Energy Loss and Straggling of Low-velocity Atoms in Matter

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Based on the dielectric function method, the analytical formulas are presented for the energy loss and the straggling of low-velocity heavy atoms with atomic number Z_1 passing through the degenerate electron gas. The spatial size Λ of the electron cloud on projectiles is newly determined according to the statistical variational method by taking into account the static screening effect of conduction electrons. The analytical formulas obtained here have the Z_1-dependences different from those by the existing theories in spite of the same velocity dependence. It is found that the screening effect on Λ enlarges thelectronic stopping of the media by a constant value regardless of Z_1.

I. INTRODUCTION

Since accelerators were developed and used to elucidate the phenomena in particle-matter interaction, the energy loss of penetrating particles has been an elementary problem to be solved. This is closely connected with the charge state of the particles having inside a material. Especially, a detailed knowledge of the energy loss of light-ion beams are greatly required to determine the composition, the depth distribution, and the location of lattice sites of the implanted atoms in the fields of ion implantation, surface-structure analysis, and plasma-first wall interaction. Moreover, the energy straggling limits ultimately the spatial resolution of the analysis using the above methods.

Intensive works on the electronic stopping and the straggling for light ions or fully stripped ions have been performed in experimental and theoretical aspects[1-23]. As regarding the energy loss of heavy-ion beams, Firsov[24] and Lindhard and Scharff (LS)[25] formulas have been often compared with the stopping-power data. As for the stopping of atomic systems, Firsov estimated the momentum exchange rate through the so-called Firsov plane between a projectile and a target. LS theory was derived by considering the polarization of the electron gas, but, as far as the author knows, there is no detailed derivation dictated anywhere. The typical feature of the presented theories on the electronic stopping powe for low-velocity particles is the velocity proportionality, while the target and projectile dependences are different from each other. As for the energy strangglling of low-velocity heavy ions, there are few theories presented. By applying the Firsov theory[24] to the straggling, Hvelpund obtained a formula[26].

So far, a few theoretical work have been performed on the electronic stopping and straggling for incident atoms ($Z_1 \gg 1$). Particularly, the r_s dependence of the straggling has not been discussed analytically. On account of such circumstances, we wish in this paper to find analytically the r_s- and Z_1-dependences of the electronic energy-loss and straggling of low-velocity atoms by means of the dielectric-function procedure within the framework of the linear response. Here, the velocity range of interest is limited to $v < Z_1^{2/3} v_0$. In this paper, the analytical formulas are derived, which are valid for typical solids. Throughout the paper, m, e, a_0, v_0, and $\hbar$ denote the electron rest mass, the elementary charge, the Bohr radius ($=0.529 \times 10^{-8}$cm), the Bohr velocity ($=2.18 \times 10^{-8}$cm), and the Planck constant divided by 2π, respectively. In addition, Z_1 and Z_2 are the atomic number of a projectile and of a target atom.

II. THEORY

2—1. The size parameter of atoms in solids

Here we wish to determine the size parameter of the bound electrons of atoms in a statistical way. So far the screening effect of conduction electrons on the light-ion stopping has been discussed[6], but this effect has never been considered. In other words, the size parameter for heavy atoms with Z_1 (>1) has been discussed under the condition that an isolated neutral atom is located in a vacuum[27] and no one has treated the effect of the background electron density on the spatial size of the bound electrons on heavy atoms. In general, the conduction electrons of a solid screens the electric field of an atom due to the dielectric response. This fact means that the electric interaction between the nucleus and the bound electron, $V_{ne}(r)$, and that between the bound electrons, $V_{ee}(r)$, are both screened by the conduction electrons whenever the atom exists in a solid. Provided that the speed of the atom is lower than the Fermi velocity v_F, this screening effect can be described successfully in terms of the screened Coulomb or Yukawa-type potentials: $V_{ne}(r) = -(Z_1e^2/r)\exp(-k_{TF}r)$ and $V_{ee}(r) = (e^2/r)\exp(-k_{TF}r)$. Here k_{TF} is the Thomas-Fermi (TF) screening wave length given by

$$k_{TF} = (4k_F)^{1/2}/(\pi a_0)^{1/2} = 1.564/(r_s^{1/2}a_0), \tag{1}$$

where k_F denotes the Fermi wave number connected with the number density, n, of the conduction electrons or the so-called r_s value through the relations: $k_F = (3\pi^2 n)^{1/3}$ and $1/n = 4\pi r_s^3 a_0^3/3$.

