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Material dependence of low-velocity stopping powers

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Excitations of valence electrons determine the electronic stopping power of solids for atomic projectiles moving with velocities v_1 so that $v_1 \lesssim v_F$, where v_F is the Fermi velocity of the valence electron gas. Current data vary among elements according to their position in the periodic system in agreement with new theoretical developments. A comprehensive description emerges that permits predictions of the stopping power of solids and plasmas for low-velocity ions.

I. INTRODUCTION

The study of the stopping power of matter for slow ions is advancing rapidly now that new experimental techniques and fresh theoretical approaches are brought to bear in response to stimuli from radiation physics, material development, fusion research, and space exploration.[1,2] During the last 50 years, a body of experimental stopping power data of solids has accrued for ions of atomic number Z_1 moving at velocities $v_1 \gtrsim v_F$, where v_F is the Fermi velocity of the valence electrons in the medium of atomic number Z_2. Such data exhibit characteristic fluctuations if displayed as a function of Z_2.[3–5] These "Z_2 oscillations" diminish with increasing ion velocity toward a smooth Z_2 dependence at velocities approaching and exceeding that of the stopping power maximum. Only two sets of data appear to be extant for protons that reach down to $v_1 \simeq 0.2 v_F$ in gold[6] and to $v_1 \simeq 0.1 v_F$ in carbon.[7] We present strong evidence that the energy loss of low-velocity ions is determined by the valence states of the media in which the projectiles move and, hence, is related to the position of the target material in the periodic system. For the first time, a firmly based description emerges that permits comprehensive predictions of low-velocity energy losses.

For the present discussion, we characterize the valence electron gas of a medium by the effective number of electrons that participate in plasma excitations[8] as detected in the optical properties or in the spectrum of characteristic energy losses of electrons in transmission.[9] To this end, we use the one-electron radius r_s (in units of $a_0 = \hbar^2/me^2 = 1$ a.u.) in the valence electron gas of metals.[10] It is a dimensionless parameter given through the relation $4\pi r_s^3 a_0^3 n/3 = 1$ by the electron density n that determines the plasmon energy $\hbar(4\pi e^2 n/m)^{1/2} = \sqrt{3} r_s^{-3/2}$ (a.u.) and the Fermi velocity $v_F = (3\pi^2 n)^{1/3}\hbar/m = (9\pi/4)^{1/3} v_0 r_s^{-1}$, where $v_0 = e^2/\hbar$ (Table I). Low-velocity stopping powers of semiconductors and insulators can similarly be described in terms of a dielectric response that includes an energy gap.[11]

The material dependence of low-velocity stopping powers is analyzed in two steps. First, we show that variations of proton stopping powers from substance to substance depend, as surmised by others,[4,12] only on the valence electron density, i.e., on r_s as indeed current many-body theories predict. Second, we demonstrate that stopping powers of ions heavier than protons, $Z_1 > 1$, do not exhibit significant material dependences if taken relative to proton stopping powers, provided the stopping-power ratios are viewed as a function of the r_s-dependent *relative* velocities between the ions and the valence electrons.

As derived first by Fermi and Teller,[13] the stopping power of a medium for $Z_1 = 1$ particles, S_p, when $v_1 \ll v_F$ is proportional to v_1. We write it in the form

$$S_p = f(r_s) v_1 / v_F \quad . \tag{1}$$

The constant $f(r_s)$ is a function only of r_s. In the following we give $f(r_s)$ and v_F in atomic units; multiplication with $e^2/a_0^2 = 51.42$ eV/Å $= 5.142 \times 10^3$ MeV/cm converts $f(r_s)$ into practical units. In the Fermi-Teller approximation

$$f(r_s) = \frac{2}{3\pi} v_F \ln v_F \quad . \tag{2}$$

Ritchie[14,15] derived S_p in the frame of linear response theory with the result

$$f(r_s) = \frac{2}{3\pi} v_F \left[\ln(1 + \pi v_F) - \left[1 + \frac{1}{\pi v_F} \right]^{-1} \right] \quad . \tag{3}$$

In a somewhat different approximation, Lindhard and Winther[16] obtained

$$f(r_s) = \frac{2}{3\pi} v_F \left\{ \ln \left[\pi v_F \left[1 + \frac{2}{3\pi v_F} \right] \right. \right. - \left. \left. \frac{3\pi v_F - 1}{3\pi v_F + 2} \right\} \left[1 - \frac{1}{3\pi v_F} \right]^{-2} \quad . \tag{4}$$

TABLE I. Values of the one-electron radius r_s and the Fermi velocity v_F, in atomic units, chosen to characterize the effective electron density in the dynamic response of the valence electron gas in the substances discussed in this paper, from Ref. 10, except for Se, where Ref. 10 quotes $r_s = 1.84$.

