ELECTRONIC ENERGY LOSS

By

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ABSTRACT

An analytic method is described to allow one to calculate the stopping power of an ion travelling through matter. This method accounts for the electronic structure of the target as well as that of the ion. This has been shown to be important for a good prediction of channeling in crystals.

The electronic shells are introduced and the concept of the effective charge is viewed under the light of these shells.

1 - INTRODUCTION

In this work we outline an analytic method that expresses the electronic energy loss of an ion travelling through matter by means of the energy transfer to each electron of the medium. This procedure allows us to distinguish among the electrons of the target according to their position in space. This approach is important to account for the energy loss of an ion when the electronic part is important and when the electronic target distribution affect the results. This is the case of axial channeling in a crystal where the electronic loss is very decisive and very different whether the ion travels close to the axis (where the electron density is lowest) or away from it. The most significative parameter is thus the impact parameter (b) between the ion and the electron in question. The formalism accounts for the possible electronic distribution of the ion.

We work in a region of not too high energy to avoid plasmon excitation. This requirement can be easily removed and the formalism extended to include plasmon response from the medium.

In section 2.1 we develop the theory and give the most important formulas for the energy loss as a function of the impact parameter b, and the local electronic density. In section 2.2, and 2.3 we outline the method when the target electron distribution is described by a Thomas-Fermi distribution and also by a Shell Quantum Dynamic like that of Hartree-Fock. Thus the affect of the shell structure of the target on the electronic-energy loss of the ion may be studied. Finally in section 2.4 of the theoretical part we address the problem of Effective Charge.

In part 3 called Results and Discussions, we present the Energy Loss per Electron and an integral form of that energy suitable to be compared with more classical gross approaches like those of Firsov, Lindhard and Oen and Robinson. We also present in section 3 the effective charge of an ion described by a shell structure obtained from Hartree-Fock calculations.

2 - THEORY

The method we describe here allows us to write the stopping power as a function of the impact parameter. To correctly describe channelling we have found [1] that the stopping power at low incident energies must take into account the electron density distribution of the target as the ion travels through the channel. This means that the impact parameter must be used in the treatment of channelling in the low keV energy range.

The energy transferred from an ion to one electron in a gas may be written as

$$\Delta E = e \int_{-\infty}^{\infty} \boldsymbol{v} \cdot \boldsymbol{E}(t)\, dt ,$$

where **v** is the velocity imposed on the electron by the electric field **E**(t) generated by the ion at the electron position. **v** is proportional to the polarization. The ion has a velocity v_0 in the laboratory system and collides with the electron with an impact parameter b as illustrated in Fig. 1.

The electron field has components E_x and E_y along the x and y axis and the electron is located at a distance **r**(t) from the ion. Thus **r** and **E** are in the same direction.

The Fourier components of **E** and **r** are given by

$$E(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} E(\omega)\, e^{-i\omega t}\, d\omega ,$$

$$r(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} r(\omega)\, e^{-i\omega t}\, d\omega .$$

Since **E**(t) and **r**(t) are real **E***(w) = **E**(-w) and **r***(w) = **r**(-w). From the electromagnetic wave equations.

$$E_x(k,\omega) = -4\pi i k_x \frac{\varrho(k,\omega)}{\varepsilon(k,\omega)\, k^2} ,$$

$$E_y(k,\omega) = -4\pi i k_y \frac{\varrho(k,\omega)}{\varepsilon(k,\omega)\, k^2} .$$

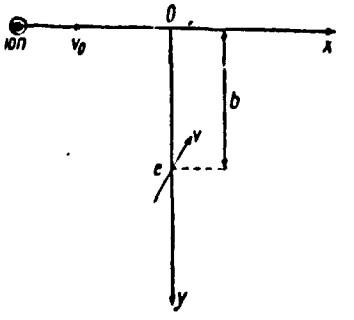

Fig. 1. Schematic of an ion with velocity v_0 approaching an electron in the medium with impact parameter b

The velocity of the electron is given by

$$v = \dot{r}(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} r(\omega)\,(-i\omega)\,e^{-i\omega t}\,d\omega$$

and

$$\Delta E = \mathrm{Re}\left\{\frac{e}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\omega\, d\omega'\, dt (-i\omega)\, e^{-i\omega t}\, r(\omega) \cdot E^*(\omega')\, e^{i\omega' t}\right\}.$$

Since $\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega' - \omega)t}\,dt = \delta(\omega' - \omega)$,

$$\Delta E = \mathrm{Re}\,\{e \int_{-\infty}^{\infty} d\omega(-i\omega)\, r(\omega) \cdot E^*(\omega)\}$$

$$= 2\,\mathrm{Re}\,\{e \int_{0}^{\infty} d\omega(-i\omega)\, r(\omega) \cdot E^*(\omega)\}.$$

The last equality is due to the fact that the integrand is its own complex conjugate for w<0, and therefore the real part for w<0 is equal to the real part for (-w).

