## Polarization Induced in a Solid by the Passage of Fast Charged Particles\*

Zeev Vager† and Donald S. Gemmell Argonne National Laboratory, Argonne, Illinois 60439 (Received 27 August 1976)

A theoretical description is given of the polarization charge-density distribution induced in a solid by the passage of a fast charged particle. The stopping power of the solid (including the effects of close collisions) is well accounted for by the braking effect of the polarization charges. Calculations based on this model for the polarization give good agreement with the results of recent experiments on the dissociation of fast molecular ions in foils.

In 1948 Bohr pointed out<sup>1</sup> that a fast positively charged particle traversing matter induces an electronic-polarization "wake" that trails behind the projectile and acts as a brake on it. Bohr gave a rough estimate showing that this braking force accounts approximately for the stopping power of the medium being traversed. The concept of a polarization wake attracted little attention in the years following Bohr's paper. However, recent work on molecular-ion stopping powers,<sup>2-5</sup> speculations on the possibility of forming "wake-riding" states,<sup>5-7</sup> and pronounced new effects seen in the motions of the breakup products formed when fast molecular-ion beams dissociate in thin foils<sup>8-10</sup> have focused renewed interest on this topic.

In this Letter a new theoretical description of the polarization wake in solids is outlined. It accounts well for the electronic stopping power of the medium (including the effects of close collisions). The theory is of particular importance in understanding the interactions of fast molecular ions with solids. As an example, we show the good agreement between calculations based on this wake model and recent experimental results<sup>9,10</sup> obtained on the dissociation of fast HeH<sup>+</sup> ions.

Consider a point particle with charge +Ze moving with velocity v along the positive z axis of a Cartesian coordinate frame fixed with respect to the solid medium. We restrict ourselves to projectile velocities that are nonrelativistic yet large compared to the velocities of most of the electrons in the medium. That is,  $v^2/c^2 \ll 1$  and, approximately,  $v \gg v_0$ , the Bohr velocity. In this range, the slowing down of the projectile over distances comparable with the extent of the polarization wake (typically  $\leq 100$  Å) is negligible. Therefore, for our present purposes, v may be treated as a constant. We employ the macroscopic frequency-dependent dielectric function  $\epsilon(\omega)$  to describe the response of the solid to the passage of the charged projectile. The Fourier components of the polarization and projectile chargedensity distributions are related by

$$\rho_{\text{DD}}(\mathbf{\tilde{r}}, \omega) = \rho_{\text{DFO}}(\mathbf{\tilde{r}}, \omega) \{ [\epsilon(\omega)]^{-1} - 1 \}, \qquad (1)$$

where  $\vec{\mathbf{r}} \equiv (x, y, z)$ . The time-dependent polarization charge-density distribution is then

$$\rho_{\text{pol}}(\mathbf{\hat{r}},t) = \frac{Ze}{2\pi\nu} \,\delta(x)\,\delta(y) \int_{-\infty}^{\infty} e^{i\omega(z/\nu-t)} \{ [\epsilon(\omega)]^{-1} - 1 \} \,d\omega.$$

This distribution is a line of charge (extending along the z axis). It does not take into account the close electronic collisions of the projectile.

Further evaluation of Eq. (2) requires a knowledge of  $\epsilon(\omega)$ . For solids capable of sustaining well-defined plasma oscillations, we may approximate  $\epsilon(\omega)$  with the high-frequency form<sup>11</sup>

$$\epsilon(\omega) = 1 - \omega_{\phi}^2 / \omega^2. \tag{3}$$

Here the plasma frequency is given by  $\omega_p = (4\pi ne^2/m)^{1/2}$ , where *n* is the average density of electrons (normally outer-shell or conduction electrons) participating in the coherent resonant motion.

