PROJECTILE SIZE DEPENDENCE OF STOPPING POWER*

D. K. Brice
Sandia Laboratories†
Albuquerque, New Mexico 87185

ABSTRACT

Recent measurements for 0-, 1-, and 2-electron ions channeled in {111} Au suggest that the electronic stopping power, dE/dx, depends on the spatial distribution of charge on the projectile. We have investigated the effect of the projectile charge distribution on dE/dx using the Lindhard dielectric theory of stopping. The charge distribution contribution is demonstrated directly within the framework of this theory. Good agreement is obtained between experiment and theory when higher order Z_1-effects, which are of comparable magnitude (~ 5-10%), are included in a self-consistent phenomenological manner.

*This work supported by the U. S. Department of Energy, DOE, under Contract DE-AC04-76-DP00789.

†A U. S. Department of Energy facility.

INTRODUCTION

The use of beams of swift atomic projectiles for the alteration and study of the near surface region of solid targets has received considerable attention over the past several years. Knowledge of the stopping power, dE/dx, is important in such studies in order to characterize both the energy deposition and the implanted ion profiles. Recent theoretical work[1-6] has shown that for a point projectile with charge Z_1e the electronic contribution to the stopping power can be written as

$$-dE/dx = N\ S_e = N\ S_o\ Z_1^2\ (L_o + Z_1\ L_1 + Z_1^2\ L_2 + \ldots) \qquad (1)$$

where N is the target atomic density and the $\{L_i\}$ are functions only of the projectile speed, v, and properties of the target material. The quantity S_o in (1) is given by

$$S_o = 4\pi e^4\ n_a/(m\ v^2) \qquad (2)$$

with n_a the number of electrons per target atom and m the electron mass. Experimental measurements have verified the importance of the higher order terms in (1) and have confirmed that the theoretical predictions for L_1 and L_2 are of the correct sign and order of magnitude.[7]

Equation (1) has also been used to describe the stopping power of projectiles which are not fully stripped of their electrons,[8,9] and are therefore not point particles, with Z_1 replaced by an effective value, Z_1^*, where

$$\left(Z_1^*/Z_1\right)^2 = 1 - \exp\left(- 0.95\ v/Z_1^{2/3}\ v_o\right) . \qquad (3)$$

In (3) v_o is the Bohr velocity, $e^2/\hbar$. Evidence suggests[10] that Z_1^* closely approximates the average charge on the projectiles at equilibrium. Values of L_1 and L_2 for such projectiles extracted from experimental data through the use of Eqs. (1)-(3) are in agreement with those obtained for point projectiles.[7] This agreement must be viewed with some caution, however, since the dE/dx values represent an average property of the beam which has a distribution of projectile charge states.

Recent measurements of dE/dx[11] show that Eqs. (1) and (2) cannot be used to describe the stopping power in the simple approximation in which Z_1 is replaced by the net charge, $q = Z_1 - Z_e$, with Z_e the number of electrons carried by the projectile. Results of these measurements for 0-, 1-, and 2-electron projectiles with $1 \geq Z_1 \geq 9$, which were transmitted through the {111} channel of a gold target at a velocity of 8.95 v_o, are collected in Table I. A portion of the data are plotted in Fig. 1 to illustrate that the stopping power, S_e, is not constant for a fixed value of q. These data clearly show that the quantities $\{Z_1^{i+2}L_i\}$ in Eq. (1) must be replaced by functions which depend not only on the net charge, q, but also on its spatial distribution about the projectile charge center.

Ashley and Ritchie[12] have used a modified form of the Bohr theory to analyze the data of Table I, but they neglected higher-order Z_1 effects. Careful examination of the data in the table show however that the higher order effects are important (~ 10%) in determining dE/dx, and should be included in a proper analysis. In the present paper we reexamine these experimental data from the point of view of the Lindhard theory[13] as discussed by Lindhard and Winther[14] and include both charge distribution and higher Z_1 effects.

