Effective-charge theory and the electronic stopping power of solids

B. S. Yarlagadda and J. E. Robinson
Argonne National Laboratory, Argonne, Illinois 60439

Werner Brandt
*Department of Physics, New York University, New York, New York 10003**
and Argonne National Laboratory, Argonne, Illinois 60439

(Received 27 December 1977)

Electronic stopping powers S of solids for penetrating ions are analyzed on the basis of effective-charge theory, and comprehensive comparisons are made to available data for random stopping. The effective projectile-ion charges $Z_1^* e$, extracted from the data agree to within experimental uncertainties with those calculated in a statistical model, for projectile atomic number ranging from $Z_1 = 1$ to $Z_1 = 92$ and for projectile velocity $v_1 \gtrsim v_0 \equiv e^2/\hbar$. The rise of Z_1^* with v_1 fully accounts for an often-quoted apparent deviation of heavy-ion stopping power from the behavior expected in the limit $v_1 \to 0$. The Bloch and the Z_1^3 corrections to the usual formula for S are calculated and found to make no appreciable contribution to presently available data, save possibly to one bromine datum. When $v_0 \lesssim v_1 \lesssim 3v_0$ the analysis requires, and provides, an empirical velocity-dependent proton effective charge $Z_p^* e$. A theoretical account of Z_p^* is given in terms of velocity and energy criteria for electron stripping. Thomas-Fermi densities for heavy ions are used to calculate Z_1^*. Our results lead to an interpolation linear in v_1 for the range $0 \leq v_1 \lesssim v_0$ which gives satisfactory values for S in this low-velocity regime.

I. INTRODUCTION

Over the past half century a fairly complete physical understanding has developed of the electronic stopping power S of matter, i.e., the kinetic-energy loss per unit path length by ions to electronic excitations during penetration of matter. At high ion velocities, the theories of Bethe[1] and of Bloch[2] provide a quantitative account. At low ion velocities, Fermi and Teller[3] have shown on very general grounds that S must be linearly proportional to the ion velocity v_1. The proportionality constant can be estimated by various methods.[4,5] At intermediate ion velocities one has recourse to effective-ion-charge models, first introduced by Bohr[6] and by Lamb.[7] Brandt[8] has given an effective-charge theory that successfully summarizes a large body of stopping-power data for heavy ions. Extensive discussions of the field are available,[9-13] as are extensive compilations of interpolated stopping powers.[14,15]

The present study was stimulated by some recent data on heavy-ion stopping in solids, which were claimed to call into question the proportionality to v_1 expected in the low-velocity limit.[16] If in fact so, such evidence would pose very disturbing theoretical questions, and would imply important practical consequences for radiation-damage calculations. However, these data do not pertain to the low-velocity limit. They were taken in an intermediate velocity range where the effective projectile-ion charge increases with velocity. We show in the following that when this is taken into account the putative discrepancy is resolved.[17] Brice has also addressed this "discrepancy" and concluded that these data conform to his three-parameter semiempirical formulas.[16]

In the course of this investigation it became apparent that effective-charge theory provides a comprehensive description of electronic stopping power at all velocities from the high values of the Bethe limit down to those approaching the Fermi-Teller regime and for all projectile-target combinations, provided that the proton stopping power in the target is known. In scrutinizing available data,[19-49] we find that for ion velocities greater than thrice the Bohr velocity $v_0 = e^2/\hbar$ the effective projectile charge $Z_1^* e$ calculated using a velocity criterion for electron stripping[8] agrees with experiment. The leading corrections to the Z_1^{*2}-proportional energy loss formula, which are proportional to Z_1^{*3} and Z_1^{*4}, were included. It is then shown that when allowance is made for an empirical effective-proton charge $Z_p^* e$, agreement between theory and experiment extends to $v_1 \gtrsim v_0$. Both a velocity criterion and an energy-stability criterion for stripping are considered, and a theoretical account of the effective proton charge for stopping power is given. Our results lead to a simple interpolation scheme for electronic stopping powers in the range $0 \leq v_1 \lesssim v_0$.

II. ANALYSIS AND COMPARISON TO EXPERIMENT USING A VELOCITY-STRIPPING CRITERION

Effective-charge theory asserts that the electronic stopping power in a target of atomic num-

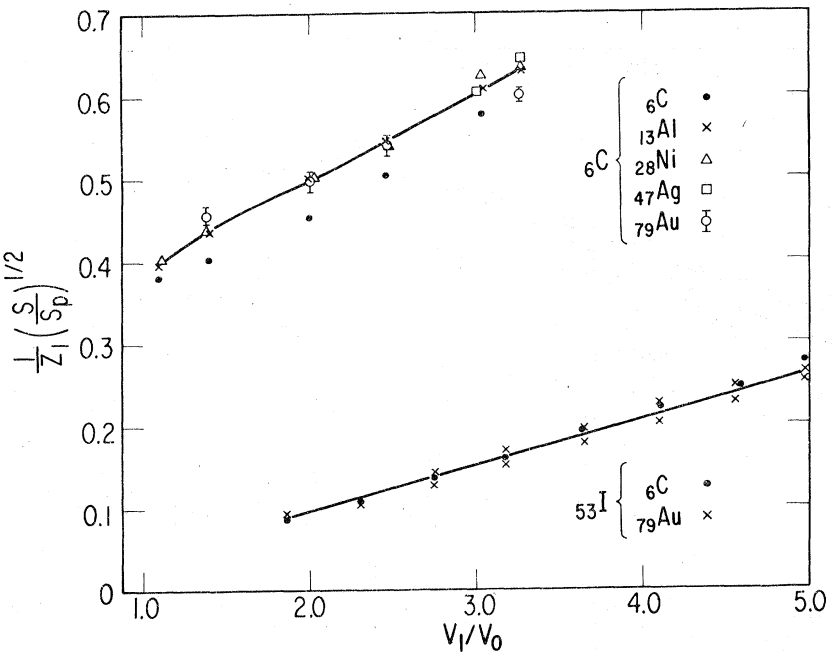

FIG. 1. Effective charge in various targets. Data references: carbon projectiles, Refs. 20, 33; iodine projectiles, Refs. 27–30. Proton stopping powers were taken from Refs. 21, 25, 40–49. The approximate target independence exhibited is representative of that for all published data.

ber Z_2 for an ion having charge $Z_1^* e$ and velocity v_1 can be written

$$S(Z_1, Z_2; v_1) = [Z_1^*(v_1)e\,]^2 S_0(Z_2; v_1), \tag{2.1}$$

when v_1 is greater than the velocity at which the stopping power for protons in the same target has a maximum.[8] S_0 is then the stopping power per unit charge taken in the limit of vanishing charge. At velocities such that the effective charge number Z_1^* is equal to the projectile atomic number Z_1, Eq. (2.1) is simply the Bethe approximation.[1] When higher-order contributions to the stopping cross section for a specified projectile charge need be retained, the right-hand side of Eq. (2.1) has additional terms to which we shall come presently. According to Eq. (2.1) we can write the basic scaling relation of effective charge theory as

$$\left(\frac{S(Z_1, Z_2; v_1)}{S_p(Z_2; v_1)}\right)^2 = \left(\frac{Z_1^*(v_1)}{Z_p^*(v_1)}\right)^2, \tag{2.2}$$

where $S_p(Z_2; v_1) \equiv S(1, Z_2; v_1)$ and $Z_p^*(v_1)e$ are, respectively, the proton stopping power and effective charge in the same target.