The polarization P is given by

$$P = Ne\, r(\omega) = \frac{1}{4\pi}\,[\varepsilon(\omega) - 1]\, E(\omega),$$

where N is the number of electrons per unit volume. Thus

$$\Delta E = \frac{1}{2\pi N} \mathrm{Re} \int_{0}^{\infty} (-i\omega)\, \varepsilon(\omega)\, E(\omega) \cdot E^*(\omega)\, d\omega.$$

The vectors A(w) and B(w) are defined as

$$A(\omega) = \varepsilon(\omega)\, E(\omega) \quad \text{at} \quad r = (0, b, 0),$$

$$B(\omega) = E^*(\omega) \quad \text{at} \quad r = (0, b, 0).$$

Thus the energy transferred to each oscillator is given by

$$\Delta E = \frac{1}{2\pi N} \mathrm{Re} \int_{0}^{\infty} (-i\omega)\, [A(\omega) \cdot B(\omega)]\, d\omega$$

2.1 Example 1: Point charge

The density $\varrho(r,t)$ for a point charge is

$$\varrho(r, t) = Z_1 e\, \delta(r - v_0 t).$$

Therefore

$$\varrho(k, \omega) = \frac{Z_1 e}{2\pi} \delta(k \cdot v_0 - \omega).$$

The vectors A and B are calculated as follows:

$$A_x(\omega) = -\frac{2iZ_1 e}{(2\pi)^{3/2}} \int k_x \frac{\delta(\omega - k_x v_0)\, e^{ik_y b}}{k^2}\, dk$$

$$= -\frac{2iZ_1 e\omega}{(2\pi)^{3/2} v_0^2}\, a_x(\omega, b),$$

where

$$a_x(\omega, b) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{ik_y b}}{\frac{\omega^2}{v_0^2} + k_y^2 + k_z^2}\, dk_y\, dk_z .$$

and similarly with the other components of A and B.

Carrying out the integration in k_z first and later in k_y, a_x becomes

$$a_x(\omega, b) = 2\pi K_0\left(\frac{\omega b}{v_0}\right),$$

where K_0 is the modified Bessel function. Similarly,

$$a_y(\omega, b) = \frac{2i\omega}{v_0} K_1\left(\frac{\omega b}{v_0}\right),$$

where again K_1 is a modified Bessel function. In the calculation of B_x and B_y we must incorporate an expression for the dielectric constant, $\varepsilon(k,w)$. In the Random Phase Approximation (RPA) [2, 3] the dielectric constant may be written as $\varepsilon = \varepsilon_1 + i\varepsilon_2$, where

$$\varepsilon_1(k, \omega) = 1 + \frac{3\omega_p^2}{v_F^2 k^2}\left\{\frac{1}{2} + \frac{k_F}{4k} \times \right.$$

$$\times \left[\left(1 - \frac{\omega - (hk^2/2m)^2}{k^2 v_F}\right) \ln\left|\frac{\omega - kv_F - hk^2/2m}{\omega + kv_F - hk^2/2m}\right| + \right.$$

$$\left.\left. + \left(1 - \frac{\omega + (hk^2/2m)^2}{k^2 v_F^2}\right) \ln\left|\frac{\omega + kv_F - hk^2/2m}{\omega - kv_F + hk^2/2m}\right|\right]\right\},$$

$$\varepsilon_2 = \frac{\pi}{2}\left(\frac{\omega}{kv_F}\right)\frac{3\omega_p}{v_F^2 k^2} \qquad \text{for } \omega < kv_F - \frac{hk^2}{2m},$$

