Energy loss of ions moving near a solid surface

You-Nian Wang*
Department of Physics, University of Waterloo, Ontario, Canada N2L 3G1

W.-K. Liu†
Department of Physics, The University of Newcastle, Newcastle-upon-Tyne NE1 7RU, England

(Received 4 December 1995)

The energy loss of an ion moving parallel to a solid surface is studied within the dielectric function formalism. Based on the specular-reflection model, the surface response function can be expressed in terms of the bulk dielectric function, and the effect of the exchange-correlation interaction of electrons in the solid is taken into account by the local-field correction dielectric theory. For low-velocity ions, semianalytical expressions of the energy loss are obtained. In the high-velocity limit, the contributions of the surface plasmon to the energy loss are studied using the hydrodynamic approximation (HA) and the plasmon pole approximation (PLA) to the bulk dielectric function. It is found that at low velocity, the exchange-correlation interaction of electrons enhances the magnitude of the energy loss, but at high velocity, its effect is less important, and both the HA and the PLA provide an adequate description for surface-plasmon description. [S1050-2947(96)08306-0]

PACS number(s): 34.50.Bw, 34.50.Dy, 61.85.+p

I. INTRODUCTION

An energetic ion approaching a solid surface experiences a wake potential arising from the surface electronic excitations it induces in the medium. The gradient of the wake potential will then act back on the ion and cause it to lose its energy. During the past decades, a number of studies on the energy loss of the ion moving in the bulk matter have been reported [1–3]. Compared with the bulk electronic excitation, exact treatment the surface electronic excitation is very difficult due to the loss of translational symmetry in the direction perpendicular to the surface. The well-known specular-reflection model (SRM), introduced by Ritchie and Marusak [4] in the study of the surface-plasmon dispersion relations, and independently discussed by Wagner [5], can discribe the surface electronic excitations reasonably well. The SRM assumes that the electrons of the solid are specularly reflected by the surface and interference between the outgoing and the reflected components can be neglected. This allows one to use the method of images to determine the wake potential and the corresponding energy loss.

In the SRM, the surface response is expressed in terms of the bulk dielectric function. Using the SRM and a modified hydrodynamic approximation to the bulk dielectric function, Ferrell *et al.* [6] studied the energy loss of a slow ion moving in vacuum parallel to a solid surface. Their dielectric function agrees with the low-frequency expansion of the full random-phase approximation (RPA) of the dielectric function and can describe the damping of collective modes with an empirical parameter γ. Subsequently, Núñez *et al.* [7] extended the work of Ferrell *et al.* to normal incident ion trajectories and also analyzed the case when the ion moves in the interior of the solid. Using the RPA dielectric function Gumbs and Glasser [8] have presented a general expression of the energy loss, but did not give detailed numerical results.

The RPA dielectric function does not include the exchange-correlation interaction of electrons in the solid, and hence is valid only in the weakly coupling limit where $r_s \leqslant 1$. Here $r_s = [3/(4\pi n_0 a_0^3)]^{1/3}$, n_0 is the electron-gas density in the solid, and a_0 is the Bohr radius. In metals, the value of r_s ranges about from 1.5 (Au,W) to 5.88 (Cs), and thus the RPA dielectric function may not provide accurate values for the energy loss, especially for slow ions.

The purpose of the present work is to study effects of the exchange-correlation interaction of electrons on the energy loss using the local-field correction (LFC) dielectric function [9]. For slow ions moving in bulk matter, it has been shown [10–13] that the values of the energy loss predicted by the LFC dielectric function are larger than those given by the RPA dielectric function. We expect a similar conclusion also holds for the energy loss when the ion moves near solid surfaces.

The organization of this paper is as follows. In Sec. II, we will give a general expression of the energy loss for the ion traveling parallel to a solid surface using the SRM, and incorporate the influence of the exchange-correlation interaction of electrons on the energy loss with the LFC function. In Sec. III we present semianalytical expressions of the energy loss for the low-velocity case. The contributions of the surface plasmon to the energy loss will be considered in Sec. IV using the plasmon-hole approximation (PLA) and the hydrodynamic approximation (HA) to the bulk dielectric function.

*Permanent address: Department of Physics, Dalian University of Technology, Dalian 116023, People's Republic of China.

