Projectile-charge dependence of stopping powers

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Recent stopping-power data of solids with atomic number Z_2 ranging from 13 to 79 for ions ranging in atomic number Z_1 from 1 to 9 and in velocity from $7v_0$ to $12v_0$ are analyzed in terms of Z_1^3 effects and effective ion charges. They are found to be consistent with current theory. High-velocity forms of the Z_1^3 -proportional stopping-power contributions are calculated by the method of moment integrals.

I. INTRODUCTION

The stopping power of matter for particles of charge $Z_1 e$ moving with velocity v_1 is proportional to Z_1^2 in the Bethe theory of energy loss.¹ The theory has been extended to include the polarization of the target atoms by the projectile which, to lowest order, gives a polarization term proportional to $Z_1^{3,2}$. The results of this development were confirmed in a quantum-mechanical harmonicoscillator approximation which leads to identical formulas.³

When averaged over the target atom, the Z_1^3 -dependent terms contain a scaled minimum-impact parameter, denoted as b. It is of order unity and essentially independent of the atomic number Z_2 of the substance in which the projectile moves. Adjusting on relative stopping powers⁴ of ₁₃Al and ₇₃Ta for ${}_1^1$ H and ${}_2^4$ He yielded a first trial value b = 1.8.

In new experiments Andersen, Bak, Knudsen, and Nielsen⁵ extended the measurements to relative stopping powers of 13Al, 29Cu, 47Ag, and 79Au for ${}^{1}_{1}\text{H}$, ${}^{4}_{2}\text{H}$, and ${}^{6}_{3}\text{Li}$ ions in the range $v_{1} = 7v_{0}$ to $v_1 = 12v_0$, where $v_0 = e^2/\hbar$. Data have been reported by the Oak Ridge group⁶ on the stopping of ${}^{1}_{1}$ H, ${}^{4}_{2}$ He, ${}_{3}^{6}$ Li, ${}_{5}^{10}$ B, ${}_{6}^{12}$ C, ${}_{7}^{14}$ N, ${}_{8}^{16}$ O, and ${}_{9}^{18}$ F ions in ${}_{79}$ Au targets. It is the purpose of this Comment to present an analysis of these data in terms of current theory, and to assess the importance of polarization effects and projectile charge states on the stopping power of matter. In Sec. II, the cutoff parameter b is determined on the light-ion data. Alternative models for the polarization terms, depending on the choice of cutoff parameter, are examined in Sec. III and found to be in need of inner-shell corrections for their application. The data analysis for heavy ions in Sec. IV agrees with that for light ions provided one invokes effective-charge theory.

II. LIGHT IONS

We consider the stopping power $S = -dE_1/dx$ of a medium composed of atoms with atomic number Z_2 at density *n* for particles of atomic charge Z_1e and nonrelativistic velocity v_1 , or kinetic energy $E_1 = \frac{1}{2}M_1v_1^2$, where M_1 is the mass of the particle. Then

$$S = (4\pi Z_1^2 e^4 n Z_2 / m v_1^2) L , \qquad (1)$$

where the stopping number $L = L_B + Z_1 L_1 + Z_1^2 L_2 + \dots$ contains

$$L_{B} = L_{0} + \Phi = \ln \frac{2mv_{1}^{2}}{I_{0}} - \frac{C_{0}}{Z_{2}} + \Phi\left(\frac{Z_{1}e^{2}}{\hbar v_{1}}\right), \qquad (2)$$

the Bethe-Bloch stopping number per target electron⁷ in terms of the mean ionization potential $I_0 = K_0 Z_2$ of the medium, K_0 being the Bloch constant. The term C_0/Z_2 accounts for inner-shell corrections. The function $\Phi(\xi)$ is given in terms of ψ , the logarithmic derivative of the Γ function,

$$\Phi(\xi) = \psi(1) - \operatorname{Re}\psi(1+\xi) . \tag{3}$$

It connects the classical theory, valid when $\xi \gg 1$, with the quantum-mechanical theory, valid when $\xi \ll 1$.

