 5N_e^2)a_0^4}{32(Z_p e)^8}\frac{2m}{\hbar^2 Z_2} G_5 , \tag{8}$$

$$G_m = \sum_n (E_n - E_0)^m |\mathbf{d}_{n0}|^2 \quad (m = 3,5) . \tag{9}$$

In Eq. (9), G_m denotes the excitation-energy moments of the dipole transition probability. In the case of the higher (but nonrelativistic) velocities, i.e., $v \gg Z_1 v_0$, one finds $q^2_{\max} \gg C$ holds true. Thus, Eq. (6) reduces to

$$\begin{aligned}L(Z_1,Z_2,v) &= L_0(Z_1,Z_2,v) + \Delta L(Z_1,Z_2,v) , \\ L_0(Z_1,Z_2,v) &= (Z_1 - N_e)^2 \ln(2mv^2/I) \\ &\quad + (2Z_1 N_e - N_e^2)\ln[v/(Z_p v_0)] \\ &\quad + Z_1 N_e - \tfrac{11}{12}N_e^2 , \\ \Delta L(Z_1,Z_2,v) &= \alpha_{-2}(Z_1 v_0/v)^2 \\ &\quad + (\alpha_{-4} + \beta_{-4})(Z_1 v_0/v)^4 + O(v^{-6}) ,\end{aligned} \tag{10}$$

where $\beta_{-4} = Z_1 N_e/2$. Note that q_0 cancels out in the total stopping power S. The terms including the factors α_{-2} and α_{-4} indicate the shell corrections of incidence of H-like and He-like ions at high velocities. They are contributed from the distant collision. On the contrary, the term including the factor β_{-4} indicates the effect of shielding the nuclear charge of the projectile by the bound electron on the close collision between the target electrons and the projectile.

Kim and Cheng[5] have treated a basic theory of the electronic stopping power for partially stripped ions. They took into account the projectile excitation, which is neglected here, as well as the target excitation. It is noted that the leading-order expression $L_0(Z_1,Z_2,v)$ of the present formula (10) can also be derived if one follows a general expression of [Ref. 5, Eq. (24)] together with the use of hydrogenic $1s$ wave function.

Let us focus on the leading-order terms of $L(Z_1,Z_2,v)$, which is obtained by omitting the correction $\Delta L(Z_1,Z_2,v)$ of the negative order of v. The expression (10) is very instructive. The first term of $L_0(Z_1,Z_2,v)$, which seemingly corresponds to the Bethe-like expression, includes only the net charge of the projectile. This term might seem to come only from the distant-collision contribution. However, the truth is that this term is contributed from both the distant and close collisions. The second term involves the logarithm of the ratio of the ion velocity v to the $1s$ orbital velocity $Z_p v_0$. The residual terms are composed of Z_1 and N_e but do not include kinematic parameters. It is obviously possible to write $L_0(Z_1,Z_2,v)$ in the form of $(Z_{\text{eff}})^2\ln(2mv^2/I_{\text{eff}})$ when the effective charge Z_{eff} and the effective mean excitation energy I_{eff} are defined.[5] The author thinks the present expression $L_0(Z_1,Z_2,v)$ is simpler and more explicit than the form of $(Z_{\text{eff}})^2\ln(2mv^2/I_{\text{eff}})$ in that an original meaning of each term is easily understood. Thus the stopping power for H-like and He-like particles can be obtained explicitly. As a central conclusion, $L_0(Z_1,Z_2,v)$ in Eq. (10) has to replace the $Z_1^2 L_0(Z_2,v)$ in Eq. (2) in case of H-like and He-like particles being treated. As a special case, the stopping power for a hydrogen atom takes

$$S = (4\pi e^4/mv^2)NZ_2[\ln(v/v_0) + \tfrac{1}{12}] . \tag{11}$$

Here it seems remarkable that Eq. (11) does not depend on I but depends on only the number density N and the atomic number Z_2 of the target. This is because a frozen-charge state is presumed here. If the projectile excitation is involved, a logarithmic term like $\ln(2mv^2/I_{\text{eff}})$

is expected to appear again.[5] Regarding heavy H-like ions (large Z_1), the first term of Eq. (10) becomes dominant in comparison with other ones so that the net charge approximation is valid in general. This is, of course, reasonable because in the case of large Z_1 ions the spatial radius of the bound electron is so short that the screening becomes complete.

Let us consider the possibility of experimentally confirming the result (10) for incidence of a hydrogenlike ion. In the derivation of the above formulas, a frozen-charge state is assumed during the passage. Also, the case of $v > Z_1 v_0$ was considered. This condition means that the H-like projectile can rarely pick up an electron from the target. That is to say, the electron loss cross section σ_L is much larger than that of the electron capture cross section σ_C. Under this condition, the charge state of the H-like ions is in a preequilibrium state and its fraction decreases like $\exp(-N\sigma_L z)$ with increasing the foil thickness z. In this regime of z, the H-like ions are considered to hold the initial charge state during their passage. Therefore, the charge exchange events cannot contribute to the electronic stopping for H-like ions. Figure 1 shows the stopping power of carbon ($I=77.3$ eV, $Z_2=6$) for He^+ ($Z_1=2, a=0.5a_0$) at $v=2-50v_0$, which is calculated from Eq. (10) without the correction terms including the factor α_{-4}, β_{-2}, and β_{-4}. According to a recent experimental result,[8] the energy loss of 32-MeV $^3He^+$ ions incident on thin ($2-100$ $\mu g/cm^2$) carbon foils can be deduced to 83.8 ± 8.1 eV ($\mu g/cm^2$). This measurement was made under the frozen-charge state so that the contribution of the projectile-excitation mechanism could be ignored. The stopping power calculated from the present formula (10) gives 93.0 eV ($\mu g/cm^2$), which is in good agreement with the data. At this energy the Z_1^3 and Z_1^4 corrections are expected to change the stopping power by only 1% at most. Consequently the contribution of the $L_0(Z_1,Z_2,v)$ is found to be more dominant again.

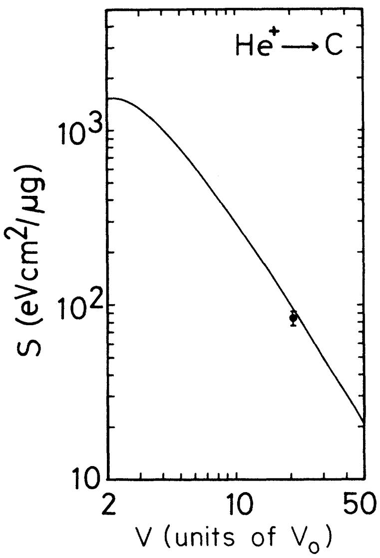

FIG. 1. The stopping power of carbon ($I=77.3$ eV) for a He^+ ion as a function of velocity. The theoretical result $S=(4\pi e^4/mv^2)L_0(Z_1,Z_2,v)$ is drawn (——) together with the data (Ref. 8).

In conclusion, the analytical expression for the electronic stopping power for hydrogenlike and heliumlike projectiles in a frozen-charge state were presented on the basis of the first-order perturbation theory. The correction term $\Delta L(Z_1,Z_2,v)$, which includes the shell correction at high energies, is also estimated. The expression $L_0(Z_1,Z_2,v)$ of Eq. (10) is to be employed as the leading-order expression for the stopping number of materials for hydrogenlike and heliumlike projectiles, instead of the $Z_1^2\ln(2mv^2/I)$ of Eq. (2).

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