Material	r_s	v_F	Material	r_s	v_F	Material	r_s	v_F
$_4$Be	1.78	1.08	$_{25}$Mn	1.71	1.12	$_{46}$Pd	1.51	1.27
$_5$B	1.83	1.05	$_{26}$Fe	2.07	0.93	$_{47}$Ag	1.53	1.25
$_6$C	1.66	1.16	$_{27}$Co	1.91	1.00	$_{50}$Sn	2.23	0.86
$_{13}$Al	2.12	0.91	$_{28}$Ni	1.80	1.07	$_{51}$Sb	2.06	0.93
$_{14}$Si	1.97	0.97	$_{29}$Cu	1.83	1.05	$_{55}$Cs	5.88	0.33
$_{22}$Ti	1.93	0.99	$_{32}$Ge	2.02	0.95	$_{79}$Au	1.49	1.29
$_{24}$Cr	1.55	1.24	$_{34}$Se	2.22	0.86	$_{83}$Bi	2.17	0.88

We denote $f(r_s)$ in Eq. (4) as f_{LW} and compare, in Fig. 1, other approximations relative to it. Curve I displays Eq. (2), and curve II Eq. (3) in multiples of Eq. (4) which appears as curve III. Curve IV results if $f(r_s)$ is calculated[11,16] in terms of the Lindhard dielectric function.[17] A recent formulation by Ferrell and Ritchie[15] treats the stopping power in terms of electron scattering off exponentially screened point charges. The result is shown as curve V. A new approach by Echenique, Nieminen, and Ritchi[18] replaces the heuristic exponential screening by a self-consistent treatment within the Hohenberg-Kohn density functional formalism,[19] with the result displayed as curve VI.

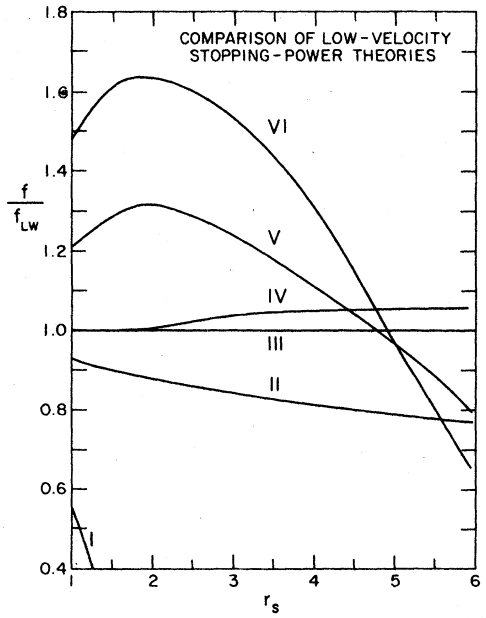

FIG. 1. Low-velocity stopping power theories, Eq. (1), in the form $f(r_s)/f_{LW}(r_s)$, where $f_{LW}(r_s)$ is Eq. (4), represented by line III at unity. The curves are I: Fermi-Teller theory, Eq. (2); II: linear response theory, Eq. (3); IV: general linear response theory, Refs. 11 and 16; V: scattering theory with exponential ion screening, Ref. 15; VI: scattering theory with self-consistent ion screening, Ref. 18.