The function L_1 , averaged over the statistical Lenz-Jensen model of the target atom, can be written in the compact form²

$$L_1(b;x) = F(b/x^{1/2})/Z_2^{1/2}x^{3/2}, \qquad (4)$$

where $x = v_1^2/Z_2 v_0^2 = [40E_1(\text{MeV})]/[M_1(\text{amu})Z_2]$. Table I gives values of the function $Z_2^{1/2}L_1(b;x)$ for a range of *b* values. Without including $\Phi(\xi)$, analysis of early data⁴ gave the trial value b = 1.8. Extensive recent data⁵ yield, with the inclusion of $\Phi(\xi)$, larger L_1 values corresponding to a new "best" parameter value $b = 1.4 \pm 0.1$ for targets with $Z_2 > 13$. In fitting to the data, we set

$$\frac{L-L_B}{Z_1} = L_1 \left(1 + Z_1 \frac{L_2}{L_1} + Z_1^2 \frac{L_3}{L_1} + \cdots \right) \simeq L_1, \qquad (5)$$

because exploratory calculations⁸ indicate that $\sum_{\nu=2}^{\infty} Z_1^{\nu} L_{\nu} / Z_1 L_1$ can have positive or negative values depending on stopping conditions, but that the absolute value in this velocity range may be $\ll 1$.

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1.0 1.21.4 1.6х b 1.8 2.00.1 3.241.81 1.10 0.7160.4910.3520.2 3.23 1.90 1.18 0.774 0.530 0.377 0.4 2.791.78 1.170.800 0.561 0.404 2.371.08 0.773 0.6 1.590.557 0.4100.8 2.041.42 1.010.728 0.539 0.404 1.0 1.78 1.270.927 0.686 0.511 0.392 2.0 0.8210.639 1.060.5040.400 0.321 4.00.566 0.463 0.381 0.316 0.264 0.222 6.0 0.3750.3150.266 0.227 0.194 0.167 8.0 0.276 0.2350.2020.175 0.1520.133100.2160.186 0.1620.142 0.1240.110200.0967 0.0859 0.0768 0.0692 0.0625 0.0567 40 0.0416 0.0379 0.0344 0.0317 0.02920.027060 0.0250 0.0230 0.0211 0.0196 0.0182 0.0170 80 0.0174 0.0160 0.0148 0.0138 0.0129 0.0121 100 0.01310.01200.0093 0.0112 0.0105 0.0098

TABLE I. Z_1^3 -dependent stopping number function L_1 , Eq. (4), in a target of atomic number Z_2 tabulated in the form $Z_2^{1/2}L_1$ (b; x) as a function of $x = v_1^2/v_0^2 Z_2$ for various parameters b. Note that $x = [40E_1 \text{ (MeV)}]/[M_1 \text{ (amu) } Z_2]$. The function F (w) is tabulated in Ref. 2.

III. Z_1^3 TERMS

The polarization stopping number L_1 was evaluated first with an inner cutoff distance a_{ω} proportional to the orbital radius r of the electrons responding with frequency $\omega(r)$.² When averaged over the atom this yields the empirically determined dimensionless parameter $b \simeq 1.4$. Other models equate a_{ω} with the harmonic-oscillator amplitude⁹ $a_{\omega} = (\hbar/2m\omega)^{1/2}$, and the quantum-mechanical minimum-impact parameter¹⁰ $a_{\omega} \simeq \hbar/2mv_1$. When one averages these models over the target atom, one can write

$$L_{1} = \frac{3\pi e^{2}G}{4mv_{1}^{3}} \int_{0}^{\infty} g(\omega)\omega \,d\omega \ln \frac{2mv^{2}}{\hbar\omega} - \frac{C_{1}}{Z_{2}}$$
(6)
$$= \frac{3\pi e^{2}G}{4mv_{1}^{3}\hbar} W_{1} \ln \frac{2mv^{2}}{I_{1}} - \frac{C_{1}}{Z_{2}},$$
(7)