$$= \frac{\pi}{4}\left(\frac{k_F}{k}\right)\left(1 - \frac{\omega - hk^2/2m}{k^2 v_F^2}\right)\frac{k_F^2}{k^2} \qquad \text{for } kv_F - \frac{hk^2}{2m} \leq \omega \leq kv_F + \frac{hk^2}{2m},$$

$$= 0 \qquad \text{for } \omega > kv_F + \frac{hk^2}{2m}.$$

Since A.B must be pure imaginary and A_x is real while A_y is pure imaginary, we just need the imaginary part of B_x and the real part of B_y. Thus

$$\mathrm{Im}\,(b_x) = \int\int_{-\infty}^{\infty} \frac{dk_y\,dk_z \cos k_y b\, \mathrm{Im}\left(\frac{1}{\varepsilon^*}\right)}{\left(\frac{\omega^2}{v_0^2} + k_y^2 + k_z^2\right)} - \int\int_{-\infty}^{\infty} \frac{dk_y\,dk_z \sin k_y b\, \mathrm{Re}\left(\frac{1}{\varepsilon^*}\right)}{\left(\frac{\omega^2}{v_0^2} + k_y^2 + k_z^2\right)}.$$

Since $\mathrm{Re}(1/\varepsilon^*)$ is symmetric with respect to k_y, the second term is zero. In region (1) where $Z \leqq 1$,

$$\mathrm{Im}\left(\frac{1}{\varepsilon^*}\right) = \frac{2\gamma\omega\pi^2 k^3}{4\pi^2\omega^2 k^2 + (4\delta k_F + \pi k^2)^2 k^2} \qquad k \leqq 2k_F,$$

$$= 0 \qquad k > 2k_F,$$

where

$$\delta = 1/a_B, \qquad \gamma = 1/a_B^2 v_B,$$

a_B the Bohr radius, and v_B the Bohr velocity. Let us introduce cylindrical coordinates so $dk_y\,dk_z = k'dk'd\varphi$ and $k'^2 = k_y^2 + k_z^2$ and $k^2 = k'^2 + w^2/v_0^2$. In $\mathrm{Im}(1/\varepsilon^*)$ terms with w^2 may be neglected even in the case where $k' \longrightarrow 0$ since for $w \longrightarrow 0$ and $k' \longrightarrow 0$, $\mathrm{Im}(1/\varepsilon^*) \longrightarrow 0\,(w)$ independently of terms containing w^2.

Thus

$$\mathrm{Im}\left(\frac{1}{\varepsilon^*}\right) = \frac{2\omega\pi^2\gamma k'}{(4k_F\delta + k'\pi)^2} \qquad k' < 2k_F,$$

$$= 0 \qquad k' > 2k_F.$$

We may now write

$$\mathrm{Im}\,(b_x) = 4\omega\pi\gamma\beta_1(k_F, b),$$

where

$$\beta_1 = \frac{1}{\pi}\int_0^{k'_{max}} dk' \frac{1}{(a^2 + k'^2)^2} \int_0^{\pi} d\varphi \cos(k'b\cos\varphi)$$

$$= b^3 \int_0^{x_{max}} \frac{J_0(x)}{(a^2 + x^2)^2}\,dx,$$

where $a = 2\sqrt{k_F\delta/\pi}$ and $x = ab$ and $x = k'b$.

Similarly

$$\mathrm{Re}\,(b_y) = \mathrm{Re}\int_0^{\infty} dk' k'^2 \int_0^{2\pi} \frac{\cos\varphi\, e^{-ibk'\cos\varphi}}{\left(\frac{\omega^2}{v_0^2} + k'^2\right)\varepsilon^*(\omega, k')}\,d\varphi.$$

Now

$$\int_0^{2\pi} \cos\varphi\, e^{-ibk'\cos\varphi}\,d\varphi = \int_0^{2\pi} \cos\varphi\cos(k'b\cos\varphi)\,d\varphi -$$

$$- i\int_0^{2\pi} \cos\varphi \sin(k'b\cos\varphi)\,d\varphi.$$

From symmetry considerations the first term is zero. So we are left with the second term and consequently we must use the imaginary part of $(1/\varepsilon^*)$ again.