THEORY

Let the quantities $Z_1^{i+2} L_i$ in (1) be replaced by functions G_i so that

$$-dE/dx = N\ S_o(G_o + G_1 + G_2 + \ldots) \quad . \tag{4}$$

Also, let the projectile consist of a positive point charge, Z_1e, with Z_e electrons having a spatial distribution $\rho_e(r)$ which is not altered by passage through the target medium. Then, Lindhard theory[13] yields

$$N\ S_o\ G_o = -\frac{e^2}{\pi}\ \mathrm{Im}\int_0^\infty \frac{dk}{k}\left[Z_1^2 - 2\ Z_1\ \rho_e(k) + \rho_e^2(k)\right]\ \times$$

$$\int_{-kv}^{kv} wdw\left\{\frac{1}{\varepsilon(k,w)} - 1\right\} \quad , \tag{5}$$

where $\rho_e(k)$ is the Fourier transform of $\rho_e(r)$. This expression has previously been used[15] to examine the effects of charge capture on dE/dx at low projectile speeds. It shows that effective charge theory can be strictly applied to the first term on the right of (4) only when $\rho_e(k)\to Z_e$, which implies a delta-function distribution at the projectile nucleus. Equations (4) and (5) will be used in the next section to analyze the data in Table 1.

CALCULATIONS AND DATA ANALYSIS

A. Bare Nuclei

The experimental data in Table I for $Z_c = 0$ have been fit by a least mean mean square method to an equation of the form of Eq. (1), with resultant values

$$S_e = 4.12\ Z_1^2 + 0.1475\ Z_1^3 - 0.0105\ Z_1^4\ (10^{-15}\ \text{eV-cm}^2/\text{atom}) \quad . \qquad (6)$$

All the data in Table 1 were obtained for well-channeled ions, i.e., particles which did not wander far from the midpoint of the channel. For these particles the stopping medium is well approximated by a free electron gas. Under such conditions the first term on the right hand side of (6), along with Eq. (5), can be used to determine the electron density $n(= n_a N)$ in the channel center. The resultant value is $n = 4.00 \times 10^{23}$ electrons/cm^3 which corresponds to 6.75 electrons per gold atom. This is a reasonable result since a free gold atom has 11 loosely bound electrons. The static screening length for this n-value is $\lambda = 0.427$ Å.

From this electron density and equation (6) the corresponding L_i-values are $L_o = 5.23$, $L_1 = 0.187$, and $L_2 = -0.0133$. These results for L_1 and L_2 are about twice the measured values for the nonchanneled beam,[7] while the value for L_o is about three times that for the nonchanneled beam. This is expected since free electrons in the channel have a larger interaction cross section than do the bound electrons which make a significant contribution in the nonchanneled case.

B. 1- and 2-Electron Projectiles

Datz, et al,[11] have argued that the electrons on the 1- and 2-electron projectiles remain in the K-shell during their passage through the target material. The charge distributions of these electrons thus correspond to 1s-like states for which

$$\rho_c(k) = Z_c\, k_o^4/(k_o^2 + k^2)^2 \, , \tag{7}$$

with $k_o = 2/a$, where a is the radius of the 1s wave-function. For isolated projectiles $a = a_o/Z_1$ for the 1-electron ions and $a = a_o/(Z_1 - 0.3125)$ for the 2-electron ions,[16] where a_o is the Bohr radius of hydrogen. Due to the dielectric response of the medium these radii are expected to increase inside the target material. The increase will be a maximum at low projectile velocities, and thus an upper limit to the values for the radii can be obtained by minimizing the electric field energy plus the electron kinetic energy with respect to variations in a. This minimization has been carried out using the low velocity approximation to the Lindhard dielectric response function with the result that the radii are expected to expand by no more than 5% from their isolated ion values. Since this amount of expansion affects the calculated stopping power values by less than 0.5% this effect has been ignored in the calculations and the isolated atom values for a have been used.

i. S_oG_o (Modified Z_1^2 term)

