Electronic stopping power for slow atoms in solids

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(Received 25 January 1991)

Using the linear-response dielectric theory, we have investigated the electronic stopping power for slow atoms in solids. The effect of the electrons bound to the projectile is considered according to the Brandt-Kitagawa (BK) model [Phys. Rev. B **25**, 5631 (1982)]. Using a local-field-correction dielectric function, the correlation and exchange interaction of the electron gas in solids is also taken into account. An analytical formula for the stopping power is obtained, and various theoretical results are compared with each other and with available experimental data.

I. INTRODUCTION

In recent years the energy loss of heavy ions in condensed matter has been of special interest in implantation experiments such as the surface modification of metal materials using ion beams. When the ion velocity is smaller than the Fermi velocity of the electron gas (the valence-electron system in a solid), the following two effects have to be considered in calculating electronic stopping power. First, a slow ion can interact with many electrons of the electron gas along its path, so the correlation and exchange interaction of electrons at short range will be important. Many investigators [1-3] have calculated stopping power based on the random-phase-approximation (RPA) theory, which is valid for the weak-coupling limit of electron correlations, i.e., $r_s < 1$ [where r_s is related to the density n_0 of the electron gas by $1/n_0 = 4\pi(r_s a_0)^3/3$, $a_0 = 0.529 \times 10^{-8}$ cm is the Bohr radius]. In the electron gas of a metal, however, the values of r_s range from 1.5 to 5.88, so the RPA theory may not provide an accurate value of the stopping power. Second, because of capture, some electrons in the electron gas will be bound to ions, so the ions cannot be regarded as bare, and are almost neutral atoms.

The first effect has been considered in a previous paper [4]. The analytical forms for the stopping power and energy-loss straggling of slow protons moving in a strongly coupled degenerate electron gas were obtained using linear-response theory. The short-range correlation and exchange interaction of electrons was included via a static local-field correction (LFC) dielectric function [5], which yielded results that differ significantly from predictions based on RPA dielectric theory, and agree quite well with experimental data.

An attempt to include the effect of electrons bound to the projectile was performed by Brandt and Kitagawa [6] (BK) who used a nonlocal-density distribution of electrons bound to ions. Similar to BK's work, Kaneko [7] recently investigated the energy loss of low-velocity heavy atoms; in this work the static screening effect of conduction electrons in the solid on the size parameter of heavy atoms was also included. However, in both works the RPA dielectric function was used.

In the present paper, the effects of bound electrons considered by BK are compared to effects of the correlation-exchange interaction of the electron gas considered in our work. In Sec. II, the basic equations are presented and the analytical formula of stopping power is derived. In Sec. III, our results are compared with other theories and with experimental data.

II. BASIC EQUATIONS

Within the framework of the linear-response theory, the stopping power $-dE/dx$ for a projectile with atomic numbers Z_1 moving in a homogeneous degenerate electron gas is given by

$$\frac{-dE}{dx} = 2(\pi v^2)^{-1} \int_0^\infty dk [\rho^2(k)/k] \times \int_0^{kv} d\omega\, \omega\, \mathrm{Im}[-1/\epsilon(k,\omega)] , \tag{2.1}$$

where v is the projectile velocity, $\epsilon(k,\omega)$ is the longitudinal dielectric function of the electron gas, and $\rho(k)$ is the Fourier transform of the charge distribution of the projectile. For a neutral atom the form of $\rho(k)$ was given by BK [6] as

$$\rho(k) = Z_1 e (k\Lambda_0)^2/[1+(k\Lambda_0)^2] . \tag{2.2}$$

Here Λ_0 is the screening length determined according to the statistical variational method

$$\Lambda_0 = 0.56 a_0 / Z_1^{1/3} . \tag{2.3}$$

In the following discussion the LFC dielectric function [5]