By integrating by parts

$$\int_0^{\pi/2} \cos\varphi \sin(k'b\cos\varphi)\,d\varphi = k'b \int_0^{\pi/2} \sin^2\varphi \cos(k'b\cos\varphi)\,d\varphi ,$$

then

$$\mathrm{Re}(b_y) = 4\omega\tau\gamma\beta_2(k_F, b) ,$$

where

$$\beta_2 = b^2 \int_0^{x_{max}} dx \frac{xJ_1(x)}{(a^2 + x^2)^2} .$$

2.2 Example 2: Cloud Charge

Assume a cloud of electrons around the Nucleus Z_1 with a density distribution

$$\varrho_c(r, t) = \frac{eN_1Z_2^3}{\pi} e^{-2Z_2|r - v_0t|} .$$

This distribution corresponds to a hydrogen 1s type of electron wave function where Z_2 is an effective charge that may be determined by some minimization procedure as in the variational method explained by Schiff, [4] or as in the paper of Ferrel and Ritchie [5]. N_1 stands for the number of electrons in the cloud. The Fourier transform of $\varrho_c(r,t)$ is

$$\varrho_c(k, \omega) = \frac{N_1Z_2^4 e\,\delta(k \cdot v_0 - \omega)\,8}{(k^2a_B^2 + 4Z_2^2)^2\,\pi} .$$

As in the example 1 we must calculate the vectors A and B which we separate into two parts

$$A = A_p + A_c ,$$
$$B = B_p + B_c .$$

A_p and B_p were derived in the example 1 since they are due to the point charge Z_1 or nuclear part. We now proceed to calculate A_c and B_c due to the cloud distribution of the N_1 bound electrons. The total charge density may be, of course, written as

$$\varrho = \varrho_p + \varrho_c = Z_1e\,\delta(r - v_0t) - \frac{N_1eZ_2^3}{\pi} e^{-2|r - v_0t|/a_0}$$

and the total loss is

$$\Delta E = \frac{1}{2\pi N_1} \mathrm{Re} \int_0^\infty (A \cdot B)(-i\omega)\,d\omega .$$

In this part we are just going to calculate A_c and B_c. They result in:

$$(A_c)_z = \frac{-4\pi ie}{(2\pi)^{3/2}} \int k_z \frac{\varrho_c\, e^{ik_z b}}{k^2}\, dk = \frac{32\pi i}{(2\pi)^{3/2}} N_1 e Z_2^4 \int k_z \frac{e^{ik_z b}\, \delta(k_z v_0 - \omega)\, dk}{(k^2 + 4Z_2^2)^2\, k^2}$$

$$= \frac{32\pi i N_1 e Z_2^4 \omega}{(2\pi)^{3/2} v_0^3} (a_c)_z ,$$

where $$(a_c)_z = \int \frac{e^{ik_y b}\, dk_y\, dk_z}{k^2 (k^2 + 4Z_2^2)^2} ,$$

where again

$$k^2 = \left(\frac{\omega}{v_0}\right)^2 + k_y^2 + k_z^2 .$$

Similarly

$$(A_c)_y = \frac{4\pi i}{(2\pi)^{3/2}} \int \frac{k_y\, 8 N_1 e Z_2^4\, e^{ik_z b}\, \delta(k_z v_0 - \omega)}{k^2 \pi (k^2 + 4Z_2^2)^2}\, dk$$

$$= \frac{4\pi i}{(2\pi)^3} \frac{8 N_1 e Z_2^4}{\pi} (a_c)_y ,$$

where $$(a_c)_y = \int \frac{k_y\, e^{ik_y b}\, dk}{\left[\frac{\omega^2}{v_0^2} + k_y^2 + k_z^2\right]\left[\frac{\omega^2}{v_0^2} + k_y^2 + k_z^2 + 4Z_2^2\right]^2} .$$

2.3 Quantum Mechanics Description for the Projectile-Electron Cloud

The Fourier transform of the projectile density $\rho(k,w)$ can be analytically determined from the Hartree-Fock $\rho(r)$. According to Clementi and Roetti [6], the electron wave function may be written

$$\Phi_{ilm} = \Sigma_n X_{nlm} C_{iln},$$
$$X_{nlm}(r,\theta,\Phi) = R_{nl}(r)\, Y_{lm}(\theta,\Phi)$$

Here, the index i refers to the ith orbital; the subscript n refers to the nth basis function of magnetic quantum number m and angular momentum l. R_{nl} represents the radial parts of the wave functions and Y_{lm} the spherical harmonics.