Rearranging Eq. (2.2) as

$$\left(\frac{1^2}{Z_1^2}\,\frac{S(Z_1, Z_2; v_1)}{S_p(Z_2; v_1)}\right)^{1/2} = \frac{Z_1^*(v_1)/Z_1}{Z_p^*(v_1)/1}, \tag{2.3}$$

and plotting experimental values of the left-hand side of Eq. (2.3) as a function of v_1 reveals that the right-hand side is insensitive to the target material within an uncertainty of about 10%, as is shown in Fig. 1 for two representative examples. Accordingly, the effective charge numbers Z_1^* and Z_p^* are taken to be independent of the target. In the following, we shall refer to Z_1^* as the effective charge number or the effective charge, which are the same in atomic units with $e = 1$. The data shown in Fig. 1 and in subsequent graphs are based on scrutiny of all measurements available to us.[20–49] As is well known, stopping-power data can differ by as much as 20%, particularly in the velocity range of the proton stopping-power maximum. When representative numbers are needed, we balance such data to provide them.

In Fig. 2 we plot the left-hand side of Eq. (2.3) using all such data as a function of the reduced ion velocity $(v_1/v_0 Z_1^{2/3})$. If $Z_p^*(v_1)$ were unity this would yield $Z_1^*(v_1)/Z_1$. The effective-charge fraction Z_1^*/Z_1 according to Brandt[8] is shown as the solid line in Fig. 2 and tabulated in Table I. The velocity criterion for electron stripping, $v(r) \leq v_1$, was used, with the "local-orbital velocity" at r in the projectile taken to be $v(r) = b v_F(r)$. The local Fermi velocity, $v_F(r) = [3\pi^2 \rho(r)\,]^{1/3}$ in atomic units, was taken to be given by the Thomas-Fermi (TF) approximation for the electronic density $\rho(r)$ of a neutral atom, and the parameter value $b = 1.26$ was chosen. At high velocities ($v_1 \gtrsim 3v_0$) the data are well represented by the theoretical curve for $b = 1.26$. The parameter value $b = 1.33$ gives a better fit to the heavy-ion data at low $v_1/v_0 Z_1^{2/3}$ values.[50] When $v_1 \lesssim 3v_0$, the light ion plots tend to deviate upward from the $b = 1.26$ curve as v_1 is reduced. The available heavy-ion data correspond to ion

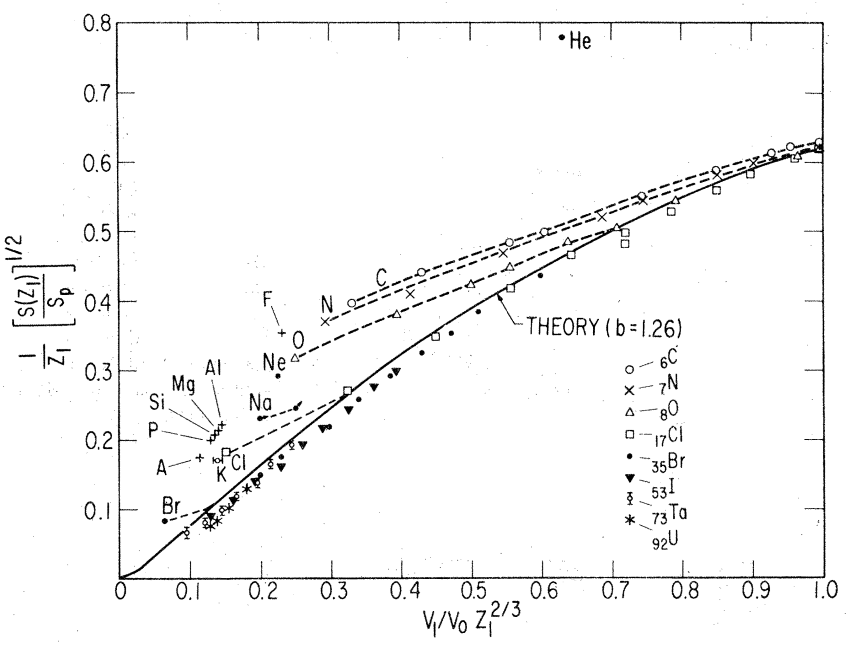

FIG. 2. Empirical effective-charge fractions obtained from data using Eq. (2.3) with $Z_p^*=1$. The theoretical curve calculated by the velocity stripping criterion (Ref. 8) with $b=1.26$ is adequate at high velocities for lighter projectiles, say $Z_1 \leq 17$, while $b=1.33$ is more satisfactory for heavier projectiles, e.g., for Br. Data references: He, Refs. 22, 25, 37, and 41; C, Refs. 20 and 33; N, Refs. 21–25, 33, and 11; O, Refs. 20 and 32–35; Ne, Ref. 38; K, Ref. 38; Cl, Ref. 32; Br, Ref. 27, 28, 30 and 39; I Refs. 27–30; Ta, Ref. 31; U, Refs. 16 and 27. Proton stopping powers, Refs. 21, 25, and 40–49. Some data used in the analysis have been omitted from the figure for clarity of presentation.

TABLE I. Fractional effective charge by Brandt's procedure. Calculated as discussed in the text and taken from Ref. 8. In this model Z_1^*/Z_1 is a universal function of $(1/b)(v_1/v_0 Z_1^{2/3})$.

	$v_1/v_0 Z_1^{2/3}$	
Z_1^*/Z_1	$b=1.26$	$b=1.33$
0.012	0.023	0.024
0.034	0.050	0.053
0.070	0.093	0.098
0.101	0.129	0.136
0.155	0.189	0.100
0.197	0.238	0 .251
0.256	0.312	0.330
0.305	0.375	0 .396
0.344	0.432	0.456
0.391	0.504	0.532
0.447	0.600	0.633
0.480	0.660	0.697
0.515	0.731	0.771
0.554	0.816	0.862
0.598	0.924	0.975
0.645	1.057	1.116
0.698	1.233	1.302
0.756	1.474	1.556
0.819	1.824	1.928
0.852	2.092	2.208
0.886	2.432	2.567
0.919	2.936	3.098
0.952	3.767	3.977
0.981	5.620	5.932

velocities $v_1 \gtrsim 2.5 v_0$, but we conjecture that similar low-velocity departures from Brandt's curve for $b=1.33$ would be found for heavy ions, as is signaled by an incipient trend of the data for chlorine, potassium, and bromine projectiles.