We test these theories in Fig. 2 by plotting $S_p/f_{LW}(r_s)$ as a function of $v_1/v_F = 0.521 r_s v_1/v_0$. The data for 20 different solids, covering Z_2 from $_4$Be to $_{83}$Bi but only the fairly narrow r_s range from 1.49 ($_{79}$Au) to 2.23 ($_{50}$Sn), are displayed in Fig. 2.[20] Over this r_s range, the curves V(FR) and VI (ENR) in Fig. 1 remain essentially constant so that $f_{FR} \simeq 1.31 f_{LW}$ and $f_{ENR} \simeq 1.63 f_{LW}$. Indeed, when plotted as in Fig. 2 the proton data follow a universal trend without residual systematic material dependences within their scatter. Specifically, we could not isolate the effect of the energy gap in the valence band in reducing the stopping power of semiconductors.[11] The broken line in Fig. 2 represents the Lindhard-Winther (LW) linear response approximation,[16] Eq. (4). The line of dots and dashes describes the Ferrell-Ritchie (FR) scattering approximation,[15] given as curve V in Fig. 1. Only the nonlinear, self-consistent scattering calculation (curve VI in Fig. 1) by Echenique, Nieminen, and Ritchie[18] (ENR) drawn as a solid line in Fig. 2 is in satisfactory agreement with all measurements. This comparison leaves no room for an effective proton charge Z_p^* that is smaller than $Z_1 = 1$ (which would require that the solid line lies above the points in Fig. 2), as we deduced in Ref. 21 from a comparison of proton and heavy-ion stopping power data. A new

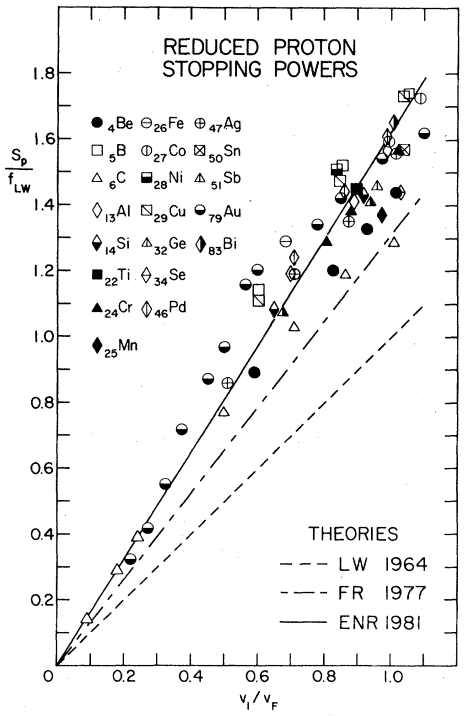

FIG. 2. Stopping powers for protons in the reduced form S/f_{LW} vs v_1/v_F, where f_{LW} is Eq. (4). Experimental data from Ref. 20. Theoretical lines depict low-velocity stopping powers, Eq. (1), in the form $S/f_{LW}=(f/f_{LW})(v_1/v_F)$. The constants f/f_{LW} are shown in Fig. 1. The broken line represents the Lindhard-Winther (LW) approximation, Eq. (4), curve III in Fig. 1, the line of dots and dashes the Ferrell-Ritchie (FR) approximation, curve V in Fig. 1, the solid line the Echenique-Nieminen-Ritchie (ENR) approximation, curve V in Fig. 1.

element, therefore, must be introduced in the analysis of heavy-ion data.

It is convenient to define an effective ion stopping-power charge Z_1^* and an effective charge fraction $\zeta \equiv Z_1^*/Z_1$ in terms of the stopping power $S \equiv -dE/dx$ of a medium,[21,22]

$$\zeta \equiv \frac{Z_1^*}{Z_1} = \frac{1}{Z_1}\left(\frac{S}{S_p}\right)^{1/2} , \tag{5}$$

where the stopping power for protons, S_p, is determined in the same material and at the same velocity as S. Effective ion charges occur because of the stripping of bound electrons from the ion when moving through a medium. Therefore, the relative velocity, v_r, between the ion moving with velocity v_1 and the velocities of the valence electrons in the medium is relevant for ζ. In a homogeneous uniform electron gas, v_r becomes[23]

$$v_r(v_1,r_s) = \begin{cases} \frac{3}{4}v_F\left(1+\frac{2}{3}\frac{v_1^2}{v_F^2}-\frac{1}{15}\frac{v_1^4}{v_F^4}\right), & \text{for } v_1 \leqslant v_F \\ v_1\left(1+\frac{1}{5}\frac{v_F^2}{v_1^2}\right), & \text{for } v_1 \geqslant v_F \end{cases} . \tag{6}$$