†Permanent address: Department of Physics, University of Waterloo, Ontario, Canada N2L 3G1.

A short summary will be given in Sec. V. Atomic units (a.u.) will be used throughout this work.

II. ENERGY LOSS FOR AN ION NEAR A SOLID SURFACE

We consider a particle of charge Z_1 moving with velocity $\mathbf{v}$ parallel to a solid surface. The surface is defined by the $z=0$ plane. The solid lies in the region $z<0$ and the vacuum is in the region $z>0$. We shall use the notations $\mathbf{r}=(\mathbf{R},z)$ and $\mathbf{k}=(\mathbf{Q},k_z)$, where $\mathbf{r}$ and $\mathbf{k}$ are the position vector and wave vector, respectively, and $\mathbf{R}$ and $\mathbf{Q}$ represent their components parallel to the surface. The particle thus produces a charge density $\rho_{\rm ext}(\mathbf{r},t)=Z_1\delta(\mathbf{R}-\mathbf{v}t)\delta(z-z_0)$, where $(\mathbf{v}t,z_0)$ is the position vector of the particle, and the Fourier transform of the external charge density is thus given by $\rho_{\rm ext}(\mathbf{k},\omega)=Z_1 e^{ik_z z_0}2\pi\delta(\omega-\mathbf{Q}\cdot\mathbf{v})$.

We now choose the x-axis along the direction of $\mathbf{v}$. The energy loss is proportional to the gradient of the wake potential $\Psi_{\rm ind}(\mathbf{r},t)$ along the x-axis at the projectile site,

$$S_e=Z_1\frac{\partial\Psi_{\rm ind}}{\partial x}(x=vt,y=0,z=z_0). \tag{1}$$

Using the SRM and applying the method of images, the surface wake potential at $(\mathbf{r},t)$ can be expressed as [14,15]

$$\Psi_{\rm ind}(\mathbf{r},t)=Z_1\int\frac{d^2\mathbf{Q}}{(2\pi)^2}e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{v}t)}\frac{2\pi}{Q}G(Q,z,z_0,\omega), \tag{2}$$

where $\omega=\mathbf{Q}\cdot\mathbf{v}$. Explicit expression of the response function $G(Q,z,z_0,\omega)$ can be found in Refs. [14–16]. Employing the two-dimensional polar coordinates in momentum space (Q,φ) so that $\omega=Qv\cos\varphi$, we obtain a general expression of the energy loss from Eqs. (1) and (2) as

$$S_e=\frac{2Z_1^2}{\pi v}\int_0^\infty dQ\int_0^{Qv}\frac{\omega\,d\omega}{\sqrt{Q^2v^2-\omega^2}}F(Q,z_0,\omega) \tag{3}$$

in which $F(Q,z_0,\omega=-\mathrm{Im}\,G(Q,z,z_0,\omega)|_{z=z_0}$, where Im G denotes the imaginary part of G. When the particle moves in vacuum ($z_0>0$), the function $F(Q,z_0,\omega)$ is given by

$$F(Q,z_0,\omega)=\mathrm{Im}\left[\frac{\varepsilon_s(Q,\omega)-1}{\varepsilon_s(Q,\omega)+1}\right]e^{-2Qz_0}, \tag{4}$$

while for the particle traveling in the interior of the solid ($z_0<0$),

$$F(Q,z_0,\omega)=-\mathrm{Im}\left[\varepsilon_s(Q,\omega)+\varepsilon_s(Q,2z_0,\omega)-\frac{2\varepsilon_s^2(Q,z_0,\omega)}{\varepsilon_s(Q,\omega)+1}\right], \tag{5}$$

where

$$\varepsilon_s(Q,z,\omega)=\frac{2Q}{\pi}\int_0^\infty\frac{dk_z}{k^2}\frac{\cos(k_z z)}{\varepsilon(k,\omega)}, \tag{6}$$