To explore the origin of this trend we have compared the TF curve for the charge fraction with calculations based on the Lenz-Jensen (LJ) approximation[51] for the electronic density and the same velocity criterion, for $b=1$. The results, curves a(TF) and b(LJ) in Fig. 3, are virtually the same, and rule out the possibility that the upward deviations for light ions in Fig. 2 could be eliminated by using a more accurate electron density than that of the TF atom.

We have calculated the contributions to the stopping power due to the Bloch[2] and Z_1^3 terms[53] for heavy ions and for the proton in the form of a correction factor C such that Eq. (2.3) is supplanted by

$$\frac{1}{C}\left(\frac{1^2}{Z_1^2}\frac{S(Z_1,Z_2;v_1)}{S_p(Z_2;v_1)}\right)^{1/2} = \frac{Z_1^*(v_1)/Z_1}{Z_p^*(v_1)/1} . \qquad (2.4)$$

We have

$$C = \left(\frac{1+(1/L_0)[Z_1^* L_1 + \Psi(Z_1^* e^2/\hbar v_1)]}{1+(1/L_0)[L_1+\Psi(e^2/\hbar v_1)]}\right)^{1/2}, \qquad (2.5)$$

where $L = L_0 + Z_1^* L_1$ is the stopping number per target electron and Ψ is the Bloch correction which

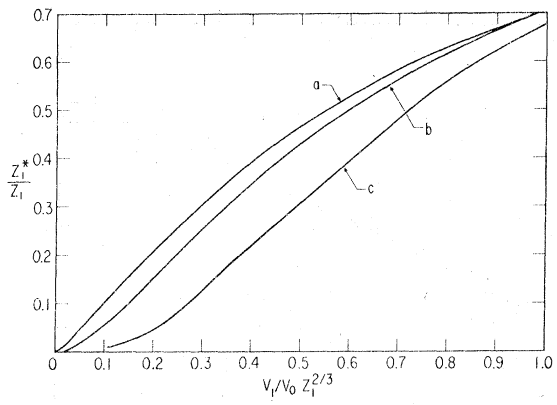

FIG. 3. Effective charge in different models, calculated using the velocity stripping criterion (Ref. 8) with $b=1$ and (a) Thomas-Fermi charge-density profile, and (b) a Lenz-Jensen profile (Ref. 51). (c) Represents the Knipp and Teller (Ref. 4) calculation using a Thomas-Fermi profile and stripping criterion differing from that used for (a) and (b) (Ref. 52).

interpolates between the quantum-mechanical limit ($Z_1^*/v_1 \ll 1$) and the classical limit ($Z_1^*/v_1 \gg 1$) of stopping-power theory. In terms of the digamma function $\psi(z)=\Gamma'(z)/\Gamma(z)$, $\Psi(x)=\psi(1)-\mathrm{Re}\psi(1+ix)$. In the high-velocity limit, L_0 becomes $\ln(2mv_1^2/I_0)$, I_0 being the average excitation energy of the target, and L_1 is the coefficient of the so-called Z_1^3 effect.

No experimental point in Fig. 2 deviates significantly from Brandt's curve unless $v_1 \lesssim 3v_0$, therefore for numerical estimates, we evaluate upper limits of C, Eq. (2.5), in the low-velocity domain where target ion cores do not contribute to stopping, and L_0 can be approximated by $\ln(2mv_1^2/\hbar\omega_p)$. Here, ω_p is the resonance (plasmon) frequency of the target valence electrons of density $3/4\pi r_s^3$ with r_s in atomic units. For the typical value $r_s=2$, we have $\hbar\omega_p=0.612$ a.u. and

$$L_1=(e^2\omega_p/mv_1^2)I(\hbar\omega_p/2mv_1^2)$$
$$=0.612(v_0/v_1)^3 I[0.306(v_0/v_1)^2]. \qquad (2.6)$$

The function $I(x)$ is given in Ref. 53, and we have here chosen $\hbar/2mv_1$ for the impact parameter cutoff a_ω of Ref. 53.

We find considerable cancellation between the Z_1^3 and the Bloch contributions, in that they happen to be comparable in magnitude but opposite in sign for all ions. Values of C obtained from Eqs. (2.5) and (2.6) are overestimates at $v_1<3v_0$ for the heavier projectiles, say for $Z_1>17$. For such Z_1 and v_1, the alternative choice $(\hbar/2m\omega_p)^{1/2}$ of impact parameter cutoff decreases C by roughly 20%, and, moreover, $Z_1{}^*L_1$ is becoming large enough that the perturbation expansion of L should include

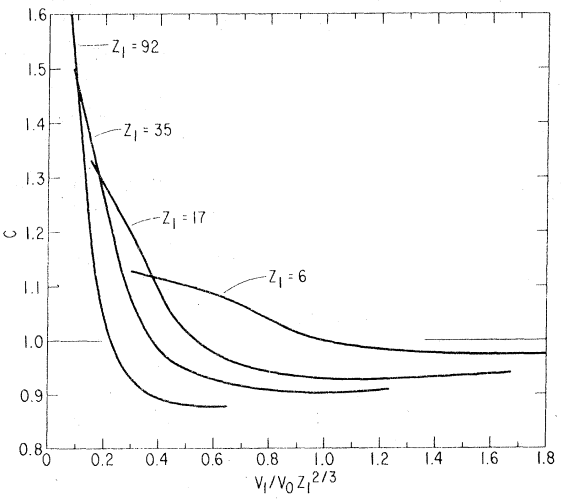

FIG. 4. Z_1^{*3} and Bloch stopping-power corrections for ions of atomic number Z_1, in terms of the correction factor C defined by Eq. (2.5) as discussed in the text.

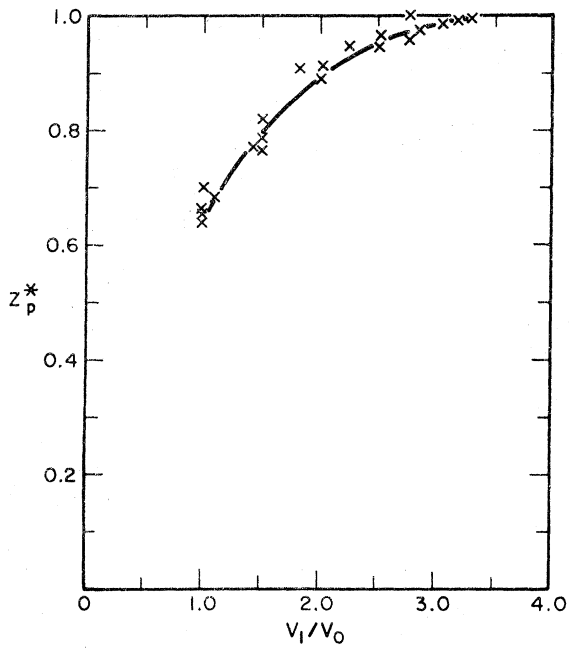

FIG. 5. Empirical effective proton charge for stopping power. Points are Z_p^* values obtained using theoretical Z_1^*/Z_1 and experimental S in Eq. (2.4). Averages over targets, e.g., the solid lines in Fig. 1, were used for S, so that each point represents several data. Only values deduced from light projectile S data are shown in the plot, since heavy-ion data are available only for velocities too high to give significant deviations from theory for $Z_p^*=1$, as Fig. 2 shows. The solid line is drawn through the points to aid the eye; smooth values of Z_p^* are given in Table II.