On the average, electrons with orbital velocities larger than v_r remain bound to the moving ion. If, at a given v_r the ion carries N electrons, the ionic charge is $Q=Z_1-N$, and the degree of ionization or, for short, the ionization is

$$q = \frac{Q}{Z_1} = 1 - \frac{N}{Z_1} . \tag{7}$$

A comprehensive function for the ionization $q(y_r)$ in the statistical approximation in terms of the reduced velocity variable $y_r = v_r/Z_1^{2/3}v_0$ was derived and tabulated in Ref. 21; it is displayed as the solid curve in Fig. 3.[24]

To compare with experiment, one needs to know the relation between ζ, Eq. (5), and q. The stopping electrons in the medium encounter a fully screened ion of charge Q only in distant collisions. In close collisions, the electrons penetrate into the screening cloud bound to the ion. One expects on general grounds, therefore, that $\zeta > q$. To pursue this argument, we have calculated the relation between ζ and q in linear response theory,[2,25] with the result that, at low velocities,

$$\zeta(y_r) = q(y_r) + C(r_s)[1-q(y_r)]\ln\left[1+\left(\frac{4\Lambda(y_r)}{r_s}\right)^2\right] . \tag{8}$$

The constant $C(r_s)\simeq 0.5$ is a weakly dependent function of r_s in the range of interest.[2] The screening radius of the coterie of N electrons moving with the projectile of ionization q in a statistical approximation is given by

$$\Lambda(y_r) = \frac{2c_2[1-q(y_r)]^{2/3}a_0}{Z_1^{1/3}\{1-c_1[1-q(y_r)]\}} \tag{9}$$

with variational constants $c_1=0.240$ and $c_2=0.143$. The second term in Eq. (8) is significant only for slow light ions and becomes small for heavy ions, $Z_1>10$, for media with large r_s, and in all cases at velocities so that $y_r \gtrsim 1$. To compare Eq. (5) with theory, we have multiplied the experimental ratios $Z_1^{-1}(S/S_p)^{1/2}$ with q/ζ calculated according to Eq. (8) at the same v_r. This factor accounts for the trends that were found earlier[22] empirically and attributed then to an effective proton charge $Z_p^*<1$. The inference of an effective proton charge is not borne out by the evidence presented in Fig. 2.