$$\epsilon(k,\omega) = 1 - P(k,\omega)/[1+G(k)P(k,\omega)] \tag{2.4}$$

will be used, where $G(k)$ is the LFC function to the RPA dielectric function [in which $G(k)=0$], which includes the correlation and exchange interaction of electrons, and $P(k,\omega)$ is Lindhard's polarizability. In the low-frequency ($u = \omega/kv_F \ll 1$) and long-wavelength ($z = k/2k_F \ll 1$) limit we obtain

$$P(k,\omega) = -\chi^2[(1-z^2/3) + i\pi u/2]z^2 , \tag{2.5}$$

$$G(k)=4\gamma_0 z^2 , \tag{2.6}$$

where $v_F=(1.92/r_s)v_0$ and $k_F=(1.92/r_s)/a_0$ are the Fermi velocity and the Fermi wave number, respectively, $v_0=2.18\times10^8$ cm/s, and $\chi^2=0.166r_s$. The parameter γ_0 is connected to the correlation energy $E_c(r_s)$ of electron gas by

$$\gamma_0=\tfrac{1}{4}-(\alpha\pi r_s^5/24)\frac{d[r_s^{-2}dE_c(r_s)/dr_s]}{dr_s} , \tag{2.7}$$

$$r_s\frac{dE_c(r_s)}{dr_s}=b_0(1+b_1x)/(1+b_1x+b_2x^2+b_2x^3) , \tag{2.8}$$

where $\alpha=(4/9\pi)^{1/3}$, $x=\sqrt{r_s}$, $b_0=0.062\,181\,4$, $b_1=9.813\,79$, $b_2=7.8224$, and $b_3=0.736\,411$.

For low-velocity projectiles, i.e., $v\ll v_F$, the stopping power can be written as [4]

$$\frac{-dE}{dx}=(4k_F^2\chi^2/3)(v/v_F)\int_0^1 dz\,\rho^2(z)z^3F(z) , \tag{2.9}$$

$$F(z)=[(1-\beta\chi^2/3)z^2+\chi^2]^{-2} , \tag{2.10}$$

where $\beta=1+12\gamma_0$. In RPA dielectric theory [1,2], the approximation $\beta=1$ is made. However, the values of β for densities in the range of valence electron density in solids are about 4.0–5.0 (see Table I).

In order to simplify the expression for $-dE/dx$, we make an approximation for $\rho(k)$. Since $(2k_F\Lambda_0)<1$ [6], $\rho(k)$ can be written as

$$\rho(k)=Z_1e(2k_F\Lambda_0)^2z^2 . \tag{2.11}$$

Substituting Eq. (2.11) into Eq. (2.9) and finishing the integration, we obtain

$$\frac{-dE}{dx}=(4Z_1^2e^2k_F^2\chi^2/3)(2k_F\Lambda_0)^4(v/v_F)C(r_s)$$
$$=4.64Z_1^{2/3}[C(r_s)/r_s^4](v/v_0) , \tag{2.12}$$

where the result is in keV/Å. The analytical expression for $C(r_s)$ is found to be

$$C(r_s)=\begin{cases}1/(8\chi^4) & \text{for } \beta\chi^2/3=1\\ \frac{1}{2}(t/\chi^2)^2[3t^2I(t)+\frac{1}{2}(1-3t)/(1+t)] & \text{for } \beta\chi^2/3\neq1\end{cases} \tag{2.13}$$

TABLE I. Comparison of values $C(r_s)$ with $C_K(r_s)$ and $C_{BK}(r_s)$ for various r_s values. Values of β are also shown.

r_s	β	$C(r_s)$	$C_K(r_s)$	$C_{BK}(r_s)$
1.0	4.2596	0.2318	0.1528	0.1123
1.5	4.3664	0.2347	0.1216	0.0967
2.0	4.4638	0.2413	0.1063	0.0836
2.5	4.5539	0.2535	0.0910	0.0728
3.0	4.6376	0.2713	0.0789	0.0640
3.5	4.7160	0.2955	0.0697	0.0566
4.0	4.7890	0.3283	0.0610	0.0504
4.5	4.8581	0.3766	0.0544	0.0452
5.0	4.9258	0.4431	0.0489	0.0407
5.5	4.9886	0.5418	0.0440	0.0369
6.0	5.0480	0.6987	0.0390	0.0336

in which the function

$$I(t)=\ln(1+1/t)-1/(1+t) , \tag{2.14}$$

with $t=\chi^2/(1-\beta\chi^2/3)$.