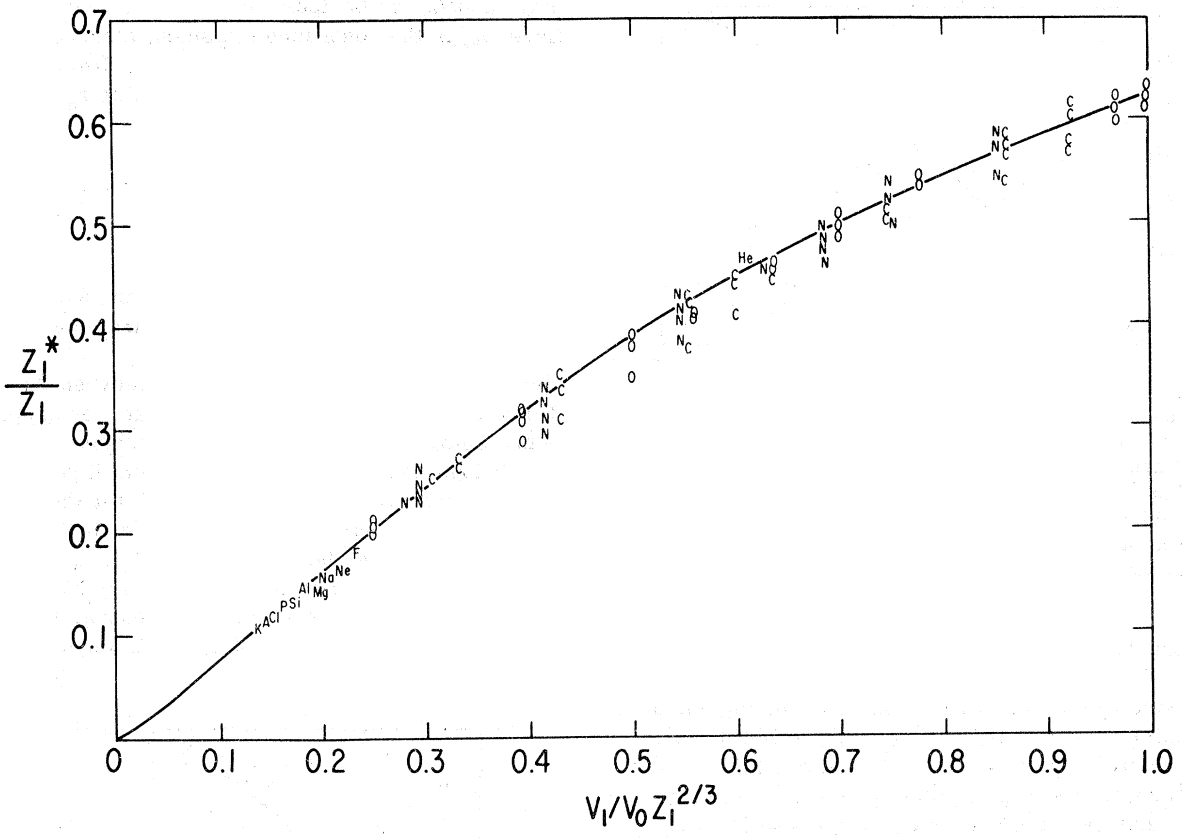

FIG. 6. Effective ion charges obtained using the empirical Z_p^*. Comparison to the $b = 1.26$ curve of Fig. 2 with points obtained from light-ion experimental data by using Eq. (2.4) and the average $Z_p^*(v_1)$ given by the solid line in Fig. 5. Target dependence for a given projectile is indicated by, e.g., several points at the same velocity. The heavy-ion data shown in Fig. 2 remain unchanged because, for them, $Z_p^* \approx 1$.

higher-order terms which are expected to reduce the correction to L_0. In Fig. 4 we show representative results of the calculation using Eq. (2.5). Examination of Fig. 4 in conjunction with Fig. 2 shows that the experimental points for the lighter ions are not brought significantly closer to the theoretical curve, and that the experimental points for heavy ions given by available data at $v_1 \lesssim 3v_0$ remain unchanged. Only the lowest-velocity datum point for Br, at $v_1 = 0.856v_0$, is affected significantly in that division by C brings it close to the solid curve of Fig. 2 (but still above a curve for $b = 1.33$). In this sense the rise of the Br plot at the lowest velocity measured can be taken to signal a distinguishable Z_1^3 contribution. The results summarized in Fig. 4 indicate that this is the *only* available heavy-ion datum which can be so interpreted.

We extract empirical values for $Z_p^*(v_1)$ by using Eq. (2.4) and the theoretical charge fraction $Z_1^*(v_1)/Z_1$, and exhibit the result in Fig. 5. An effective proton charge $Z_p^*(v_1)$ emerges which is independent of both the heavier projectiles and the target materials to which the data pertain. The solid curve in Fig. 5, which represents the locus of the data exhibited, approximates a continuation of the theoretical curve of Fig. 3 to higher arguments for $Z_1 = 1$. In Fig. 6 we have replotted the experiment-

TABLE II. Empirical proton effective charge. Values of the smoothed $Z_p^*(v_1)$ data represented by the solid line in Fig. 5.

V_1/V_0	Z_p^*
1.0	0.65
1.25	0.73
1.50	0.80
1.75	0.85
2.00	0.90
2.25	0.93
2.50	0.95
2.75	0.97
3.00	1.00
3.25	1.00

al data according to Eq. (2.4) using the mean values of $Z_p^*(v_1)$ given by the solid line of Fig. 5 and listed in Table II. They follow the theoretical curve for $Z_1^*(v_1)/Z_1$ within the uncertainty of the data.

We conclude that, when combined with Fig. 5, all available experimental data for solid targets are brought into accord with the theoretical curve at all velocites $v_1 \gtrsim v_0$ for Z_1 ranging from 2 to 92.