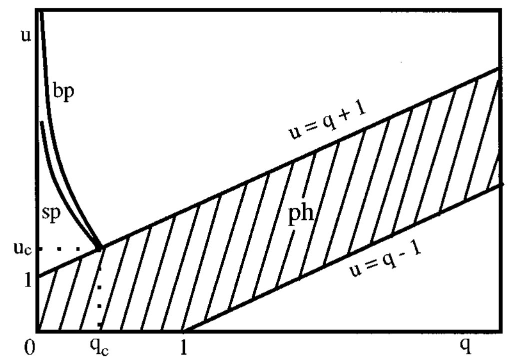

FIG. 1. Excitation spectrum in $q-u$ space. The region denoted by ph corresponds to the single-particle excitations; surface-plasmon and bulk-plasmon dispersion curves are labeled by sp and bp, respectively.

and $\varepsilon_s(Q,\omega)\equiv\varepsilon_s(Q,0,\omega)$ is the surface dielectric function [17].

From Eq. (3), we observe that within the SRM, the energy loss can be calculated if the bulk dielectric function $\varepsilon(k,\omega)$ is known. In a previous study [8], the RPA was used to investigate the energy loss for the low velocity behavior. To go beyond the RPA, the effects of the exchange-correlation interaction of electrons in the solid can be included approximately by a static local-field correction $G(k)$, so that the bulk dielectric function can be expressed as [9–11]

$$\varepsilon(k,\omega)=1-\frac{P(k,\omega)}{1+G(k)P(k,\omega)}. \tag{7}$$

Here $P(k,\omega)$ is the Lindhard polarizability and a parametrized expression of $G(k)$ has been given by Utsumi and Ichimaru [9]. Recently, this LFC bulk dielectric function was employed to calculate the surface wake potential [16]. Here, let us mention that a dynamic local-field correction $G(k,\omega)$ has been used to calculate the energy loss for slow ions in solids [12]. In this case, the imaginary part of $G(k,\omega)$ reduces values of the energy loss.

For numerical computations we introduce the dimensionless variables $q=Q/(2k_F)$, $u=\omega/(Qv_F)$, $\overline{q}=k/(2k_F)$, and $\overline{u}=\omega/(kv_F)=qu/\overline{q}$, where $k_F=(3\pi^2n_0)^{1/3}$ is the Fermi wave number, and in atomic units $v_F=k_F$ is the Fermi velocity. The polarizability $P(k,\omega)$ can be written in terms of the variables $\overline{q}$ and $\overline{u}$ as

$$P(k,\omega)=-(\chi^2/\overline{q}^2)[f_1(\overline{q},\overline{u})+if_2(\overline{q},\overline{u})], \tag{8}$$

where $\chi^2=1/(\pi k_F)$. Explicit expressions for the dimensionless functions $f_1(\overline{q},\overline{u})$ and $f_2(\overline{q},\overline{u})$ can be found in Ref. [10]. Using the variables q and u, Eq. (3) can be reduced to

$$S_e=\frac{8Z_1^2k_F^2}{\pi}\left(\frac{v_F}{v}\right)\int_0^{v/v_F}\frac{u\,du}{\sqrt{(v/v_F)^2-u^2}}\int_0^\infty q\,dq\,F(q,z_0,u). \tag{9}$$

In general, at high particle velocity, the contributions to the energy loss come from three parts: the single-particle–hole excitations (ph) in which $\mathrm{Im}[-1/\varepsilon(k,\omega)]\neq0$, the surface-plasmon excitations (sp) in which $1+\varepsilon_s(Q,\omega)=0$, and the bulk-plasmon excitations (bp) in which $\varepsilon(k,\omega)=0$ (see Fig. 1). When the particle is traveling in vacuum, only the single-particle–hole excitations and the surface-plasmon excitations contribute to the energy loss, which we will study in detail in Sec. IV. At low velocity, the energy loss is determined only by the single-particle–hole excitations for both the ion moving in vacuum and in the solid.

III. LOW-VELOCITY APPROXIMATION

In this section, we consider the low-velocity case in which $v/v_F < u_c$, where u_c is the threshold value for plasmon excitations (see Fig. 1 and discussion in Sec. IV). In this case, only single-particle–hole excitations will contribute to the energy loss, which from Eq. (9) becomes

$$S_e^{\mathrm{ph}} = \frac{8Z_1^2 k_F^2}{\pi}\left(\frac{v_F}{v}\right)\int_0^{v/v_F}\frac{u\,du}{\sqrt{(v/v_F)^2-u^2}} \times \int_{q_{\min}}^{u+1} q\,dq\,F(q,z_0,u), \tag{10}$$

where $q_{\min}=0$ for $u \leqslant 1$ and $(u-1)$ for $u>1$.