The formula (2.12) exhibits the following notable features. First, the stopping power $-dE/dx$ displays a $Z_1^{2/3}$ dependence. Second, the target r_s dependence of $-dE/dx$ behaves as $C(r_s)/r_s^4$. Finally, $-dE/dx$ is proportional to the projectile velocity, i.e., to v/v_0.

Using the RPA dielectric function, Kaneko has also obtained an analytical expression for the stopping power for a heavy atom,

$$\frac{-dE}{dx}=(4Z_1^2e^2\chi^2k_F^2/3)(2k_F\Lambda)^4(v/v_F)C_K(r_s) , \tag{2.15}$$

where

$$\Lambda=\Lambda_0/[1-1.63(\Lambda_0/a_0)^2/r_s] \tag{2.16}$$

is the size parameter of the bound electrons of atoms, and

$$C_K(r_s)=\tfrac{1}{4}\{1-4\chi^2+\chi^4[6\ln(1+1/\chi^2)-2/(1+\chi^2)]\} . \tag{2.17}$$

From Eq. (2.16) it is found that $\Lambda>\Lambda_0$, which results when the static screening effect of conduction electrons in the solid on the size parameter of the projectile is considered. The screening effect on Λ can enlarge the stopping power. When $\beta=0$ is assumed in Eq. (2.13), the function $C(r_s)$ reduces to the values of $C_K(r_s)$ obtained by Kaneko.

The stopping power of solids was also calculated by Brandt and Kitakawa using the RPA dielectric function. We discuss two formulas: slow-ion (BK1) and neutral (BK2) projectiles. For a slow ion the stopping power (called BK1) is

$$\frac{-dE}{dx}=(4Z_1^2e^2\chi^2k_F^2/3)(v/v_F)I(\chi^2)\xi^2 , \tag{2.18}$$

where ξ is the fractional effective charge of the ion,

$$\xi=q+(1-q)\{1/[(1+\chi^2)I(\chi^2)]-2\chi^2\}\ln[1+(2k_F\Lambda_q)^2] , \tag{2.19}$$

in which Λ_q is the screening length of charge distribution of the ion with degree of ionization q

$$\Lambda_q=0.48(1-q)^{2/3}a_0/\{Z_1^{1/3}[1-(1-q)^{2/3}/7]\} . \tag{2.20}$$

According to Table II in Ref. 6, q can be expressed as

$$q=0.9699-0.9874\exp[-v_r/(v_0Z_1^{2/3})] . \tag{2.21}$$

v_r is the relative velocity between the ion and electrons in solids; for slow ions [8], i.e., $v\le v_F$

$$v_r=3v_F[1+2(v/v_F)^2/3-(v/v_F)^4/15] . \tag{2.22}$$

For neutral projectiles, i.e., ionization degree $q=0$ is assumed, Eq. (18) can be reduced to

$$\frac{-dE}{dx}=(4Z_1^2e^2\chi^2k_F^2/3)(v/v_F)\times\{\ln[1+(2k_F\Lambda_0)^2]\}^2C_{\mathrm{BK}}(r_s) \quad (2.23)$$

(called BK2), where

$$C_{\mathrm{BK}}(r_s)=\tfrac{1}{2}I(\chi^2)\{1/[(1+\chi^2)I(\chi^2)]-2\chi^2\}^2 . \quad (2.24)$$

Even if $\beta=0$ is assumed in Eq. (2.13), our result cannot be reduced to Eq. (2.24). The reason is that in the BK treatment the approximation $(2k_F\Lambda_0)<1$ is not used in the expression of charge distribution $\rho(k)$, but is used in the final integration result of stopping power (which is contrary to our treatment).