III. PROTON SCREENING AND STRIPPING CRITERIA

We must now test whether the empirical Z_p^* is physically reasonable and whether its values can be estimated within the framework of effective-charge theory. In doing so it is necessary to take note of a few points which relate specifically to condensed-matter targets or to protons. Most commonly, discussions of effective charges have been couched in terms appropriate to gas targets, and Z_1^* interpreted as a steady-state average over a large number of discrete capture-loss processes.[9] Moreover, the use of a statistical model for an ion in isolation is suspect for light ions, let alone a hydrogen ion. In a solid, however, the screening corresponding to that due to the highest occupied orbitals of an isolated projectile is built up out of a macroscopic number of target electron wave functions each of which has microscopic amplitude at the projectile. In consequence, in a *solid* target, Z_1^* can vary continuously with small fluctuations, and statistical models are well justified even for the screened proton. Of course, a model useful and adequate for stopping power need not apply to other phenomena. In any bulk metal, if we were to include all of the screening charge density which accompanies a moving ion, we would always find $Z_1^*=0$, in that perfect screening at large distances is built into the dielectric response function. We here deal with a "stopping power Z_1^*" as perceived by the medium over distances comparable to the adiabatic screening length v_1/ω_p.

A. Stripping criteria

Velocity criteria for stripping stem ultimately from Bohr's discussion[6] of effective charge in terms of the v_1 dependence of capture and loss cross sections. They can be written in the form that projectile electrons of orbital velocity v such that $v<v_1$ are considered stripped, and the primary question is what to use as an electron "orbital velocity" v. In ordinary TF approximation, with $v(r)=bv_F(r)$, such a criterion can be rewritten in the form of an energy-stability condition. The parameter b then has the appearance of correcting the TF ion energy for correlation effects. Lamb's approach[7] primarily provides an energy criterion. We shall now sketch a heuristic derivation of such a criterion and its relation to a velocity criterion.

We consider an ion of atomic number Z_1 moving with a constant velocity v_1 in the bulk of a solid and take the entire system to be in its ground state for given v_1 and fixed total number of electrons. We take N_1 electrons moving with the ion, and seek a condition on N_1 for the total system electronic energy to be a minimum. It is conceptually important to remember that in the rest frame of the target solid the energy of each projectile-ion electron increases as v_1^2. Any level in a static ion, however deep, eventually rises with increasing v_1 to the lowest unoccupied level of the target medium, i.e., the Fermi level in a solid. Projectile electrons can then simply fall off into the medium provided that there is a finite transition-matrix element.

Examination of those contributions to the total electronic energy of the system which change with N_1 reveals that for $v_1>v_0$ the target solid may be treated as merely a source and sink for electrons at the Fermi level.[54] It is then sufficient to retain only the total projectile ion energy written as

$$\tfrac{1}{2}(M_1+N_1m)v_1^2+E(Z_1,N_1),$$

where M_1 and m are the nuclear and electron masses, respectively. $E(Z_1,N_1)$ is the ion's ground ground-state energy in its center of mass system. The steady-state condition is then

$$\tfrac{1}{2}mv_1^2=-\frac{\partial E(Z_1,N_1)}{\partial N_1}>0, \tag{3.1}$$

which applies to any target medium with the stipulation that differences rather than differentials are used if the electron energy and number are discrete. For discrete N_1, $-\partial E(Z_1,N_1)/\partial N_1$ is just the ionization potential at N_1 and Eq. (3.1) becomes Lamb's stripping criterion.[7,9]

In a one-electron approximation, Koopmans's theorem[55] assures us that $\partial E/\partial N_1$ is the orbital energy of the highest-lying electron on the ion. In turn, this orbital energy is equal to the self consistent potential energy $U(r)$ evaluated at the classical turning point $r\equiv r_1$, where the kinetic-energy density vanishes. Therefore, we obtain the energy-stability condition

$$\tfrac{1}{2}mv_1^2+U(r_1)=0. \tag{3.2}$$

An electron for which the left-hand side of Eq. (3.2) is positive is to be considered stripped. In a statistical model we introduce the local velocity

$v(\vec{R}+\vec{r})$ by writing $\frac{1}{2}mv^2(\vec{R}+\vec{r})+U(\vec{R}+\vec{r})$ for the energy of an electron at an arbitrary space point $\vec{R}+\vec{r}$ in the system, where $\vec{R}$ is the projectile-ion center of mass. For definiteness we take the target Fermi level as the zero of energy. Since the Fermi level of the system is not shifted from that of the target by the presence of a single projectile, for an electron in the highest occupied level of the system we have

$$\tfrac{1}{2}mv_F^2(\vec{R}+\vec{r})+U(\vec{R}+\vec{r})=0,$$

which defines a local Fermi velocity v_F. Near the moving ion the self-consistent potential U is dominated by the strong and effectively spherical field of the partially stripped projectile, independent of the position $\vec{R}$ of the ion in the system. In consequence, near the projectile we may write

$$\tfrac{1}{2}mv_F^2(r)+U(r)=0 \tag{3.3}$$

and interpret $v_F(r)$ as the local Fermi velocity "in the ion." We take the classical turning point r_1 for an electron in the ion and at the Fermi level of the system as a natural choice for the effective ion radius and $v_F(r_1)$ as the relevant "orbital velocity." Comparison of Eq. (3.2) with Eq. (3.3) for $r=r_1$ then shows that the energy criterion coincides with the velocity criterion for $b=1$. Because we have concentrated on the ground state of the system, this connection takes no account of electron transfers to states above the Fermi level of the solid. Inclusion of such processes requires parameter values $b>1$.

B. Screening charge density

The screening of a static proton in metals has been studied in quantitative detail,[56] and these studies fully justify use here of a local-density approximation and a statistical model. Accurate static-charge-density profiles are close to those of hydrogenic 1s functions at all points inside the first node of the Friedel oscillations which occurs occurs close to the classical turning point.[56,57] We use charge-density profiles appropriate to a static proton also for a moving proton. Since Z_1^* is given by Z_1 minus an integral over the screening cloud, an accurate account of shape changes due to the finite velocity[58] v_1 is not crucial. As in the calculations of $Z_1^*(v_1)/Z_1$ of Sec. II, we shall use neutral-atom charge densities truncated according to a stripping criterion.