When the projectile velocity v is much less than the Fermi velocity v_F the polarizability $P(\overline{q},\overline{u})$ and the LFC function $G(\overline{q})$ can be written approximately as [10]

$$P(\overline{q},\overline{u}) \approx -\frac{\chi^2}{\overline{q}^2}\left(1-\frac{\overline{q}^2}{3}+i\,\frac{\pi}{2}\,\overline{u}\right), \tag{11}$$

$$G(\overline{q}) \approx 4\gamma_0 \overline{q}^2, \tag{12}$$

where γ_0 is a parameter related to the correlation energy of the electron gas [9]. Inserting Eqs. (11) and (12) into Eq. (6), we can write the real and imaginary parts of ε_s as

$$\mathrm{Re}\,\varepsilon_s(Q,z,\omega) \approx f_r(q,z), \tag{13}$$

$$\mathrm{Im}\,\varepsilon_s(Q,z,\omega) \approx -u f_i(q,z), \tag{14}$$

where

$$f_r(q,z) = \frac{2q}{\pi}\int_0^{\sqrt{1-q^2}} d\overline{q}_z\left(a_0+\frac{a_1}{\overline{q}_z^2+q^2+\tau}\right)\cos(2k_F z\overline{q}_z), \tag{15}$$

$$f_i(q,z) = \frac{2q}{\pi}\int_0^{\sqrt{1-q^2}} d\overline{q}_z\,\frac{a_2 q}{(\overline{q}_z^2+q^2+\tau)^2}\,\frac{\cos(2k_F z\overline{q}_z)}{\sqrt{\overline{q}_z^2+q^2}}, \tag{16}$$

$$a_0 = \frac{\frac{4}{3}\gamma_0\chi^2}{1-\frac{1}{3}\beta\chi^2}, \tag{17}$$

$$a_1 = \frac{1-4\gamma_0\chi^2-\frac{4}{3}\gamma_0\chi^2\tau}{1-\frac{1}{3}\beta\chi^2}, \tag{18}$$

$$a_2 = \frac{\frac{1}{2}\pi\chi^2}{(1-\frac{1}{3}\beta\chi^2)^2}, \tag{19}$$

$$\beta = 1+12\gamma_0, \tag{20}$$

and

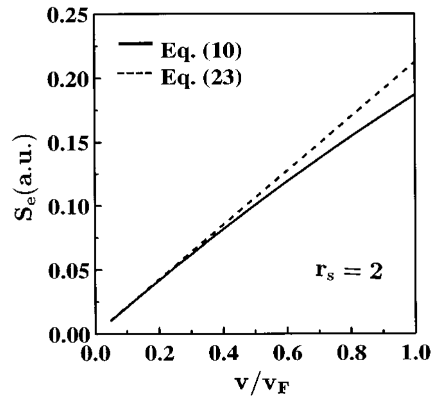

FIG. 2. Comparison of the full numerical result [Eq. (10)] for the energy loss with that of the semianalytical formula [Eq. (23)] for a slow proton moving in the interior of the solid with $z_0=-k_F^{-1}$. Both calculations employ the LFC bulk dielectric function and $r_s=2$. (1 a.u.=51.4 eV/Å).

$$\tau = \frac{\chi^2}{1-\frac{1}{3}\beta\chi^2}. \tag{21}$$

Substituting the above results into Eq. (10), we find the energy loss due to the single-particle–hole excitation is proportional to the projectile, velocity v,

$$S_e^{\mathrm{ph}} = 4Z_1^2 k_F^2\left(\frac{v}{v_F}\right)\int_0^1 dq\,\frac{q f_i(q)}{[1+f_r(q)]^2}\,e^{-4k_F z_0 q} \quad (z_0>0), \tag{22}$$

$$S_e^{\mathrm{ph}} = \frac{4Z_1^2 k_F}{3\pi}\left(\frac{v}{v_F}\right)C(r_s) + 2Z_1^2 k_F^2\left(\frac{v}{v_F}\right)\int_0^1 H(q,z_0)q\,dq \quad (z_0<0), \tag{23}$$