Eq. (5) has been used to calculate the contribution of S_oG_o to (4). Lindhard's dielectric response function[13] divides (k,ω)-space into regions corresponding to "close" collisions and "distant," or resonant, collisions. Eq. (7) was used to describe the electron charge distribution for the close collisions. For the distant collisions the projectile was assumed to be a point charge with effective charge $q = Z_1 - Z_e$. Calculated values for S_oG_o are given in Table I.

ii. S_oG_1 (Modified Z_1^3 term)

Ashley, et al,[1] have argued that the Z^3-corrections to dE/dx come primarily from distant collisions. Correspondingly, we have used the value of L_1 obtained for the bare nuclei along with the net charge, q, to represent this contribution to Eq. (3). Calculated values for S_oG_1 are given in Table I.

iii. S_oG_2 (Modified Z_1^4 term)

Values for $\Delta = -S_oG_2$ were obtained by subtracting the above contributions to S_e from the experimental data. These values of Δ are listed in Table I. It was assumed that Δ could be separated into contributions from "close" and "distant" collisions by writing

$$\Lambda = 0.0105\ [f\ Z_1^4 + (1 - f)\ q^4] \tag{8}$$

where f is the fraction of collisions which are "close," i.e., collisions in which the unshielded nucleus determines Λ. The constant 0.0105 characterizes the Z^4 correction for point projectiles (see Eq. [6]). A value for f is thus obtained for each experimental value of Λ, and these values are plotted in Fig. 2 as a function of the radius of the projectile electron cloud.

This analysis of the Λ-values is satisfying from a physical point of view. One can view the collisions between projectile and target electrons as divided into two categories: (1) those collisions which occur inside the charge cloud radius, for which $Z_1^* = Z_1$, and (2) those collisions which occur outside the charge cloud radius, for which $Z_1^* = q$. The larger the charge cloud radius, the more likely is a collision of type (1) and thus the fraction, f, of the collisions for which $Z_1^* = Z_1$ is expected to be an increasing function of the charge cloud radius. The agreement of the f-values as *a function of a for* both the 1- and 2-electron projectiles suggests that such a geometic argument is reasonable.

CONCLUSIONS

Lindhard theory[13] has been used to study the projectile size dependence of the electronic contribution to the stopping power. An expression for the Z^2 contribution to dE/dx, i.e., the term S_oG_o in Eq. (4), has been presented which explicitly demonstrates the dependence of this term on the projectile charge distribution. The Z^3 correction to dE/dx, i.e., the term S_oG_1 in Eq. (4), has been described by effective charge theory, since this term results primarily from "distant" collisions.[1] The experimental data of Datz, et al,[11] have been analyzed using these descriptions of the Z^2 and Z^3 contributions to dE/dx, and experimental values for the Z^4 correction have been extracted. It is shown that the Z^4 term also is dependent on the spatial distribution of projectile charge, although explicit dependences are not mathematically represented here.

The results of this analysis indicate that accurate theoretical representations of the stopping power for atomic projectiles which are incompletely stripped of their electron clouds must include a consideration of the spatial distribution of the electronic charge on the projectiles.