Let us determine statistically the size parameter of the bound electron cloud under the static screening mentioned. We assume that N_e electrons are bound in an atom and their spatial distribution, $\rho(r)$, is described by[27]:

$$\rho(r) = N_e/(4\pi\Lambda^3)(\Lambda/r)\exp(-r/\Lambda). \tag{2}$$

Now consider the total energy of the bound electron system in a statistical treatment when the atom exists in a solid. The total energy E can be expressed in terms of the local electron density $\rho(r)$ in the following form:

$$E = E_k + E_{ne} + \mu E_{ee}, \tag{3}$$

with the kinetic energy

$$E_k = (3\hbar^2/10m)(3\pi^2)^{2/3}\int\{\rho(\vec{r})\}^{5/3}d^3r, \tag{4}$$

the electron-nucleus interaction energy

$$E_{ne} = \int V_{ne}(\vec{r})\rho(\vec{r})d^3r, \tag{5}$$

and the electron-electron interaction energy

$$E_{ee} = (1/2)\int V_{ee}(\vec{r}-\vec{r}')\rho(\vec{r})\rho(\vec{r}')d^3r d^3r'. \tag{6}$$

In eq. (3), the factor μ is a variational parameter. Now let us minimize $E(\mu, \Lambda, N_e)$ with respect to N_e and Λ as follows:

$$\partial E(\mu, \Lambda, N_e)/\partial\Lambda = 0, \quad \partial E(\mu, \Lambda, N_e)/\partial N_e\Big|_{N_e = Z_1} = 0 \tag{7}$$

As a result, we get the following result for a neutral atom[29]

$$\Lambda = \Lambda_0/[1 - 1.63\Lambda_0^2/(r_s a_0^2)], \tag{8}$$

with $\Lambda_0 = 0.560\, Z_1^{-1/3}a_0$. The formula (8) is valid as long as $k_{TF}\Lambda_0 < 1$ is fulfilled. It is realized that the parameter Λ reduces to the Brandt-Kitagawa (BK) value Λ_0, when there exists no background of the conduction electrons around the atom.

2—2. Stopping and straggling cross sections

The probability of energy transfer to a degenerate free electron gas from the projectile atom is described by the RPA dielectric function $\varepsilon(k, \omega)$[5]. The electronic stopping cross section S and the straggling parameter Ω^2 for an atom with velocity v and with the bound electron distribution $\rho(r)$ can be expressed by

$$S=(1/n)dE/dx=4\pi e^4/(mv^2)L_1, \tag{9}$$

$$L_1=-2/(\pi\omega_p^2)\int_0^\infty dk/k|Z_1-\rho(k)|^2\int_0^{kv}d\omega\ \omega\ \mathrm{Im}\{1/\varepsilon(k,\omega)-1\}, \tag{10}$$

and

$$\Omega^2/(nx)=4\pi e^4/(mv^2)L_2, \tag{11}$$

$$L_2=-2\hbar/(\pi\omega_p^2)\int_0^\infty dk/k|Z_1-\rho(k)|^2\int_0^{kv}d\omega\ \omega^2\mathrm{Im}\{1/\varepsilon(k,\omega)-1\}. \tag{12}$$

