Application of Lindhard's dielectric theory to the stopping of ions in solids

G. Jafring
U.S. Army Electronics Technology and Devices Laboratory (ERADCOM), Fort Monmouth, New Jersey 07703

J. F. Ziegler and M. J. Nuss
IBM-Research Yorktown Heights, New York 10598

(Received 30 November 1978; accepted for publication 28 September 1979)

Lindhard's dielectric theory of energy loss is applied to the stopping of energetic ions in solids. The Lindhard formalism, in combination with the local density approximation and the concept of effective charge, is used to calculate the stopping powers of heavy ions in many targets and over a wide range of projectile energies. Theoretically calculated stopping powers are compared with available experimental data.

PACS numbers: 61.80.Jh

INTRODUCTION

For many years, the stopping of energetic ions in matter has been a subject of great interest to theoretical and experimental physicists. Bohr, Bethe, and Bloch were the pioneering theoretical investigators of charged particle stopping in matter. Some 30 years after the development of Bethe-Bloch theory, Lindhard presented an elegant dielectric formulation of stopping theory for a charged particle penetrating a free-electron gas.

The Lindhard dielectric formalism probably stands as the most complete "first principles" theory of energy loss to date. However, the application of Lindhard's theory to real solids becomes a formidable task since the direct numerical integration of the Lindhard stopping equation is slow and cumbersome due to the presence of singularities in the integrand. This paper represents the first attempt to apply, with precision, the Lindhard theory of stopping to actual solids.

The original work of Lindhard was extended by Bonderup and Winther (L-W) who obtained an analytic expansion for the stopping power in the limit of high and low projectile velocity relative to the Fermi velocity of an electron gas; the Bethe stopping power (with a redefined mean ionization potential) plus shell corrections were obtained in the high-velocity limit whereas a linear dependence of velocity with stopping power was shown at low velocity.

Bonderup used the L-W expansions to include the local density approximation of Lindhard and Scharff (L-S) so as to extract the Bethe-Bloch terms, commonly referred to as the mean ionization potential and the shell corrections. In the local density approximation, each volume element of the solid is considered to be an independent plasma of uniform density, so that the total electronic stopping power is obtained by spatially averaging a specific stopping power over the target electron charge distributions. Bonderup, in his calculations, uses the Lenz-Jensen atomic charge distribution to describe the target electrons. His calculation was subsequently refined by Rousseau, Chu, and Powers (RCP) who utilized Hartree-Fock-Slater (HFS) charge distributions to describe the spatially varying electron density, thereby predicting the presence of oscillations in the stopping power when plotted versus target atomic number.

In this paper, we evaluate the Lindhard dielectric theory of stopping power within the local density approximation and the concept of effective charge. A comparison of Lindhard's stopping powers with the experiment for 0.4-MeV/amu heavy ions in solid targets is given; comparative agreement between theory and experiment over a wide range of projectile energies is discussed.

LINDHARD'S THEORY OF STOPPING POWER

For an ion of charge $z e$ moving with velocity $v$ in a medium of uniform density $\rho$, the energy loss due to electron excitation can conveniently be written in the form

$$-\frac{dE}{dx} = \frac{4\pi}{m} \left( \frac{z e}{v} \right)^2 \rho L(p, v),$$

(1)

where $L$ is the stopping number and $m$ is the mass of the electron. In the dielectric formalism, $L$ is written as

$$L = \frac{i}{\pi \omega_0} \int \frac{dk}{k} \int_{k_F}^{k_F'} \omega \, d\omega \, \epsilon''(k, \omega),$$

(2)

where $\omega_0$ is the plasma frequency, i.e.,

$$\omega_0 = \frac{4\pi e^2 \rho}{m},$$

(3)

and $\epsilon''(k, \omega)$ is the wave number and frequency dependent longitudinal dielectric constant.

Lindhard obtained the dielectric constant for a free-electron gas within first-order perturbation theory as

$$\epsilon(k, \omega) = 1 + \frac{8\pi e^2}{\hbar^2 k} \sum \epsilon F(E_n) \times \left( \frac{1}{k^2 + 2k k_x - (2m/\hbar^2)(\omega + i\gamma)} \right.$$

$$+ \left. \frac{1}{k^2 - 2k k_x + (2m/\hbar^2)(\omega + i\gamma)} \right),$$

(4)

where $E_n$ and $k_x$ represent the energy and wave vector for an electron in the $n$th state and $\gamma$ is a small positive value. For a free-electron gas at zero temperature,

$$F(E_n) = 1 \quad \text{for} \quad E_n < E_F,$$

$$F(E_n) = 0 \quad \text{for} \quad E_n > E_F,$$

(5)

and the summation in Eq. (4) can be evaluated to get
\[
e(u,v) = 1 + (\chi^2/z^2) \left[ f_1(u,v) + i f_2(u,v) \right],
\]

where

\[
f_1(u,v) = \frac{1}{2} + \frac{1}{8z} \left[ 1 - (z - u)^2 \right] 
\times \ln \left[ (z - u + 1)/(z - u - 1) \right] 
+ \frac{1}{8z} \left[ 1 - (z + u)^2 \right] 
\times \ln \left[ (z + u + 1)/(z + u - 1) \right],
\]

and

\[
f_2(u,v) = \frac{1}{4} \pi u,
\]

for \( z + u < 1 \)

\[
f_1(u,v) = \frac{\pi}{8z} [1 - (z - u)^2],
\]

for \( |z - u| < 1 < z + u \)

\[
f_2(u,v) = 0,
\]

for \( |z - u| > 1 \).