REFERENCES

1. J. C. Ashley, R. H. Ritchie, and W. Brandt, Phys. Rev. B5, 2393 (1972).
2. J. D. Jackson and R. L. McCarthey, Phys. Rev. B6, 4131 (1972).
3. K. W. Hill and E. Merzbacher, Phys. Rev. A9, 156 (1974).
4. J. Lindhard, Nucl. Inst. Methods 132, 1 (1976).
5. H. Eshensen (Thesis, University of Aarhus, 1977), unpublished.
6. C. Bashas, W. Brandt, and R. H. Ritchie, Bull. Am. Phys. Soc. 22, 487 (1977).
7. H. H. Andersen, J. F. Bak, H. Knudsen, and B. R. Nielsen, Phys. Rev. A16, 1929 (1977).
8. R. H. Ritchie and W. Brandt, Phys. Rev. A17, 2102 (1978).
9. L. E. Porter, Phys. Rev. A16, 1812 (1977).
10. H. D. Betz, Rev. Mod. Phys. 44, 465 (1972).
11. S. Datz, J. Gomez del Campo, P. F. Dittner, P. D. Miller, and J. A. Biggerstaff, Phys. Rev. Lett. 38, 1145 (1977).
12. J. C. Ashley and R. H. Ritchie, Proceedings of the Moscow Conf. on Atomic Collisions in Solids, 1977, to be published.
13. J. Lindhard, Mat. Fys. Medd. Dan. Vid. Selsk. 28, No. 8 (1954).
14. J. Lindhard and Aa. Winther, Mat. Fys. Medd. Dan. Vid. Selsk. 34, No. 4 (1964).
15. T. L. Ferrel and R. H. Ritchie, Phys. Rev. B16, 115 (1977).
16. See, for example, L. I. Schiff, Quantum Mechanics, 2nd ed. (McGraw Hill, New York, 1955) p. 174.

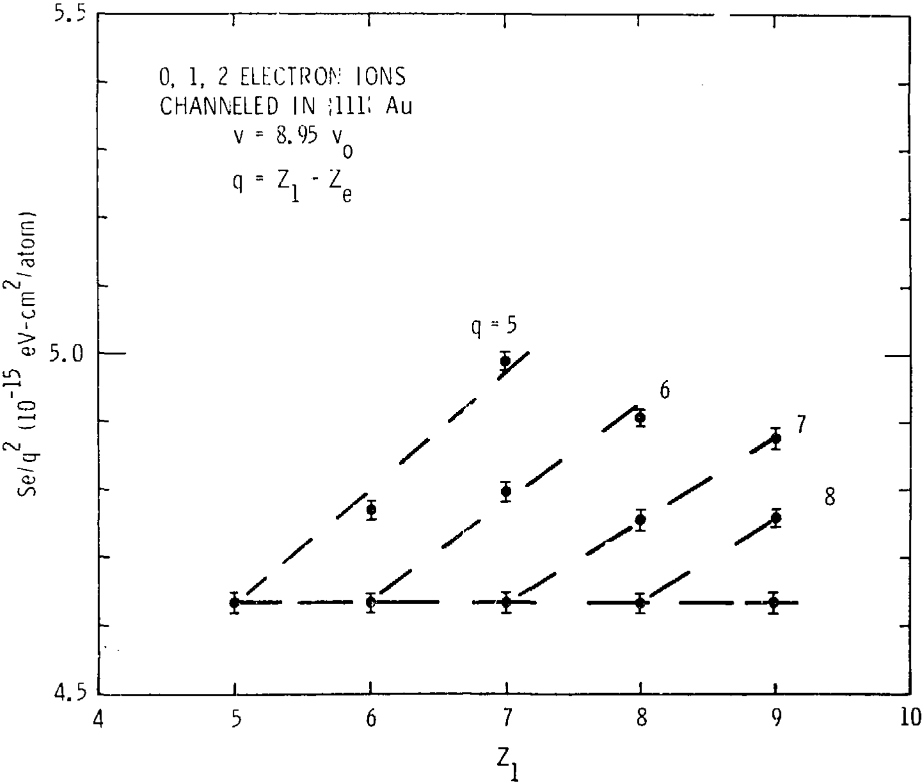
Table I. Experimental and Theoretical Contributions to S_e for 0-, 1-, and 2- Electron Projectiles Channeled in {111} Au at $v = 8.95\ v_o$. Units 10^{-15} eV-cm^2/atom.