In the aboves, n and ω_p denote the number density of the free electrons and the plasma frequency defined by $\omega_p=(4\pi ne^2/m)^{1/2}$. The form factor $\rho(k)$ of the projectile is defined by the Fourier transform of the spatial electron distribution $\rho(\vec{r})$ as $\rho(\vec{k})=\int d^3r\rho(\vec{r})\exp(-i\vec{k}\vec{r})$. From (2), one has

$$\rho(\vec{k})=Z_1/[1+(\Lambda k)^2]. \tag{13}$$

For low velocity ions, L_1 is finally expresed as follows:

$$L_1=(4E_F/\hbar\omega_p)^2\chi^2(1/3)(v/v_F)^3\times I_1, \tag{14}$$

$$I_1/Z_1^2=(1-\alpha)^2g(\pi v_F/v_0)+\alpha^2g(4k_F^2\Lambda^2)+2\alpha(1-\alpha)\times [\alpha ln(1+4k_F^2\Lambda^2)+(1-\alpha)ln(1+\pi v_F/v_0)], \tag{15}$$

where $\chi^2=v_0/(\pi v_F)$ and $\alpha=1/\{1-(2k_F\Lambda\cdot\chi)^2\}$.

In a similar way, L_2 is reduced to have the form

$$L_2=(4E_F/\hbar\omega_p)^2\chi^2(1/4)(v/v_F)^4\times I_2, \tag{16}$$

$$\begin{aligned}I_1/Z_1^2=1&-(\alpha^3/2)\beta^2(7-3\beta)\chi\arctan(1/\chi)\\&+(\alpha^3/2)(7\beta-3)/(2k_F\Lambda)\arctan(2k_F\Lambda)\\&+(1/2)\alpha^2\beta^2\chi^2/(\chi^2+1)+(1/2)\alpha^2/[(2k_F\Lambda)^2+1],\end{aligned} \tag{17}$$

where $\beta=(\alpha-1)/\alpha$, and $g(y)=ln(1+y)-y/(1+y)$.

The parameter χ is expressed by the r_s value of the electron gas as $\chi=1/[1.92\pi/r_s]^{1/2}$. By considering the range of r_s values for metals to be $1.5<r_s<5.8$, one finds that χ ranges from 0.05 (r_s=1.5) to 0.98 (r_s=5.8). In order to find simpler and useful expressions for I_1 and I_2, let us consider the quantity $R=2k_F\chi\Lambda$ in α. Through an simple calculation, R is written as Λ/a_{TF}, where a_{TF} is the Thomas-

Fermi screening length of the from: $a_{TF}=k_{TF}^{-1}$. On the other hand, as shown in (8), the size parameter Λ depends on Z_1 roughly like $Z_1^{-1/3}$ according to the statistical model. Then, R and $2k_F\Lambda$ $(=R/\chi)$ can be found to be smaller than unity for large Z_1 values. Actually, taking into account eqs. (8) with $v_F/v_0=1.92/r_s$, one finds that $\Lambda \ll a_{TF}$ leads to $Z_1 \gg 1.13$ ($r_s=1.5$) and $Z_1 \gg 0.15$ ($r_s=5.8$). These conditions cover all projectile atoms except for hydrogen. Thus we can tell it reasonable to regard α and β as unity and zero, respectively, and to expand I_1 and I_2 in a power series of $2k_F\Lambda$. Physically speaking, this result means that the screening length of the conduction electrons is rather longer than the size of the bound electrons. Consequently, the conduction electrons feel the strongly-screened electric field of the projectile nucleus. In the lowest order of R, one can estimate eqs. (15) and (17) to be

$$I_1=(Z_1^2/2)(2k_F\Lambda)^4[1-4\chi^2+\chi^4\{6\,ln(1+\pi v_F/v_0)-2\pi v_F/(\pi v_F+v_0)\}] \tag{18}$$

$$I_2=(3/2)Z_1^2[1-1/(2k_F\Lambda)\arctan(2k_F\Lambda)]. \tag{19}$$

The number density of the conduction electrons, n, is given by $n=N_{free}N$, where N_{free} is the the number of the conduction electrons per atom. At a glance, one notices the size parameter Λ play a very important part in the electronic stoppingand straggling. Moreover, it affects the stopping rather strongly than the straggling.