where G = 1 if $a_{\omega} = (\hbar/2m\omega)^{1/2}$ and G = 2 if $a_{\omega} = \hbar/2mv_1$; $g(\omega)$ is the differential-oscillator strength distribution of the target atom normalized such that $\int_0^{\infty} g(\omega) d\omega = 1$, and C_1/Z_2 denotes inner-shell corrections of L_1 . Equation (7) introduces energies W_1 and I_1 as

$$W_1 = k_1 Z_2 = \hbar \int_0^\infty g(\omega) \omega \, d\omega \,, \tag{8}$$

$$\ln I_1 = \ln K_1 Z_2 = W_1^{-1} \hbar \int_0^\infty g(\omega) \omega \, d\omega \, \ln \hbar \omega \,. \tag{9}$$

Similarly, the Bethe stopping number is

$$L_{0} = \int_{0}^{\infty} g(\omega) d\omega \ln \frac{2mv_{1}^{2}}{\hbar\omega} - \frac{C_{0}}{Z_{2}} = \ln \frac{2mv_{1}^{2}}{I_{0}} - \frac{C_{0}}{Z_{2}} , \qquad (10)$$

such that

$$\ln I_0 = \ln K_0 Z_2 = \int_0^\infty g(\omega) \, d\omega \ln \hbar \omega \,. \tag{11}$$

One may evaluate the constants K_0 , k_1 , and K_1 from moment integrals,¹¹⁻¹³ s(k), defined

$$s(k) = \int_0^\infty g(\omega)(\hbar\omega)^k d\omega , \qquad (12)$$

and normalized such that s(0) = 1. Treating s(k) as an analytical function of k, one obtains the approximations

$$W_1 = s(1)$$
, (13)

$$\ln I_1 = s^{-1}(1) \left(\frac{ds(k)}{dk} \right)_{k=1},$$
(14)

$$\ln I_0 = \left(\frac{ds(k)}{dk}\right)_{k=0}.$$
 (15)

Tables of s(k) are available for some elements.^{14,15} For illustration, we give the constants for a few atoms in Table II. The Bloch constants K_0 so obtained agree well with experimental data.¹⁶

In terms of the Lenz-Jensen statistical model of the atom with density $\rho^{\rm LJ}$, one can estimate with $\omega(r) = \chi [4\pi e^2 \rho^{\rm LJ}(r)/m]^{1/2}$, χ being a constant ~1, the spectral function²

$$g^{\mathrm{LJ}}(\omega) = \int \rho^{\mathrm{LJ}}(r) \delta(\omega - \omega(r)) d^3r , \qquad (16)$$

and calculate the corresponding constants from Eqs. (8), (9), and (11), as listed in Table II. The

TABLE II. Atomic constants in L_0 and L_1 , as estimated from Eqs. (13)-(15) from moment integrals s(k), for $-2 \le k \le 2$. Values of s(k) for $Z_2=36$ and 54 from Ref. 14, empirical K_0 values from Ref. 16 and for H calculated in Ref. 1. The constants for $Z_2=2$, 10, and 18 are from Ref. 15. The last line is calculated for the Lenz-Jensen (LJ) statistical atom, according to Eq. (16) with x = 1.29 chosen for K_0 to agree with experiment.

Element	Z_2	K ₀ (emp) (eV)	<i>K</i> ₀ (eV)	k_1 (eV)	<i>K</i> ₁ (eV)
Н	1	(15.0)	14.8	18.1	24.8
He	2	21.0	19.4	26,2	40.5
Ne	10	13.1	13.1	43.0	150.9
Ar	18	11.7	9.85	52.9	263.3
Kr	36	10.6	10.2	55.6	264
Xe	54	10.3	10.2	60.6	299
LJ			9.8	30.6	97.6

constants for atoms up to Z = 54, calculated by the method of moment integrals, are larger and have additional Z_2 dependences, presumably because of the contributions of the innermost shells that are not well described by the Lenz-Jensen approximation. Over the range of x values under discussion, $1 \le x \le 11$, these differences can only be studied and the relative merits of the two model approximations represented by the parameter G be assessed when, in analogy to C_0/Z_2 for L_0 , innershell corrections C_1/Z_2 are developed for L_1 .