where $f_r(q)=f_r(q,0)$, $f_i(q)=f_i(q,0)$,

$$C(r_s) = \frac{1}{2(1-\frac{1}{3}\beta\chi^2)^2}\left[\ln\left(1+\frac{1}{\tau}\right)-\frac{1}{1+\tau}\right], \tag{24}$$

and

$$H(q,z_0) = f_i(q,2z_0) - \frac{4f_r(q,z_0)f_i(q,z_0)}{1+f_r(q)} + \frac{2f_r^2(q,z_0)f_i(q)}{[1+f_r(q)]^2}. \tag{25}$$

The first term on the RHS of Eq. (23) represents the energy loss for a slow ion in an infinite medium and the second term comes from the surface contribution.

In Fig. 2 we compare the results of the semi-analytical formula, Eq. (23), with the full numerical results of Eq. (10) for a proton moving in the interior of the solid with $z_0=-k_F^{-1}$. In the small velocity region, both results are in good agreement. However, as the velocity increases, the semianalytical results become larger than the exact values.

Using Eqs. (22) and (23) the dependence of the energy loss S_e on the separation of the proton from the surface z_0 is shown in Fig. 3 for $v=0.5v_F$ and $r_s=2$. When the proton moves in vacuum the values of the energy loss increase rapidly as the distance z_0 from the surface decreases. When the

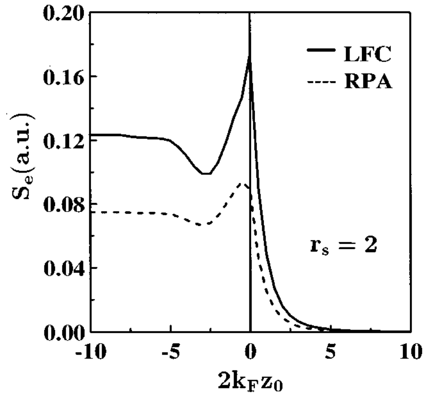

FIG. 3. The dependence of the energy loss on the position of a slow proton ($v=0.5v_F$). Solid curve: employing the LFC bulk dielectric function. Dashed line: employing the RPA bulk dielectric function.

proton is traveling inside the solid side, S_e shows some oscillations near the surface and approaches asympotically the bulk value as the separation $|z_0|$ increases. The qualitative behavior of the RPA results is similar to those of the LFC, but the values of the LFC energy loss are always larger than the RPA values, especially inside and near the surface. Hence, near the surface, there is an enhancement of the energy loss due to the effect of the exchange-correlation interaction.

IV. CONTRIBUTIONS OF SURFACE PLASMONS

In this section, we will only consider an ion moving parallel to the solid surface in vacuum. If the ion velocity is high enough, surface plasmons can be excited. The surface-plasmon dispersion relation is given by the real root of the equation

$$D_r(q,u)\equiv 1+\varepsilon_s(q,u)=0, \tag{26}$$

yielding the dispersion curve $q=q_r(u)$. The threshold value u_c is obtained by solving Eq. (26) simultaneously with $u=1+q$. Thus, surface plasmons will be excited when $u=v/v_F>u_c$ (see Fig. 1). In this case, there is an additional contribution from the surface plasmons to the energy loss.

$$S_e^{\rm sp}=-8Z_1^2k_F^2\left(\frac{v_F}{v}\right)\int_{u_c}^{v/v_F}du\ \frac{uq_r(u)}{\sqrt{(v/v_F)^2-u^2}}\times e^{-2q_r(u)z_0}\left(\frac{\partial D_r}{\partial q}\right)^{-1}\Bigg|_{q=q_r(u)}. \tag{27}$$

TABLE I. Values of u_c as functions of r_s.

r_s	u_c (PLA)	u_c (HA)
2.0	1.264 394 6	1.288 912 7
3.0	1.309 125 6	1.333 643 6
4.0	1.345 025 3	1.368 847 0
5.0	1.375 517 2	1.398 277 4
6.0	1.402 290 4	1.423 758 6

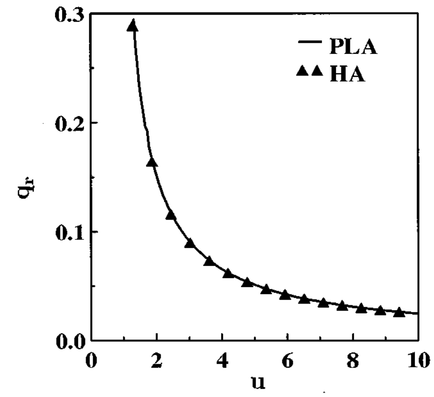

FIG. 4. Surface-plasmon dispersion relations using the PLA and the HA bulk dielectric function.