In the Hartree-Fock calculation Clementi et al., in agreement with Roothaan et al.[7], used the following form:

$$R_{nl}(r) = \Sigma_j a_j r^{n_j} e^{-\alpha_j r}$$

The radical density (electrons per unit volume) is

$$\rho(r) = \Sigma_{nl} N_{nl} R_{nl}^2(r)/4\pi,$$

where N_{nl} is the number of electrons in the (n,l)th shell. Naturally, the integral of $\rho(r)$ over the whole space is N, the total number of electrons in the atom.

It is customary to use a shell density $\rho_{nl}(r)$ such that

$$N = \Sigma_{nl} \int_0^\infty \rho_{nl}(r)\, dr .$$

Thus, $\rho_{nl}(r) = N_{nl} r^2 R_{nl}(r)$.

The product (rR_{nl}) is sometimes indicated by ρ_{nl} .

In general (e.g., for deformed shells), ρ will depend on the angular coordinates. However, in this work the time-dependent part of ρ is obtained by assuming a rigid motion of the whole cloud system, with ρ a function only of the radial coordinate.

Therefore,

$$\rho(r) \longrightarrow \rho(r-v_1 t),$$

where v_1 is the velocity of the ion with nuclear charge Z_1 and r is now the vector position. The Fourier transform of $\rho(r-v_1 t)$ is

$$\hat{\rho}(k,w) = \frac{1}{4\pi^2} \int e^{i(k\cdot r - wt)}\, \rho(r-v_1 t)\, dr\, dt .$$

Using the change of variable $u = r - v_1 t$, we obtain

$$\hat{\rho}(k,w) = \sqrt{(2\pi)}\, \delta(k\cdot v_1 - w)\, D(k), \text{ where}$$

$$D(k) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} e^{ik\cdot u}\, \rho(u)\, du .$$

Hence, the time-dependent part of appears only in the delta function. (Now we revert to the usage $k = |k|$, $r = |r|$.)

According to the previous description of (r), its radial part (or average over angle) is for each shell of the form.

$$\rho(r) = \Sigma_\lambda a_\lambda r^{\beta_\lambda} e^{-\gamma_\lambda r} .$$

The Fourier transform of this function is

$$D(k) = \frac{1}{2\pi k} \Sigma_\lambda a_\lambda \left[(1+\beta_\lambda) \frac{\gamma_\lambda^2 + \beta_\lambda}{(\gamma_\lambda^2 + k^2)^{2+\beta\lambda}} \sum_{i=0}^{(1+\beta_\lambda)/2} (-1)^i \binom{\beta_\lambda + 2}{2i+1} \left(\frac{k}{\beta_\lambda}\right)^{2i+1} \right] .$$

2.4 Concept of Effective Charge

Almost all formalisms (including ours) yield a stopping power

$$S = z_1^2 \, f\,(v_1, z_2, b),$$

in which the function f does not involve the charge z_1. It is found experimentally that the ratio between the stopping power S for the z_1 ion and S_p for a proton is nearly independent of the quantum structure of the target element. Specifically, we may define an effective charge z_1^* by

$$S = z_1^{*2} f_p(v_1, z_2, b),$$

with z_1^* almost independent of the detailed shell structure of the target. This observed independence is closely related to one of the conclusions of the present work, namely that only the valence electrons are relevant to the value of z_1^*.

It is worth noting that we do not address here the relation between the actual charge of an ion inside the material and the charge measured outside. In transmission experiments it is possible to analyze the ion and determine its charge, but the relation between the charge inside the material and outside it is difficult to determine. It touches upon quantum mechanical problems of the variation of the Hamiltonian of an ion as it goes from the bulk toward the surface and out of the target material. We will simply regard z_1^* as being defined by the previous equation.

Inasmuch as the results which follow are (as in Ref. 8) for boron in silicon, we will now refer specifically to boron as the ion and silicon as the target. As the boron atom moves through the silicon target material (fig. 2) it may excite an electron at position b. This electron belongs to the silicon, whose local electron density is $\rho(r)$, r being the distance between the silicon nucleus and the electron. The local density determines the response function of the medium for the target electron, which sees an effective Coulomb field from the ion which is lower than the field due to the point charge z_1 (5, for boron).