IV. HEAVY IONS

The Oak Ridge stopping-power data⁶ of ions, $1 \leq Z_1 \leq 9$, moving at $v_1 = 8.94v_0$ and $v_1 = 11.98v_0$ in random ₇₉Au foils, were treated in a manner similar to that described in Sec. II. The data for channeled ions require separate considerations.¹⁷ According to effective-charge theory,¹⁸ one may write

$$S = Z_1^{*2}(v_1)S_0, \qquad (17)$$

where $Z_1^*(v_1)$ is the effective charge of the ion which depends on v_1 but only weakly on the medium. S_0 is the stopping power per unit charge in the limit $Z \rightarrow 0$. Setting $Z_1^* \simeq Z_1 [1 - \exp(0.95v_1/Z_1^{2/3}v_0)]$, the data, S, are plotted in Fig. 1 in the form

$$L = \frac{mv_1^2}{4\pi e^4 n Z_2} \frac{S}{Z_1^{*2}} - \Phi\left(\frac{Z_1^* e^2}{\hbar v_1}\right)$$
(18)

as a function of Z_1 . Extrapolation to $Z_1 \rightarrow 0$ yields $L_0(8.94v_0) = 1.44 \pm 0.04$ and $L_0(11.9v_0) = 1.86 \pm 0.05$. By comparision, Eq. (10) gives for $_{79}$ Au, with $I_0 = 797$ eV and $C_0/Z_2 = 0.27$ at $v_1 = 8.94v_0$, and $C_0/Z_2 = 0.38$ at $v_1 = 11.9v_0$,¹⁹ the stopping numbers $L_0(8.94v_0) = 1.43$ and $L_0(11.9v_0) = 1.87$.



FIG. 1. Experimental stopping number L, extracted from data (Ref. 6) according to Eq. (18), as a function of the charge number Z_1 of projectiles at two velocities v_1 in random ₇₉Au foils. Solid curves are drawn to aid the eye. The extrapolated values L_0 for $Z_1 \rightarrow 0$ are indicated by dashed lines. The rise of the data with Z_1 is indicative of deviations from the Bethe-Bloch stopping-power theory as listed in Table III.

This permits one to extract L_1 from the data in the form $(L - L_0)/Z_1^*$ as collated in Table III, with mean values $L_1 = 0.10$ at $v = 8.94v_0$ and $L_1 = 0.08$ at $v = 11.9v_0$. From Table I with b = 1.4, we find corresponding values of 0.104 and 0.079. The fluctuations in Table III may be indicative of contributions from L_{ν} , $\nu > 1$, but they do not exceed experimental uncertainties. The trend of the $8.94v_0$ data could signify that they may be negative, as are some results from preliminary calculations.⁸ This merits further study.

TABLE III. Empirical L_1 values given by $(L - L_0)/Z_1^*$ with $L_0 = 1.44$ at $v_1 = 8.94 v_0$ and $L_0 = 1.86$ at $v_1 = 11.8 v_0$, based on measurements of Ref. 6 as shown in Fig. 1. Uncertainties are approximately $\pm 20\%$.