Solving for the dispersion relation of Eq. (26) and then calculating $S_e^{\rm sp}$ from Eq. (27) become very tedious when the LFC dielectric function is used. Fortunately, the effect of the exchange-correlation interaction becomes less important at high velocities, and the RPA dielectric function is adequate for predicting $S_e^{\rm sp}$. Furthermore, it has been shown from the calculations of the wake potential [14,15] that in the high-velocity limit, the full RPA dielectric function can be replaced by either the HA dielectric function

$$\varepsilon(k,\omega)=1+\frac{\omega_p^2}{c^2k^2-\omega(\omega+i0^+)}, \tag{28}$$

where $c=(3/5)^{1/2}v_F$, or the PLA dielectric function

$$\varepsilon(k,\omega)=1+\frac{\omega_p^2}{c^2k^2+k^2/4-\omega(\omega+i0^+)}. \tag{29}$$

Hence, in the following discussions, we shall use the PLA and the HA dielectric function to study the contributions of the surface-plasmon excitations to the energy loss, although we will use the LFC or RPA dielectric function in computing the single-particle–hole contribution.

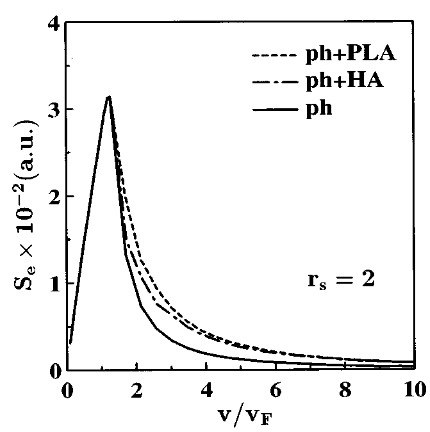

FIG. 5. Contributions to the energy loss for a proton moving in the vacuum ($z_0=k_F^{-1}$). Solid curve: LFC single-particle–hole excitation. Dashed curve: total contributions with PLA for plasmons. Dot-dashed curve: total contribution with HA for plasmons.

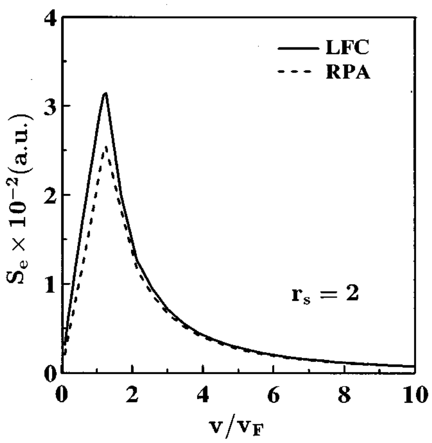

FIG. 6. Total energy loss (including both ph and sp contributions) for a proton moving in vacuum ($z_0=k_k^{-1}$) as a function of v/v_F. Solid curve: employing LFC dielectric function; dashed line: employing RPA dielectric function.

Using the HA and PLA dielectric functions, the values of u_c for various r_s are listed in Table I and the surface-plasmon dispersion curves for $r_s=2$ are shown in Fig. 4. One observes that the results of the PLA and the HA dielectric functions agree quite well. We show in Fig. 5 the contributions of single-particle–hole and surface-plasmon excitations to the energy loss for a swift proton moving in vacuum with $z_0=k_F^{-1}$. The LFC dielectric function was used in computing the single-particle–hole contribution. At low velocity, S_e first increases with ion velocity until it reaches a maximum at $v/v_F \simeq 1.26$, after which it decreases rapidly first, and then tails off almost exponentially. From Table I, we see that surface-plasmon excitations begin to contribute when $v/v_F>1.26$ for the PLA dielectric function (or $v/v_F>1.29$ for the HA dielectric function), and become more important than the single-particle–hole excitations when $v>3v_F$. Values of the energy loss obtained from the PLA dielectric function are larger than those from the HA dielectric function for $v \leqslant 6v_F$, beyond which the HA and PLA results are very similar.