In Table I it is shown that the values of $C(r_s)$ in our work are obviously increased in comparison with $C_K(r_s)$ and $C_{\mathrm{BK}}(r_s)$. The increase in values of $C(r_s)$ compared with $C_K(r_s)$ and $C_{\mathrm{BK}}(r_s)$ is caused by the effect of the correlation and exchange interaction of the electron gas. However, even though the expression $C_K(r_s)$ is not the same as $C_{\mathrm{BK}}(r_s)$, the numerical values obtained are very close.

The treatment by Lindhard and Scharff [9] (LS) is based on the Thomas-Fermi statistical model for the atom, from which they obtained the following results for the electronic stopping power for a slow projectile with velocity v:

$$\frac{-dE}{dx}=N(8\pi e^2a_0)(Z_1^{7/6}Z_2/Z)(v/v_0) , \quad (2.25)$$

with $Z=(Z_1^{2/3}+Z_2^{2/3})^{3/2}$. Here, N and Z_2 are the target atomic density and atomic number, respectively.

In the next section we will make a comparison of our theoretical predictions to both some experimental data and other theoretical predictions obtained using the LS, Kaneko, and BK approaches.

III. COMPARISON OF THE THEORY WITH EXPERIMENTAL DATA

To compare the theoretical results with experimental data, we introduce the projectile stopping cross section of the electron gas per target atom as

$$S=\left[\frac{-dE}{dx}\right]\Big/\rho_0 , \quad (3.1)$$

where ρ_0 is the target-atom mass density.

Ward *et al.* [10] have measured the electronic stopping power at the common projectile velocity $v=0.82v_0$ for all projectiles $6\le Z_1\le 20$ in five solid materials: carbon, silver, gold, nickel, and aluminum. The comparison of theoretical predictions, with experimental data of Ward *et al.* is shown in Figs. 1–5. The experimental data exhibit the Z_1 oscillation in stopping power, which is related to atomic shell structures of projectiles. Since our theory (curve labeled WM), Kaneko's theory (curve labeled K), BK theory (curves labeled BK1 and BK2), and Lindhard-Scharff theory (curve labeled LS) is based on a statistical approximation, this oscillation is not given by the theories. In the following comparison we will disregard this oscillation.

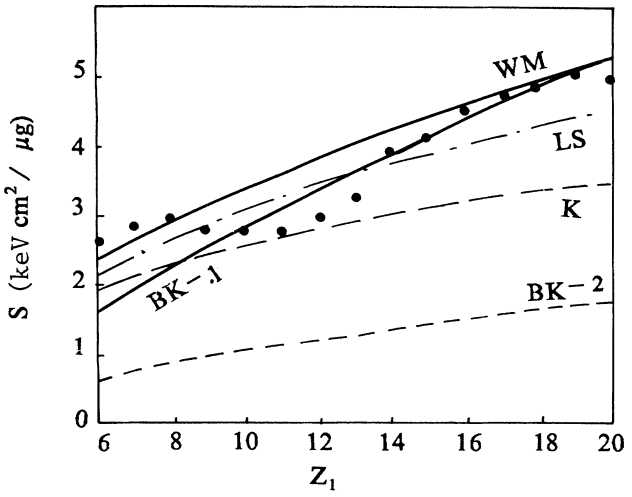

FIG. 1. Electronic stopping cross section of carbon ($r_s=1.526$, $\rho_0=2.266$ g cm^{-3}) for slow projectile atoms ($v=0.82v_0$) as a function of Z_1. WM, our results; K, the theory of Kaneko; LS, the theory of Lindhard and Scharff; BK1 (nonzero q values) and BK2 ($q=0$) theories of Brandt and Kitakawa. ●, experimental data of Ward *et al.* [10].