C. Z_p^* estimates

With a 1s screening charge-density profile truncated at radius r_1 we calculate Z_p^* as a function of

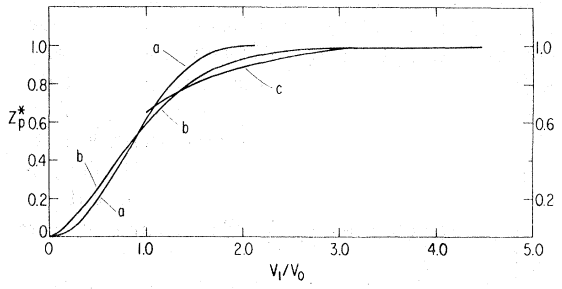

FIG. 7. Effective charge of screened proton. $Z_p^*(v_1)$ calculated as discussed in the text using (a) the velocity stripping criterion, and (b) the energetic stability criterion. The empirical Z_p^* of Fig. 5 is shown as (c).

r_1 and relate r_1 to v_1 through the stripping condition to obtain $Z_p^*(v_1)$. When we set $b=1$, as we would for a hydrogen atom, the Z_p^* obtained using the velocity criterion (Fig. 7, curve a) rises significantly more rapidly with v_1 than do the empirical values (curve c). The overall differences in slope and value are not materially reduced by varying the density profile or the value of b, and appear to be qualitative. Since such a truncated ion has no charge at $r>r_1$, the potential-energy criterion, Eq. (3.2), may be written

$$\tfrac{1}{2}mv_1^2=Z_1^*(r_1)e^2/r_1. \tag{3.4}$$

Use of Eq. (3.4) gives a $Z_p^*(v_1)$ (Fig. 7, curve b) which lies within the spread of the data about the empirical curve. The small systematic overestimate of Z_p^* is to be expected, since an energy-stability criterion assumes all energetically allowed transitions to proceed with probability one.

The two criteria give different results because a local density appropriate to a *neutral* atom was used to determine $v_F(r_1)$ for the velocity criterion. The potential which is consistent with that local density is the potential at $r=r_1$ in a neutral atom, and differs from the ion potential of Eq. (3.4) by an outer screening shift which for the proton can be substantial. For example, the electron potential energy at r_1 is deeper in the ion than in the neutral atom by about 9 eV at $v_1=v_0$ and by about 15 eV at $v_1=1.5\,v_0$.

Equation (3.4) is a Hartree approximation which neglects exchange-correlation effects, but these become appreciable only at large distances,[59] where the screening charge density oscillates between positive and negative with a period on the scale of interatomic spacings. Indeed, our results suggest that the contributions of this oscillating tail cancel sufficiently to be neglected as compared to the central region insofar as stopping power is concerned. The greater accuracy of the energy-stability criterion for Z_p^* as compared to the velo-

city criterion with $b=1$ is analogous to the familiar experience that, in any order of perturbation theory, energies are more accurate than wave functions or densities.

IV. SELF-CONSISTENT EFFECTIVE CHARGE BY THE POTENTIAL-ENERGY CRITERION

All the previous calculations are based on truncated neutral-atom electronic density for the projectile. The effective-projectile charge is obtained by stripping the projectile according to a velocity or potential-energy criterion. There will be redistributions of charge as the projectile is progressively ionized. To assess their influence we solve the TF equation for several ionic charges. We shall call the resulting relationship between Z_1^*/Z_1 and $y \equiv v_1/v_0 Z_1^{2/3}$ the self-consistent solution.

Following conventional procedures,[60] the potential-energy criterion leads to the relations

$$Z_1^*(x_0)/Z_1 = -x_0\phi'(x_0) \tag{4.1}$$

and

$$y(x_0) = 1.50329\,[-\phi'(x_0)]^{1/2}, \tag{4.2}$$

where $\phi(x)$ and x are the usual dimensionless TF potential and distance, $\phi' = d\phi/dx$ and x_0 is the radius of the TF ion defined by

$$\phi(x_0) = 0. \tag{4.3}$$

The results of this calculation are shown in Fig. 8 as curve a and compared with those for the truncated atom (curve b) and with those based on the velocity criterion (curves c and d). Satisfactory agreement of curve a with the data is obtained without any empirical parameters for $y \lesssim 0.4$ provided Z_p^* is used, as seen in Fig. 9. At higher values of y this form of self-consistent solution ceases to agree with experiment.

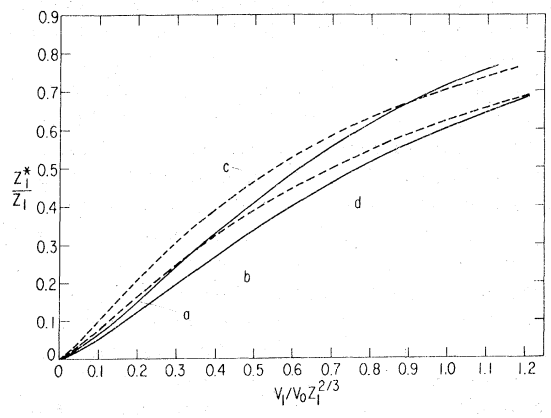

FIG. 8. Effective charge inThomas-Fermi approximation for ions. Calculated using the energy criterion for (a) a self-consistent TF ion of finite radius, and (b) a model ion obtained by truncating the TF density for a neutral atom. Calculated using the velocity criterion and the truncated TF neutral-atom density with (c) $b=1$, and (d) $b=1.26$ (same as the curve in Figs. 2 and 6).

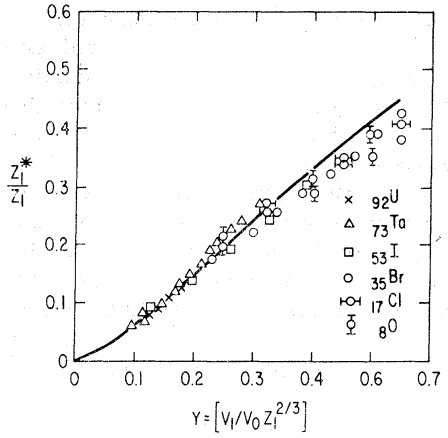

FIG. 9. Comparison of self-consistent effective charges with data. Z_1^*/Z_1 is calculated self-consistently in Thomas-Fermi approximation for an ion, as discussed in the text and shown as curve (a) in Fig. 8. Data shown are those used in Fig. 6.

We have also performed Thomas-Fermi-Dirac (TFD) calculations for several ions over the range $6 \leq Z_1 \leq 92$. The Z_1^*/Z_1 obtained by TFD lie systematically below those found in TF, but only by amounts smaller than the spread of the data, and the shape of the Z_1^*/Z_1-vs-y curve is the same.

V. INTERPOLATION FOR $0 < v_1 < v_0$

With allowance for proton screening the regime of reliable Z_1^* theory reaches down to $v_1 \approx v_0$, but we have no basis for supposing it to reach significantly lower. We now deal with interpolating to the zero-velocity limit, at which S/v_1 is constant. Our goal is a prescription for generating acceptable values of S, at all v_1, for practical computations in which fully quantitative accuracy at low velocities is not crucial. As an example, we have in mind the account of electronic losses which is required in collision cascade-simulations.

For $0 < v_1 < v_0$ no simple theory can be expected to be quantitatively accurate for all projectile-target combinations. While projectile shell-structure effects are typically 5% corrections when $v_1 > v_0$, at lower velocities Z_1-oscillation amplitudes can be 50% of the "average" S. The Lindhard[5] and the Firsov[4] theoretical estimates of the limiting

S/v_1 coefficient, despite significant successes, disagree often with each other and with experiment, and seemingly unsystematically. A detailed theoretical description of S throughout the range $0<v_1<v_0$ is still lacking, and we are for practical applications led to semiemiprical interpolation.