Finally, in Fig. 6 we show the dependence of the total energy loss on the velocity of a proton moving in the vacuum with $z_0=k_F^{-1}$, using the LFC or the RPA for the single-particle–hole excitations, and the PLA for the surface-plasmon excitation. We observe that in the low-velocity region the results predicted by the LFC dielectric function are larger than those predicted by the RPA dielectric function, but at high-velocity ($v>2v_F$), both results are in good agreement with each other as the effect of the exchange correlation diminishes.

V. SUMMARY

In this paper, we have studied the influence of electronic exchange correlation on the energy loss of an ion moving parallel to the solid surface. The energy loss is calculated within the framework of the dielectric theory, and the specular-reflection model is employed to approximate the surface response functions in terms of the bulk dielectric function. Exchange-correlation effects are approximately taken into account by the local-field correction dielectric theory. At low velocity, only single-particle–hole excitations contribute to the energy loss, and by comparing the results obtained from using the LFC and the random-phase approximation, we conclude that exchange-correlation effects tend to enhance the energy loss near the surface, especially for the ion traveling inside the solid and close to the surface. For the ion moving outside the surface at high velocity, surface-plasmon excitations also contribute to the energy loss, and their effects can be modeled by either the hydrodynamic approximation or the plasmon pole approximation. We found that at high velocity, the exchange-correlation effects are unimportant and both the HA and the PLA give similar results. It is well known that the linear-response dielectric theory is valid only for high-velocity ions with small atomic numbers ($Z_1=1$ or -1). In the future work, we will consider some nonlinear effects on the surface wake and the energy loss for slow ions.

ACKNOWLEDGMENTS

This work is partially supported by a Natural Sciences and Engineering Research Council (NSERC) of Canada Research Grant (W.K.L.), and by the Natural Science Foundation of China and the Ion Beam Laboratory of the Shanghai Metallurgy Institute (Y.N.W.). Y.N.W. wishes to acknowledge the hospitality of the Department of Physics; University of Waterloo during his visit, and W.K.L. thanks the University of Newcastle.

[1] J. Lindhard and A. Winther, K. Dan. Vidensk. Mat. Fys. **34**(4) (1964).
[2] R. H. Ritchie, Phys. Rev. **114**, 644 (1959).
[3] W. Brandt and M. Kitagawa, Phys. Rev. B **25**, 5631 (1982).
[4] R. H. Ritchie and A. L. Marusak, Surf. Sci. **4**, 234 (1966).
[5] D. Wagner, Z. Naturforsch, Teil A **21**, 634 (1966).
[6] T. L. Ferrel, P. M. Echenique, and R. H. Ritchie, Solid State Commun. **32**, 419 (1979).
[7] R. Núñez, P. M. Echenique, and R. H. Ritchie, J. Phys. C **13**, 4229 (1980).
[8] G. Gumbs and M. L. Glasser, Phys. Rev. B **37**, 1391 (1988).
[9] K. Utsumi and S. Ichimaru, Phys. Rev. A **26**, 603 (1982).
[10] Y. N. Wang and T. C. Ma, Nucl. Instrum. Methods B **51**, 216 (1990).
[11] T. C. Ma, Y. N. Wang, and T. Cui, J. Appl. Phys. **72**, 3838 (1992).
[12] I. Nagy, J. Làzzló, and Giber, Z. Phys. A **321**, 221 (1985).
[13] B. Dabrowski, Phys. Rev. B **34**, 4989 (1986).
[14] F. J. García de Abajo and P. M. Echenique, Phys. Rev. B **46**, 2663 (1992).
[15] F. J. García de Abajo and P. M. Echenique, Phys. Rev. B **48**, 13 399 (1993).
[16] Y. N. Wang and W.-K. Liu, Chem. Phys. Lett. (to be published).
[17] D. M. Newns, Phys. Rev. B **1**, 3304 (1970).