In Fig. 1, theoretical results are compared with experimental data for carbon film. For carbon, we choose $r_s=1.526$ [11] and four valence electrons per atom to produce the density $\rho_0=2.266$ g cm^{-3}. We can see that our results, Kaneko's results, and the BK1 results are

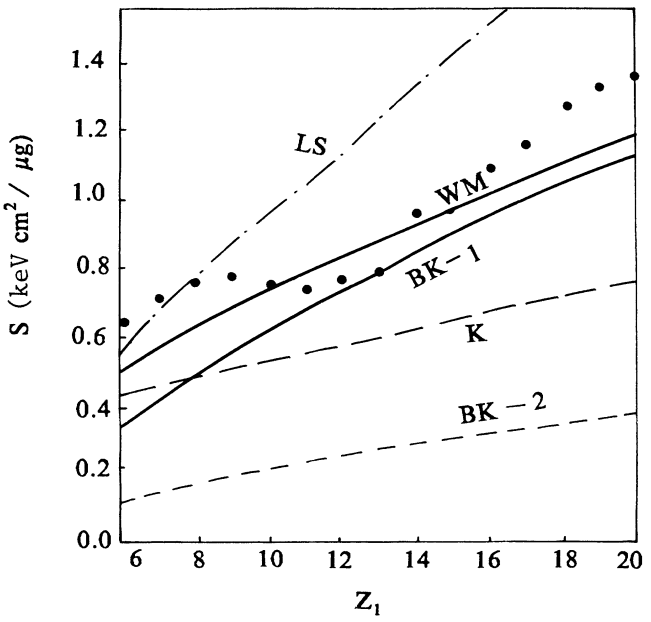

FIG. 2. Electronic stopping cross section of silver ($r_s=1.53$ and $\rho_0=10.47$ g cm^{-3}). The same notation as in Fig. 1 is used.

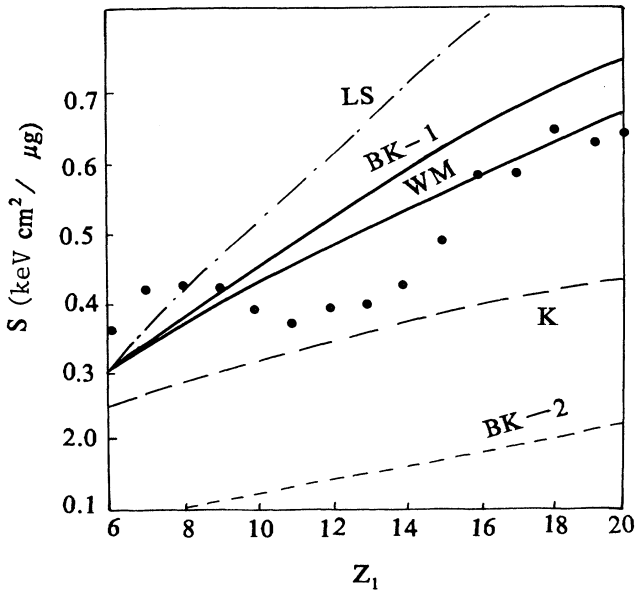

FIG. 3. Electronic stopping section of gold ($r_s=1.49$ and $\rho_0=19.31$ g cm^{-3}). The same notation as in Fig. 1 is used.

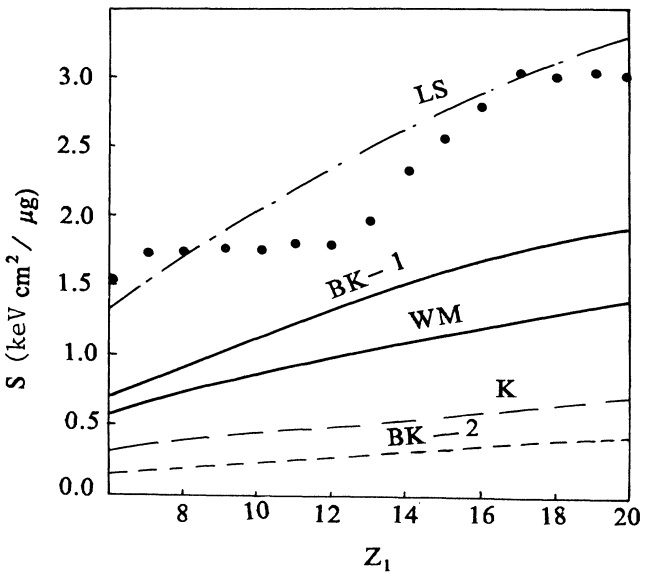

FIG. 5. Electronic stopping cross section of aluminum ($r_s=2.07$ and $\rho_0=2.70$ g cm^{-3}). The same notation as in Fig. 1 is used.