		L	L_1		
Projectile	Z_1	$v_1 = 8.90 v_0$	$v_1 = 11.8 v_0$		
Н	1	0.10	0.078		
He	2	0.10	0.083		
\mathbf{Li}	3	0.10	0.070		
в	5	0.10	0.078		
С	6	0.096			
N	7	0.095			
Ο	8	0.091			
\mathbf{F}	9	0.088			

In conclusion, current nonrelativistic stoppingpower data in the ranges $1 \le Z_1 \le 9$, $7 \le v_1/v_0 \le 12$, consistent with the theory of Z_1^3 effects, assuming that effective-charge theory applies. Comparison of experiments with calcula-

tions of the polarization stopping number L_1 by the method of moment integrals and the assessment of the relative merits of the various cutoff models require the development of inner-shell

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- ¹H. A. Bethe, Ann. Phys. (Leipz.) 5, 325 (1930).
- ²J. C. Ashley, R. H. Ritchie, and W. Brandt, Phys. Rev. B 5, 2393 (1972); Phys. Rev. A 8, 2402 (1973); 10, 737 (1974); J. C. Ashley, V. E. Anderson, R. H. Ritchie, and W. Brandt, Z_1^3 Effects in the Stopping Power of Matter for Charged Particles: Tables of Functions, Document No. 02195 (National Auxiliary Publication Service, New York, 1974).
- ³K. W. Hill and E. Merzbacher, Phys. Rev. A <u>9</u>, 156 (1974).
- ⁴H. H. Andersen, H. Simonsen, and H. Sørensen, Nucl. Phys. A 125, 171 (1969).
- ⁵H. H. Andersen, J. F. Bak, H. Knudsen, B. R. Nielsen, Phys. Rev. A 16, 1929 (1977).
- ⁶S. Datz, J. Gomez del Campo, P. F. Dittner, P. D. Miller, and J. A. Biggerstaff, Phys. Rev. Lett. <u>38</u>, 1145 (1977).
- ⁷H. A. Bethe and J. Ashkin, *Passage of Radiations* through Matter in Experimental Nuclear Physics, edited by E. Segrè (Wiley, New York, 1960), Vol. I, p. 166.
- ⁸G. Basbas, W. Brandt, and R. H. Ritchie, Bull. Am. Phys. Soc. 22, 487 (1977).
- ⁹J. D. Jackson and R. L. McCarthy, Phys. Rev. B <u>6</u>, 4131 (1972).

corrections to the Z_1^3 -proportional stopping-power contributions.

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- ¹⁰H. Esbensen, thesis (University of Aarhus, Denmark, 1976) (unpublished); J. Lindhard, Nucl. Instrum. Methods 132, 1 (1976).
- ¹¹W. Brandt, Phys. Rev. 104, 691 (1956).
- ¹²C. L. Pekeris, Phys. Rev. <u>115</u>, 1216 (1959).
- ¹³A. Dalgarno, Proc. Phys. Soc. Lond. <u>76</u>, 422 (1960).
- ¹⁴V. Fano and J. W. Cooper, Rev. Mod. Phys. <u>40</u>, 441 (1968); <u>41</u>, 724 (1969).
- ¹⁵J. L. Dehmer, M. Inokuti, and R. P. Saxon, Phys. Rev. A <u>12</u>, 102 (1975); G. D. Zeiss, W. J. Meath, J. C. F. MacDonald, and D. J. Dawson, Can. J. Phys. 55, 2080 (1977).
- ¹⁶Studies in Penetration of Charged Particles in Matter, Publication No. 1133 (National Academy of Sciences and National Research Council, Washington, D.C., 1964), p. 225.
- ¹⁷J. C. Ashley and R. H. Ritchie, in Proceedings of the International Conference of Atomic Collisions in Solids, Moscow, 1977 (unpublished).
- ¹⁸For a discussion of effective-charge theory and experiment, see Werner Brandt, in *Proceedings of the Fifth International Conference on Atomic Collisions in Solids, Gatlinburg, Tennessee, 1973, edited by S. Datz, B. R. Appleton, and C. D. Moak (Plenum, New York, 1975), p. 261 ff. For a recent data analysis see B. S. Yarlagadda, J. E. Robinson, and Werner Brandt, Phys. Rev. B 17, 3473 (1978).*
- ¹⁹E. Bonderup, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 35, 17 (1967).