Figure 3 displays data on low-velocity stopping

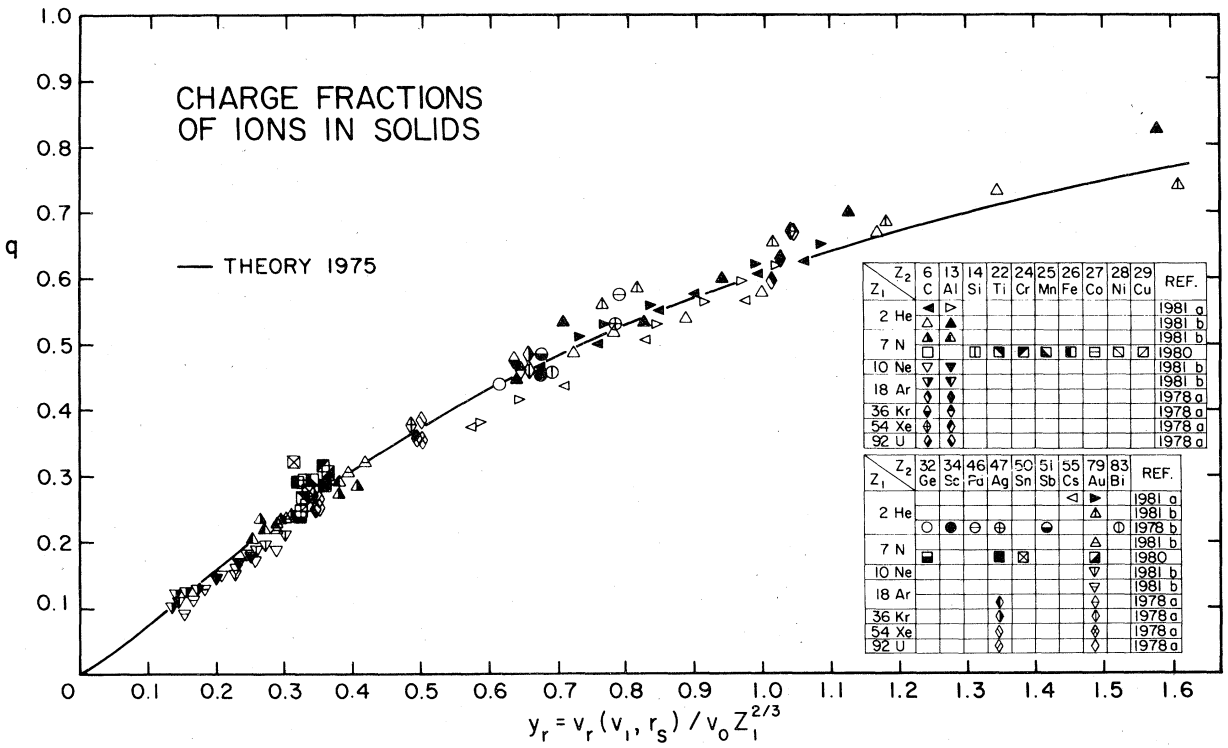

FIG. 3. Charge fraction q of ions of atomic number Z_1 moving at reduced velocities y_r with regard to the valence electrons in solids of atomic number Z_2 and r_s values listed in Table I. Theory curve from Ref. 23 with stripping parameter $b = 1.33$. Data were taken from: 1978a: Ref. 27; 1978b: Ref. 28; 1980: Ref. 5; 1981a: Ref. 23; 1981b: Ref. 26.

powers[5,23,26–28] which have been reported for $Z_1 > 1$ since the appearance of Ref. 22, with proton stopping powers from Refs. 23, 27, and 29, in the form $(q/\zeta)Z_1^{-1}(S/S_p)^{1/2}$. Only the data points for $^4_2$He and $^2_1$H ions from Ref. 23 were obtained *ceteris paribus* as intended by Eq. (5). Still, the data in Fig. 3 resolve no residual systematic trends even though they comprise measurements performed with ions ranging from $_2$He to $_{92}$U in stopping media from $_6$C to $_{83}$Bi or from $r_s = 1.49(_{79}\text{Au})$ to $r_s = 5.88(_{55}\text{Cs})$ (cf. Table I). The locus of the points forms a smooth curve within the scatter of the data. This experimental curve coincides with the Brandt theory[21] of charge fractions through velocity stripping in the Thomas-Fermi approximation.

Significant projectile- and material-dependent fine structures, smaller than the relative uncertainties in the data collated in Fig. 3, emerge in precision experiments with different ions on the same material under otherwise identical conditions.[30] These "Z_1 oscillations" are of the order of 20% in ζ or less. They signify the shell structure of moving ions which is not contained in the statistical model of the atom on which the theory of q and ζ as presented here is based. Conversely, the large "Z_2 oscillations" in the stopping powers of different materials for the same slow ions are the topic of the present paper. They apparently are not linked to the ionization of the projectile, as Fig. 3 shows; they are caused by the fact that low-velocity stopping powers of solids are determined by the valence states of their atoms, as Fig. 2 shows, and, hence, are linked to their place in the periodic system.

In summary, low-velocity stopping powers of solids of given r_s for all ions of atomic number Z_1 and velocities $v_1 < v_F(r_s)$ can be predicted comprehensively by the formula

$$S = \zeta^2 Z_1^2 f(r_s) v_1 / v_F(r_s) \quad , \tag{10}$$

where ζ is related by Eq. (8) to the ionization $q(y_r)$ that is shown in Fig. 3 and tabulated in Ref. 21; the function $f(r_s)$ is calculated within the density-functional formalism[18] and, in conjunction with Eq. (4), is displayed in Fig. 1 as curve VI. Inasmuch as ζ approaches a constant value only when $v_1/v_F \ll 1$ and is a monotonically rising function of v_1/v_F otherwise, the stopping powers for $Z_1 > 1$ increase faster than linearly with v_1/v_F in the low-velocity range $v_1/v_F \gtrsim 0.5$ explored so far with heavy ions. Residual subtle differences between the stopping powers of materials for various ions emerge in high-precision measurements performed under strictly controlled equal experimental conditions, which merit further study.

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