near the experimental data, the LS predictions tend to be low for high values of Z_1, and the BK2 results are lowest. Since the correlation and exchange interaction of the electron gas was included in the present work, our predictions are higher than Kaneko's and the BK2 results. Also it is found that nonzero-ionization q values make increases in the BK1 values of stopping power compared to those of BK2.

Figures 2 and 3 show similar comparisons for silver and gold targets, respectively. We choose [12] $r_s=1.53$ and $\rho_0=10.49$ g cm^{-3} for silver, and $r_s=1.49$ and $\rho_0=19.31$ g cm^{-3} for gold. It is found that our predictions and the BK1 results agree quite well with experimental data; however, the LS predictions are higher than the data, and Kaneko's results and the BK2 results are lower than the data, especially for high-Z_1 projectiles.

In Figs. 4 and 5 the comparisons are made for nickel and aluminum targets, respectively. We choose [12] $r_s=1.60$ and $\rho_0=8.89$ g cm^{-3} for nickel, and $r_s=2.07$ and $\rho_0=2.70$ g cm^{-3} for aluminum. We can see that the LS predictions agree well with the experimental data; and our results, Kaneko's results, and the BK1 and the BK2 results are lower than the data, especially for an aluminum target. We believe that the difference is caused by the low-velocity approximation used in the present work, Kaneko's approach, and the BK work. For aluminum the projectile velocity is high ($v=0.82v_0$). For a nickel target the Fermi velocity $v_F=1.2v_0$, and for the aluminum target $v_F=0.9v_0$, which yield $v/v_F=0.7$ and $v/v_F=0.9$, respectively. However, the approximation $v/v_F\ll 1$ was used in the present paper, Kaneko's work and the BK work.

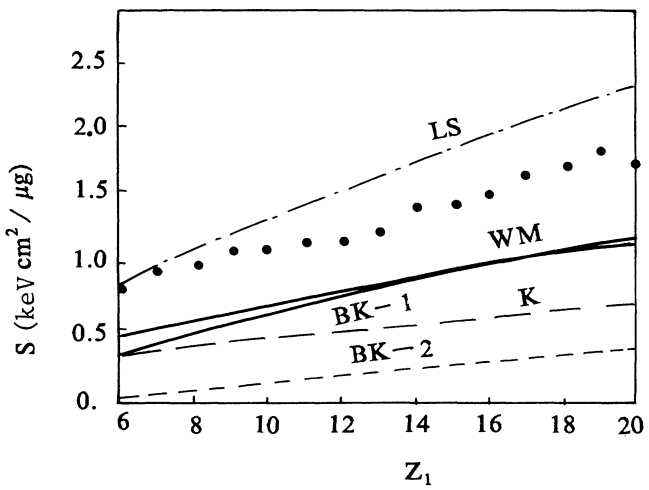

FIG. 4. Electronic stopping cross section of nickel ($r_s=1.60$ and $\rho_0=8.89$ g cm^{-3}). The same notation as in Fig. 1 is used.

In summary, the stopping power of slow projectiles has been investigated using the LFC dielectric function, and some analytical formulas obtained. The effect of correlation and exchange interaction of electrons makes the values of stopping power increase compared with Kaneko's results and the BK2 results, both of which are based on RPA dielectric theory. However, our results are very near that of BK1, which is based on nonzero-ionization q values. A comparison of our theoretical results with Lindhard and Scharff results was also made. For carbon, silver, and gold targets our theoretical predictions agree quite well with the experimental data; however, for nickel and aluminum targets, our theory, Kaneko's theory and the BK theory give poor predictions due to the low-velocity approximation.

ACKNOWLEDGMENTS

This work was funded by the Key National Laboratory of Material Modification by Beam Three, Dalian University of Technology.

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