Here the variables \( k \) and \( v \) have been replaced by reduced variables

\[
z = (k / 2k_f) \quad \text{and} \quad u = (v / kv_f),
\]

where \( k_f \) and \( v_f \) are defined by

\[
E_f = \frac{1}{2} mu^2 = \left( \frac{h^2}{2m} \right) = \left( \frac{h^2}{2m} \right) (3\pi^2\rho)^{2/3}.
\]

In addition, the parameter \( \chi^2 \) in Eq. (6) is defined by

\[
\chi^2 = \left( \frac{v}{\pi v_f} \right),
\]

where \( v_f = (e^2/h) \), the Bohr velocity. When the dielectric constant of Eq. (6) is substituted into Eq. (2), one obtains

\[
L = \frac{6}{\pi} \int_0^\infty u du \int_0^z \frac{z' f_2(u,z)}{\left[ z^2 + \chi^2 f_1(u,z) \right]^2 + \left[ \chi f_2(u,z) \right]^2}.
\]

This expression for \( L \) in Eq. (11) is the Lindhard stopping number. In this paper, we make use of stopping numbers obtained from a numerical integration of Eq. (11) as a continuous function of electron density (or \( \chi^2 \)) over a wide range of projectile velocities (or energies). While the detailed results of the calculation can be found elsewhere, some typical illustrations of the variation in stopping number with electron density and energy can be found in Fig. 1.
gives rise to a marked change in density-averaged stopping number. Inspection of Figs. 3 and 4 shows that the stopping number integral of Eq. (12) approximately follows the radial charge density in spatial variation. It should also be noted that the low-energy (100 keV/amu) projectile stopping number is influenced mainly by the outer shell electron charge distribution, whereas the high-energy projectile (10 000 keV/amu) stopping number is dependent upon the inner electron shells as well. This analysis clearly shows the importance of using solid-state charge densities in the calculation of stopping powers of solids.

**EFFECTIVE CHARGE OF ENERGETIC IONS IN SOLIDS**

In the preceding discussions, the projectile ion was assumed to be a bare nuclear point charge. However, when the projectile is an ionized atom with an intrinsic electronic charge distribution, the question of the net charge of the projectile arises. From the beginning of stopping power theory the charge of heavy ions in solids has been poorly understood. Bohr suggested that the ion might be assumed stripped of all electrons with orbital velocities less than the ion velocity. This concept is difficult to calculate in detail for heavy ions because of the difficulties in assigning velocities to the highly distorted electron orbitals of a partially stripped ion in a dense electron plasma.

The active interest in fission fragments in 1939–1941 brought about various attempts to predict heavy ion stopping powers using the concept of effective charge.11-14 Within this concept, the ion charge state was assumed to be independent of the ion-solid stopping interaction so that the ion-target stopping interaction should be represented by an experimental proton stopping power, and the ratio of a heavy ion stopping power to the proton value (for the same velocity in the material) was identified as the heavy ion effective charge (it was assumed that the proton charge was unity)...

\[ z^*/z = 1 - \exp(-v_o z^*/2), \]

where \( z^* \) is the effective charge and \( v_o = e^2 h/s \) is the Bohr velocity (2.188 x 10^8 cm/sec). This formula has been reshaped by many authors as thousands of heavy ion stopping powers have been measured. We use the form

\[ z^*/z = 1 - [\exp(-A) - 1], \]

where

\[ A = B + 0.0378 \sin\pi B, \]

\[ B = 0.886(40E/amu)^{1/2}/z^*/2, \]

where the ion energy \( E \) is in MeV, and the ion mass is in amu. The expression is considered to be accurate to about 5% for ions with atomic numbers 6–92 in solids with atomic numbers 4–79, for energies above 0.2 MeV/amu. This formula is independent of target and depends only on the ion atomic number and velocity.

**COMPARISON OF THEORY WITH EXPERIMENT: CONCLUSIONS**

Within the local density approximation and the concept of effective charge, we have applied the Lindhard stopping theory for a charged particle in a free-electron gas to the stopping of heavy ions in solids. Stopping powers [Eq. (12) with \( z \) replaced by \( z^* \)] were calculated for a wide variety of projectile energies ranging from 100 to 10 000 keV/amu and for many targets. For projectile energies of 4000 keV/amu and above, the maximum error incurred in comparing the calculated stopping powers with experiment15 for many targets is about 4%. For projectile energies below 4000 keV/amu, the maximum error increases monotonically to a value of about 30% for a projectile energy of 100 keV/amu. A typical comparison of theoretical and experimental stopping powers for many targets is illustrated in Fig. 5. Here the ratio of experimental to theoretical stopping is plotted versus
target atomic number for a projectile energy of 400 keV/amu.

The objective of this paper has been to apply the Lindhard theory of stopping to real solids. Within the assumed approximations, the results show that the theory significantly deviates from experiment in the low projectile energy (100 keV/amu < E < 4000 keV/amu) region. The reasons for this disagreement may be manifold: the use of a free-electron gas dielectric response function, the extrapolation of the uniform electron gas model to solid state systems via the local density approximation, and the use of the effective charge concept to reduce experimental stopping powers to stopping numbers. In a future paper, we plan to explore an extension of Lindhard's theory to self-consistently include heavy atom projectiles which may abrogate some of the above weaknesses.

1. N. Bohr, Philos. Mag. 28, 10 (1913).