Z_1	S_{expt}	S_oG_o (Calc.)	S_oG_1 (Calc.)	$S_o(G_o+G_1)-S_{expt}$
$Z_e = 0$				
1	4.25 ± 0.05	4.13	.15	0.03 ± 0.05
2	17.5 ± 0.2	16.5	1.2	0.2 ± 0.2
3	40.0 ± 0.3	37.2	4.0	1.2 ± 0.3
5	115.7 ± 0.8	103.4	18.4	6.1 ± 0.8
6	166.4 ± 1.1	148.8	31.9	14.3 ± 1.1
7	226.3 ± 1.5	202.6	50.6	26.9 ± 1.5
8	295.4 ± 1.9	264.6	75.5	44.7 ± 1.9
9	363.6 ± 2.4	335.0	107.5	68.9 ± 2.4
$Z_e = 1$				
6	119.2 ± 0.5	111.2	18.4	10.4 ± 0.5
7	172.8 ± 0.7	156.7	31.9	15.8 ± 0.7
8	233.2 ± 1.0	210.5	50.6	27.9 ± 1.0
9	304.6 ± 1.3	272.4	75.5	43.3 ± 1.3
$Z_e = 2$				
7	124.8 ± 0.5	118.1	18.4	11.7 ± 0.5
8	176.8 ± 0.8	163.6	31.9	18.7 ± 0.8
9	239.1 ± 1.0	217.3	50.6	28.8 ± 1.0

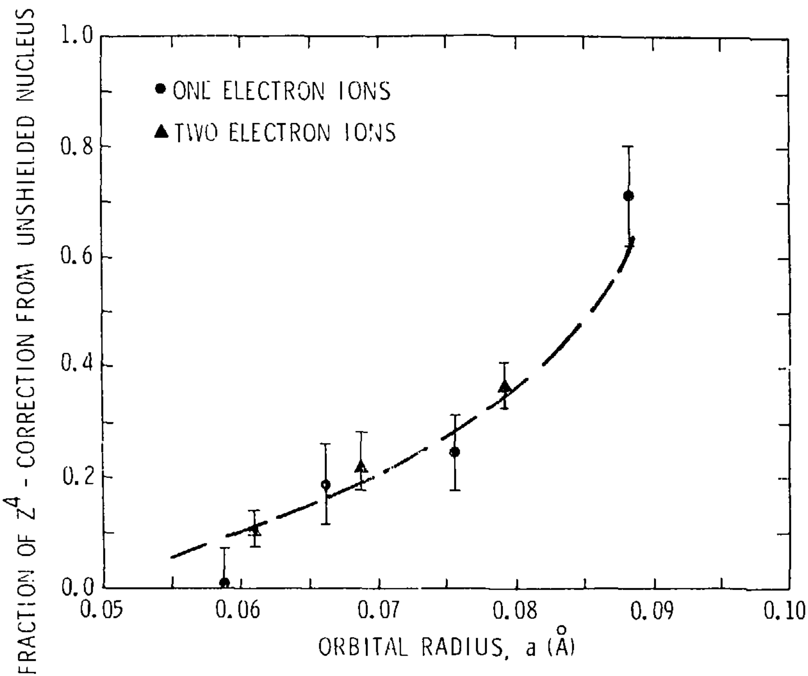
FIGURE CAPTIONS

Figure 1 Dependence of stopping cross section, S_e, on net charge, q, and nuclear charge Z_1. Dashed lines drawn through points to guide the eye. (After Datz, et al, reference 11)

Figure 2 Fraction, f, of projectile-electron collisions for which the Z^4-residual is produced by the unshielded nucleus versus projectile orbital radius.



0, 1, 2 ELECTRON IONS
CHANNELED IN {111} Au
v = 8.95 v0
q = Z1 - Ze
Se/q2 (10-15 eV-cm2/atom)
5.5
5.0
4.5
q = 5
6
7
8
4
5
6
7
8
9
10
Z1


ONE ELECTRON IONS
TWO ELECTRON IONS
FRACTION OF Z4 - CORRECTION FROM UNSHIELDED NUCLEUS
ORBITAL RADIUS, a (Å)
0.0
0.2
0.4
0.6
0.8
1.0
0.05
0.06
0.07
0.08
0.09
0.10