Metals and conductors exhibit plasma oscillations most clearly, but similar collective oscillations are also to be found in other types of solid.<sup>12</sup> Substitution of Eq. (3) into Eq. (2) yields after integration

$$\rho_{\text{pol}}(\mathbf{\tilde{r}}, t) = (Ze/a) \sin[(z - vt)/a] \delta(\mathbf{x}) \delta(\mathbf{y}) \theta(vt - z), \qquad (4)$$

where  $a = v/\omega_p$  and  $\theta(x) = 0$  for x < 0,  $\theta(x) = 1$  for  $x \ge 0$ . This spatially oscillating, linear chargedensity distribution is stationary with respect to the moving projectile and extends only behind the projectile, not in front of it. The wavelength,  $\lambda = 2\pi a$ , is typically a few tens of angstroms.

We now consider the effect of close electronic collisions. Viewed microscopically in the frame of the moving projectile, almost unbound electrons with velocity v undergo scattering at the projectile. Thus, for example, the *s*-wave scattering is described by a wave packet of extension  $\sim \hbar / mv$ . Therefore the thickness of the polarization charge distribution is of that order. We take this into account when evaluating the potential distribution corresponding to the polarization wake, by substituting  $R^2 + (\hbar / mv)^2$  for  $R^2$  (where  $R^2 = x^2 + y^2$ ). This substitution procedure serves a similar purpose in the usual derivations of the stopping power by semiclassical methods.<sup>11</sup> The expression for the potential is then



FIG. 1. Potential distribution [Eq. (5)] associated with the polarization wake of a 400-keV proton traversing carbon ( $\hbar \omega_p = 25.0 \text{ eV}$ ). Distances are shown in units of  $\lambda = 2\pi a = 14.5$  Å.

$$\varphi(R, z - vt) = -(Ze/a) \int_0^\infty \sin(\zeta/a) [R^2 + (\hbar/mv)^2 + (\zeta + z - vt)^2]^{-1/2} d\zeta,$$
(5)

an example of which is shown plotted in Fig. 1.

This potential differs significantly from previous formulations (see, e.g., Ref. 2 and Neufeld and Ritchie<sup>13</sup>) in that it extends ahead of the projectile and that the derivative taken at the projectile position yields the stopping power (-dE/dz). From Eq. (5), we find

$$-dE/dz = Ze(\partial \varphi/\partial z)|_{z=vt,R=0} \approx \frac{4\pi n Z^2 e^4}{mv^2} \ln\left(\frac{1.123mv^2}{\hbar\omega_b}\right),\tag{6}$$

which is a close approximation to the usual Bethe formula that applies in this velocity range. Experiments concerned with the interactions of fast molecular-ion beams with thin foil targets



FIG. 2. (a) Experimental and (b) calculated joint distributions in energy and angle for protons emerging (near the beam direction) from an 85-Å carbon foil bombarded by 2.0-MeV HeH  $^{\circ}$  ions. In the experimentally determined distribution there about 10 000 proton counts at the maximum. In the calculation, the hydrogen ions are assumed to be singly charged both inside the target foil and after leaving it. The helium ions are assumed to be doubly charged inside the foil and 92% doubly and 8% singly charged after emergence from the foil (Ref. 14). The two single-parameter spectra shown in both (a) and (b) are the distributions for zero shift in energy and angle. They thus correspond to cuts through the center of each two-parameter distribution.