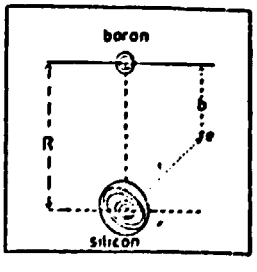

Fig. 2. The boron atom at a distance R from the silicon atom. An electron e of the silicon cloud is at a distance r from the silicon nucleus.

The difference is due to the electron charge of the boron ion, which is inside a sphere of radius b. The boron atom, which is assumed to have been singly ionized, has two shells, $(1s)_2$ and $(2s)_2$, each with two electrons. If the target electron is outside the outer $(2s)_2$ shell the field between the ion and this electron is due to $5^{(+)}+4^{(-)}=1^{(+)}$ unit of charge. However, if the target electron is inside the second shell the field at b will be due mainly to $3^{(+)}$ charges.

This simple picture, which is originally due to Brandt and co-workers (see for instance Ref. 9) is used in this paper. We work in the energy regime where the assumption that the boron atom retains 2 electrons in the (1s) shell and 2 in the (2s) shell is plausible. Also, we use a response function (dielectric constant) derived form electron-hole excitation without plasmon excitation.

The effective charge ratio calculated in this work is defined by

$$(Z_1^*/Z_1)^2 = S(R) / S_p(R) ,$$

where S(R) is the total (cloud plus point) stopping power of boron completely dressed with its 4 electrons, and $S_p(R)$ is for boron treated as a point charge with 5 protons.

3. Results and Conclusions

3.1 Point Charge Case

Except where noted, atomic units are used: that is, energy in Hartree and distances in Bohr radius.

In Fig. 3 we show ΔE, energy loss per electron, as function of the impact parameter b. The upper curve responds to the bare ion (in this case for boron Z_1=5) and the other to the ion with an electron cloud of 3,3.5 and 4 electrons. The target was Si with an average electron cloud corresponding to the one electron radius, r_s=0.1047 nm. This value corresponds to the average electron density in [110] channel of the Si crystal. All curves show a systematic oscillation with a wavelength of the order of 0.1 nm.

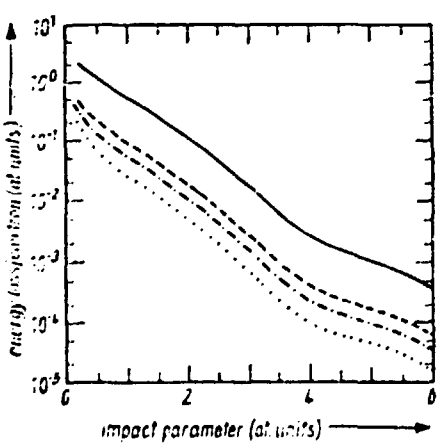

Fig. 3. Energy loss/electron as a function of impact parameter for boron incident on a silicon target with r_s=0.1047nm. Results are plotted for the boron ion modeled as a point charge (-----) and with and electron cloud of 3.0(- - -), 3.5 (-.-),and 4.0 (....) electrons. The incident velocity is $0.06v_B$, where v_B is the Bohr velocity. The impact parameter is given in terms of a_B, the Bohr radius; energy is given in terms of E_B=27.2eV.

These oscillations are of quantum origin and arise form the assumption of a zero temperature Fermi gas for the target electron gas. As the temperature rises the oscillations are damped. [8]

3.2 Cloud Charge Case

We have found that the energy loss (ΔE) per electron is very dependent upon the electronic structure of the light ion $^{10}_{5}B$. However, the internal Si structure is practically irrelevant--only the four valence electrons $(3s)_2$ and $(3p)_2$ are important. This is because the high density of its inner core generates high Fermi momenta, and so the imaginary part of the response function ε and also $Im(1/\varepsilon)$ are very small.

It is apparent from our calculations that the maximum energy transfer is experienced by those target electrons close to the boron nucleus, where the coulomb field generated by the ion is greatest. When boron is approximated by a single $(1s)_4$ shell, as in our preceding paper [8] and in the one of Brandt et al [9], we see that ΔE_{total} is increased by as much as a factor of 4 with respect to the standard case: $(1s)_2$, $(2s)_2$.