With the use of eq. (8), the stopping and the straggling cross sections of the electron gas *per atom* for an heavy atom are, respectively, reduced to be

$$\begin{aligned} S=(1/N)dE/dx &= 16\pi(k_Fa_0)(v/v_0)Z_1^{2/3}N_{free}A^4(mv_0^2a_0^2) \\ &\times[1-4\chi^2+\chi^4\{6\,ln(1+\pi v_F/v_0)-2\pi v_F/(\pi v_F+v_0)\}], \end{aligned} \tag{20}$$

and

$$\Omega^2/(Nx)=12\pi(v/v_0)^2Z_1^{4/3}N_{free}A^2(mv_0^2)^2a_0^2, \tag{21}$$

with $A=0.56/(1-0.511Z_1^{-2/3}r_s^{-1})$. The above formulas exhibit remarkable features. Firstly, the stopping cross section S and the straggling cross section $\Omega^2/(Nx)$ display the $Z_1^{2/3}$ and $Z_1^{4/3}$ dependences, respectively. Secondly, S depends on the target like $N_{free}k_F[1-4\chi^2+\chi^4\{6\,ln(1+\pi v_F/v_0)-2\pi v_F/(\pi v_F+v_0)\}]$, meanwhile the physical parameter of the free electron gas, r_s, is not incorporated into the straggling cross section per atom. Namely, only N_{free} characterizes the target dependence of $\Omega^2/(Nx)$. These results on the electronic stopping and straggling for low velocity atoms are different from those presented so far by Firsov, Lindhard and

Scharff[25], and Hvelplund[26].

The screening effect of conduction electrons is represented in the factor A of eqs. (20) and (21). It is realized that for large Z_1 the stoppig formula (20) enlarges the electronic stopping cross section by the amount ΔS in comparison with the Brandt-Kitagawa value S_{BK}. That is, we can write $S=\Delta S+S_{BK}$, where S_{BK} is defined by (20) with the use of $A=0.56$. The explicite form of ΔS is as follows:

$$\Delta S=16\pi(k_F a_0)(v/v_0)(0.2/r_s)N_{free}(mv_0^2 a_0^2)$$
$$\times[1-4\chi^2+\chi^4\{6\,ln(1+\pi v_F/v_0)-2\pi v_F/(\pi v_F+v_0)\}] \quad (22)$$

In a similar way, for large Z_1, we can estimate the magnitude of the static screening effect on the straggling. If we write $\Omega^2=\Delta\Omega^2+\Omega_0^2$, $\Delta\Omega^2$ has the form

$$\Delta\Omega^2/(Nx)=12\pi(v/v_0)^2(0.32/r_s)N_{free}(mv_0^2)^2 a_0^2, \quad (23)$$

Here $\Omega_0^2/(Nx)$ is defined by formula (21) with the use of $A=0.56$. It is remarkable that ΔS and $\Delta\Omega^2$ are independent of Z_1 and determined both by the physical parameters of a target and by the velocity of an atom. Formulas (22) and (23) show the importance of the screening effect. In general, with increasing Z_1, the present value Λ approaches the BK value Λ_0. Even in such cases, ΔS and $\Delta\Omega^2$ are never vanishing.

III. Concluding remarks

We derived the theoretical formulas for the electronic stopping and straggling cross sections of the free electron gas for low-velocity heavy atoms with the use of the statistical treatment of the bound electrons. The static screening effect of conduction electrons in a solid on the size parameter of heavy atoms is discussed. It was found that the static screening effect on the stopping and the straggling is never vanishing for large Z_1, even though Λ approaches Λ_0. These contributions, ΔS (eq. (22)) and $\Delta\Omega^2$ (eq. (23)), are newly obtained. Regarding the stopping, our theory is an extension of the Brandt-Kitagawa theory. Though the present theory cannot predict the Z_1 oscillation in the electronic stopping, it provided the values consistent qualitatively with the data. On the other hand, we gave newly an analytical expression for the energy straggling of low velocity heavy atoms. This formula will be tested by the measurement in the future.

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