VOLUME 37, NUMBER 20

provide a sensitive test of the wake potential in the neighborhood of a charged projectile. In such interactions the separations between the nuclear constituents of each molecular cluster typically do not exceed 1 or 2 Å while the cluster is inside the foil. Figure 2 shows a comparison of the experimental and calculated results (joint distribution in energy and angle) for protons emerging from an 85-Å-thick carbon foil bombarded by 2-MeV HeH<sup>+</sup> ions. Details of the experiment are given elsewhere.<sup>9,10</sup> The calculated results come from a computer simulation of the experiment. The  $\alpha$ -particle and proton motions are computed under the assumption that they are influenced only by (a) the direct Coulomb repulsion and (b) wake forces corresponding to potentials of the form given in Eq. (5). The initial internuclear separations are taken to be distributed as a Gaussian with mean value  $\bar{r}_0 = 0.79$  Å, and width 0.35 Å [full width at half-maximum (FWHM)]. These values are consistent with the population of a few vibrational levels in the ground electronic state<sup>15</sup> of HeH<sup>+</sup>. The calculated results have been smeared in the angular coordinate by the measured multiple scattering whose angular distribution has a width of  $0.09^{\circ}$  (FWHM). The plasmon energy needed to evaluate Eq. (5) was obtained by matching Eq. (6) to the measured stopping power of carbon for 400-keV protons. This gave  $\hbar \omega_p = 25.0$  $eV_{\circ}$  The associated value of *n* is equivalent to 4.5 electrons per carbon atom. (By way of comparison, characteristic energy-loss measurements for 30-keV electrons in evaporated carbon foils yield  $\hbar \omega_{p} = 25.9 \text{ eV.}^{16}$ 

The fact that the calculation reproduces the experimental results so well (not only for those shown in Fig. 2, but also for a large variety of results obtained in other molecular-ion dissociation measurements<sup>9,10</sup>) is encouraging support for the validity of the wake model outlined here. The theory can readily be expanded to take into account damping of the polarization wake, binding of the target electrons, target density, quantum mechanical and fluctuation effects, etc. A publication in preparation<sup>10</sup> describes this expanded model and makes detailed comparisons with a wide range of experimental data.

\*Work performed under the auspices of the U.S. Energy Research and Development Administration.

†On leave of absence from the Weizmann Institute of Science, Rehovot, Israel.

<sup>1</sup>N. Bohr, K. Dan. Vidensk. Selsk., Mat.-Fys. Medd. <u>18</u>, No. 8 (1948).

<sup>2</sup>W. Brandt, A. Ratkowski, and R. H. Ritchie, Phys. Rev. Lett. 33, 1325 (1974).

<sup>3</sup>N. R. Arista and V. H. Ponce, J. Phys. C <u>8</u>, L188 (1975).

<sup>4</sup>J. W. Tape, W. M. Gibson, J. Remillieux, R. Laubert, and H. E. Wegner, Nucl. Instrum. Methods <u>132</u>, 75 (1976).

<sup>5</sup>W. Brandt and R. H. Ritchie, Nucl. Instrum. Methods 132, 43 (1976).

<sup>6</sup>V. N. Neelavathi, R. H. Ritchie, and W. Brandt, Phys. Rev. Lett. <u>33</u>, 302 (1976).

<sup>7</sup>M. M. Duncan and M. G. Menendez, Phys. Rev. A <u>13</u>, 566 (1976).

<sup>8</sup>D. S. Gemmell, J. Remillieux, J.-C. Poizat, M. J.

Gaillard, R. E. Holland, and Z. Vager, Phys. Rev.

Lett.  $\underline{34},$  1420 (1975), and Nucl. Instrum. Methods  $\underline{132},$  61 (1976).

<sup>9</sup>Z. Vager, D. S. Gemmell, and B. J. Zabransky, Phys. Phys. Rev. A 14, 638 (1976).

 $^{10}$ D. S. Gemmell, Z. Vager, and B. J. Zabransky, to be published.

<sup>11</sup>See, for example, J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975), 2nd ed.

<sup>12</sup>H. Raether, in *Springer Tracts in Modern Physics*, edited by G. Höhler (Springer, Berlin, 1965), Vol. 38, p. 84.

<sup>13</sup>J. Neufeld and R. H. Ritchie, Phys. Rev. <u>98</u>, 1632 (1955).

<sup>14</sup>The helium-ion charge-state ratios are taken from the work of J. C. Armstrong, J. V. Mullendore, W. R. Harris, and J. B. Marion, Proc. Phys. Soc., London <u>86</u>, 1283 (1965).

<sup>15</sup>W. Kolos and J. M. Peek, Chem. Phys. <u>12</u>, 381 (1976).

<sup>16</sup>R. E. Burge and D. L. Mosell, Philos. Mag. <u>18</u>, 251 (1968).