At $v_1=v_0$, the S values calculated via Eq. (2.2) agree on the average with all available data, including Z_1 oscillations, to within 20%. Simply connecting the point calculated at $v_1=v_0$ to the origin by a straight line, i.e., setting for $v_1<v_0$,

$$S(Z_1,Z_2;v_1)\approx S(Z_1;Z_2;v_0)(v_1/v_0)$$
$$=[Z_1^*(v_0)/Z_p^*(v_0)]^2 S_p(Z_2;v_0)(v_1/v_0) \quad (5.1)$$

should therefore give S throughout $0<v_1<v_0$ with an accuracy comparable to that at the low end of the effective-charge theory regime. This simple recipe preserves the generality as well as the computational efficiency of Z_1^* theory. Table III collates several experimental values of $S_p(Z_2;v_0)$. In Fig. 10 we compare experimental stopping powers at $v_1\approx 0.41v_0$ in carbon and in aluminum to those calculated by the Lindhard and the Firsov presciptions and by Eq. (5.1). The solid curves are the results of interpolation according to Eq. (5.1) for $Z_1^*(v_0)$ obtained in two ways: from Brandt's method with the velocity criterion and $b=1.26$, and from the self-consistent TF ion solution (SCTF) with the potential energy criterion, corresponding, respectively, to curves d and a of Fig. 8. As these plots indicate, Eq. (5.1) yields the mean Z_1 dependence of the stopping power at $v_1\approx 0.41v_0$ in both targets, and we expect the same at other velocities and for other projectile-target combinations.

TABLE III. Proton stopping power at $v_1=v_0$ of various targets.

Target (Z_2)	$S_p(10^{15}$ eV cm^2/atom)	Ref.
$_6$C	12	40
$_{13}$Al	18	40
	17	41
$_{28}$Ni	20	42
	14	37
$_{27}$Co	15	37
$_{47}$Ag	27	43
$_{79}$Au	29	43
	20	44, 45

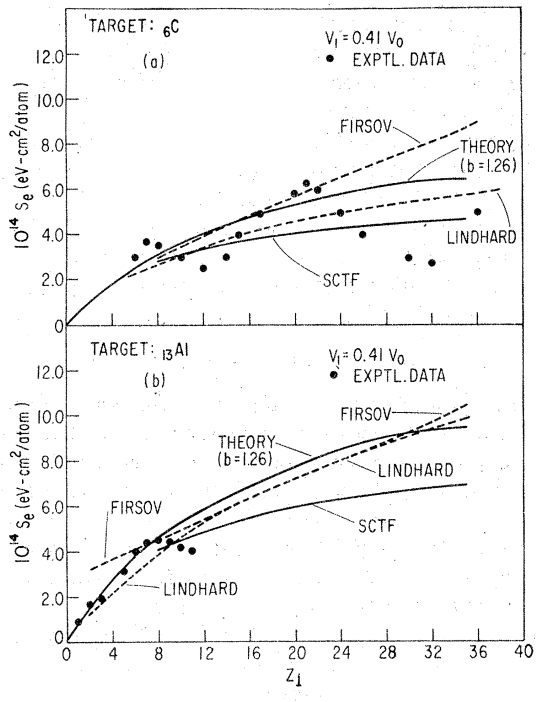

FIG. 10. Electronic stopping power at $v_1<v_0$. Solid lines: obtained by linear interpolation according to Eq. (4.1) as discussed in the text. Dashed lines: obtained from Lindhard's (Ref. 5) and from Firsov's (Ref. 6) estimates. Experimental S at $v_1=0.41v_0$ in (a) carbon targets (Refs. 39 and 40), and in (b) aluminum targets (Ref. 40). SCTF: self-consistent Thomas-Fermi approximation.

VI. CLOSING REMARKS

Simple effective-charge theory is remarkably successful, and its usefulness for practical computation seems apparent. It provides comprehensive perspective on stopping-power data taken over limited ranges of widely different projectile-target combinations and projectile velocities. In particular, some S data which were taken not to extrapolate to $S=0$ at $v_1=0$ are, in fact, high-velocity data (near $v_1=3v_0$) which along with all other data conform to theoretical expectations and are incorporated in Figs. 2 and 6. Fine structure superimposed on the mean trend of S, such as Z_1-dependent oscillations at low velocities, are not contained in the present statistical model of the projectile ion; their calculation must take into account detailed charge distributions. Our results are persuasive evidence for the validity of the factorization of electronic stopping power as stated in Eq. (2.1), on which effective-charge theory builds. Theoretical understanding of this factorization and of the conditions under which it holds is needed, and, to that end, a study is required which is firmly anchored to the foundations of stopping-power theory.

ACKNOWLEDGMENTS

We wish to acknowledge useful conversations with T. L. Gilbert, M. Guinan, O. Oen, M. T. Robinson, K. S. Singwi, and P. Vashishta. One of us (W.B.) wishes to thank R. W. Siegel and other members of the Material Science Division at ANL for their hospitality during a summer visit when this work was initiated. This work is based on research performed under the auspices of the U. S. DOE.

---

*Permanent address.

[1]H. A. Bethe, Ann. Phys. (Leipz.) 5, 325 (1930).

[2]F. Bloch, Ann. Phys. (Leipz.) 16, 285 (1933).

[3]E. Fermi and E. Teller, Phys. Rev. 72, 399 (1947).

[4]O. B. Firsov, Zh. Eksp. Teor. Fiz. 36, 1517 (1959) [Sov. Phys.-JETP 9, 1076 (1959)].

[5]J. Lindhard, M. Scharff, and H. E. Shiott, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. 33, 14 (1963); J. Lindhard and M. Scharff, Phys. Rev. 124, 128 (1961).

[6]N. Bohr, Phys. Rev. 58, 654 (1940); 59, 270 (1941).

[7]W. E. Lamb, Phys. Rev. 58, 696 (1940).

[8]W. Brandt, in *Atomic Collisions in Solids* (Plenum, New York, 1973), Vol. I, p. 261.

[9]H. Betz, Rev. Mod. Phys. 44, 465 (1972).

[10]T. E. Pierce and M. Blann, Phys. Rev. 173, 390 (1968).

[11]Ya. A. Teplova, V. A. Nikolaev, I. S. Dmitriev, and L. N. Fateeva, Zh. Eksp. Teor. Fiz. 42, 44 (1962) [Sov. Phys.-JETP 15, 31 (1962)].

[12]R. S. Nelson, *The Observation of Atomic Collisions in Crystalline Solids* (North-Holland, Amsterdam, 1968).

[13]L. C. Northcliffe, Ann. Rev. Nucl. Sci. 13, 67 (1963).

[14]L. C. Northcliffe and R. F. Schilling, Nucl. Data Sect. A 7, 4 (1970); D. K. Brice, *Ion Implantation Range and Energy Deposition Distribution* (Plenum, New York, 1975).

[15]Empirical correlation of solid-target stopping-power data on the basis of effective-charge scaling has recently been treated in detail by D. Ward, J. S. Forster, H. R. Andrews, I. V. Mitchell, G. C. Ball, W. G. Davies, and G. J. Costa, Atomic Energy of Canada Limited, Report No. AECL-5313 (1976) (unpublished). These authors are concerned with projectile energies from 0.1 to 10 MeV/nucleon, and the data which they analyze pertain primarily to velocities above those of greatest interest in the present study. With allowance for minor differences in presentation, their empirical findings agree with out theoretical results.

[16]M. D. Brown and C. D. Moak, Phys. Rev. B 6, 90 (1972). See also J. Narayan, T. S. Naggle, and O. S. Oen, Bull. Am. Phys. Soc. 20, 351 (1975).

[17]For a preliminary account, see B. S. Yarlagadda, J. E. Robinson, and W. Brandt, Bull. Am. Phys. Soc. 21, 407 (1976).

[18]D. K. Brice, Appl. Phys. Lett. 29, 10 (1976).

[19]No data pertaining to channeled projectiles have been used in the comparisons to experiment presented in the present paper. We believe that all published data for random stopping in solid targets are represented in the references that we cite, although we cannot guarantee that none has eluded our search. All data references are listed seriatim (Refs. 20–49) immediately below, and are referred to in figure and table captions as appropriate. In most instances, but by no means in all, stopping-power values taken from the interpolation tables of Northcliffe and Schilling (Ref. 14) or of Brice (Ref. 14) would have served equally as well.

[20]D. I. Porat and K. Ramavataram, Proc. Phys. Soc. Lond. 77, 97 (1961).

[21]D. I. Porat and K. Ramavataram, Proc. Phys. Soc. Lond. 78, 1135 (1961).

[22]D. I. Porat and K. Ramavataram, Proc. R. Soc. A 252, 394 (1959).

[23]P. H. Barker and W. R. Philips, Proc. Phys. Soc. Lond. 86, 379 (1965).

[24]H. Nakata, Phys. Rev. B 9, 4654 (1974).

[25]H. Nakata, Phys. Rev. B 3, 2847 (1971).

[26]H. Nakata, Can. J. Phys. 46, 2765 (1968); 47, 2545 (1969).

[27]C. D. Moak, B. R. Appleton, J. A. Biggerstaff, S. Datz, and T. S. Noggle, *Atomic Collisions in Solids* (Plenum, New York, 1975): Vol. I, p. 57.

[28]L. B. Bridwell and C. D. Moak, Phys. Rev. 156, 242 (1967).

[29]L. B. Bridwell, L. C. Northcliffe, S. Datz, C. D. Moak, and H. O. Lutz, Phys. Rev. 159, 276 (1967).

[30]C. D. Moak and M. D. Brown, Phys. Rev. 149, 244 (1966).

[31]R. Kalish, L. Grodzins, F. Chmara, and P. H. Rose, Phys. Rev. 183, 431 (1969).

[32]W. Booth and I. S. Grant, Nucl. Phys. 63, 481 (1965).

[33]L. C. Northcliffe, Phys. Rev. 120, 1744 (1960).

[34]D. Ward, R. L. Graham, and J. Geiger, Can. J. Phys. 50, 2302 (1972).

[35]H. Schmidt-Böcking, G. Rühle, and K. Bethge, *Atomic Collisions in Solids* (Plenum, New York, 1975), Vol. I, p. 83; P. G. Roll and F. E. Steigert, Nucl. Phys. 17, 54 (1960).

[36]W. K. Chu and D. Powers, Phys. Rev. 187, 478 (1969).

[37]W. White and R. M. Mueller, Phys. Rev. 187, 499 (1969).

[38]B. Fastrup, P. Hvelplund, and C. A. Sutter, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. 35, 10 (1966).

[39]P. Hvelplund and B. Fastrup, Phys. Rev. 165, 408 (1968).

[40]J. H. Ormrod, J. R. McDonald, and H. E. Duckworth, Can. J. Phys. 43, 275 (1965).

[41]G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 7, 983 (1973).

[42]R. L. Wolke, W. N. Bishop, E. Eichler, N. R. Johnson, and G. D. O'Kelley, Phys. Rev. 129, 2591 (1963).

[43]A. Valenzeula, W. Meckbach, A. J. Kestleman, and J. C. Eckardt, Phys. Rev. B 6, 95 (1972).

[44]A. H. Morton, D. A. Aldcroft, and M. F. Payne, Phys. Rev. 165, 418 (1968).

[45]S. K. Allison and S. D. Warshaw, Rev. Mod. Phys. 25, 779 (1953).

[46]W. Whaling, *Handbuch der Physik*, edited by S. Flügge (Springer- Verlag, Berlin, 1958), Vol. 34, p. 193.

[47]R. D. Moorehead, J. Appl. Phys. 36, 391 (1965).

[48]H. K. Reynolds, D. N. F. Dunbar, W. A. Wenzeland, and W. Whaling, Phys. Rev. 92, 742 (1953).

[49]S. D. Warshaw, Phys. Rev. 76, 1759 (1949).
[50]A similar variation of b was found by J. H. M. Bruning, J. K. Knipp, and E. Teller, Phys. Rev. 60, 657 (1941). Ward *et al.* (Ref. 15) parametrize the effective-charge fraction in the form $Z_1^*/Z_1 = 1 - A\exp(-Bv_1/v_0)$ and find a weak Z_1 dependence of A which is equivalen to this variation of b.
[51]P. Gombas, *Die Statistiche Theorie der Atoms und ihre Anwendungen* (Springer-Verlag, Vienna, 1949), p. 72.
[52]J. K. Knipp and E. Teller, Phys. Rev. 59, 659 (1941).
[53]J. C. Ashley, R. H. Ritchie, and W. Brandt, Phys. Rev. B 5, 2393 (1972).
[54]The restriction to $v_1 \gtrsim v_0$ is similar to but not identical with the approximation stated by Lamb as neglecting the binding of electrons in the target.
[55]See, e.g., J. C. Slater, *Quantum Theory of Molecules and Solids* (McGraw-Hill, New York, 1963), Vol. I, p. 96.
[56]See, e.g., Z. D. Popovic, M. J. Stott, J. P. Carbotte, and G. R. Piercy, Phys. Rev. B 13, 590 (1976), and references listed therein.
[57]P. Jena and K. S. Singwi, Bull. Am. Phys. Soc. 22, 467 (1977).
[58]H. Stachowiak, Bull. Acad. Pol. Sci. Ser. Sci. Math. Astron. Phys. 23, 1213 (1975).
[59]K. S. Singwi and P. Vashishta (private communication).
[60]N. H. March, *Self-consistent Fieids in Atoms* (Pergamon, New York, 1975).