Shown in Fig. 4 as a function of the nuclear impact parameter $\underline{R}$ is the stopping power $\underline{S}$, calculated by

$$S(R) = \int_0^\infty 2\pi r\, p(r)\, \Delta E(r,R)\, dr \quad ,$$

where $\Delta E(r,R)$ is the energy loss per electron at the position $\underline{r}$. Also shown in Fig. 4 is the point stopping power $S_p(R)$ corresponding to a ΔE generated exclusively by the boron point charge (5 protons). S is always smaller than S_p, due to the screening effect of the boron electron cloud. The range of $\underline{R}$ (but not of $\underline{r}$) used in these calculations is of course much broader than would be realistic for an actual boron in silicon case.

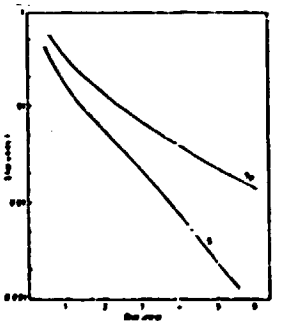

Fig. 4. Stopping power as a function of $\underline{R}$, minimum distance between the silicon and boron nuclei. S_p is due only to the boron nucleus (charge 5^+), while S is the net when the 4-electron boron cloud is included. (Boron energy = 1 kev.)

In Fig. 5 the effective charge ratio Z_1^*/Z_1 is presented for the 1-kev case; this ratio varies from ≈ 1.0 when $R \approx 0$ to ≈ 0.2 when R is large. For large R all the silicon atoms will see the boron atom as $5^{(+)} + 4^{(-)} = 1^{(+)}$ point charge. For smaller R we easily can find silicon valence electrons that see the boron screened only by its (1s) electrons; the contributions of such target electrons cause the effective charge ratio always to be strictly less than 1 and greater than 0.2.

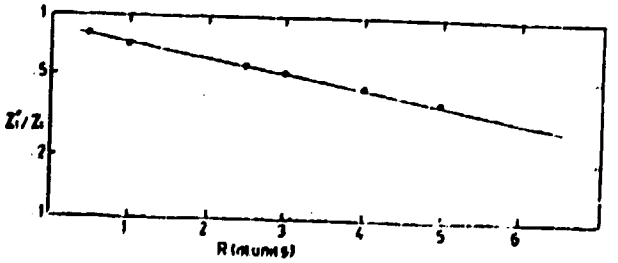

Fig. 5. Effective charge ratio for 1-kev boron on silicon as a function of $\underline{R}$, minimum distance between the silicon and boron nuclei. At 10 kev this ratio is almost unchanged.

In addition to these 1-kev calculations we have done some with E_0=10 kev. Since ΔE is proportional to V_0, the calculated values of ΔE increased by the factor $\sqrt{10}$. However, the effective charge ratio was virtually unchanged.

3.3 Comparison with Experiment and Other Work

It is very difficult to have a direct comparison of this work with experimental results. We must somewhat average the energy loss ΔE per electron over target-projectile configurations in order to obtain values which can result from experimental measurements.

As the averages are done the impact parameters b disappear from the function f of section 2.4 and the new analytic expression may show a Z_1 dependency different from that of expression S for the stopping power. Thus, when we perform the comparison of our average stopping power with the formulas given by Firsov or Oen and Robinson or Lindhard this implicit Z_1 and Z_2 dependency must be kept in mind.

Fig. 6 provides a comparison with our average stopping power with these given by Firsov [11] and Oen and Robinson [12].

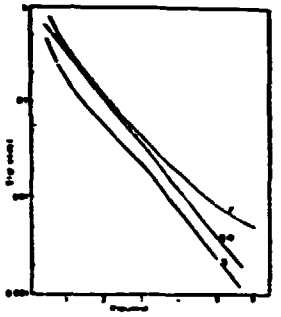

Fig. 6. Stopping power S calculated in this work, compared with the predictions of Firsov (F) and of Oen and Robinson (O-R) (exponential). R is the minimum distance between the silicon and boron nuclei. (Boron energy = 1 kev.)

The Firsov predictions were derived from the formula

$$S(R) = \frac{(Z_1+Z_2)^{5/3} \cdot 4.3 \cdot 10^{-8} \cdot V_1}{(1 + 0.31 \cdot (Z_1+Z_2)^{1/3} \cdot R)^5}$$

in ev/Å, where V_1 is in cm/sec and R in A. His predictions are seen to exceed our S(R) by a factor of two (at a typical distance of 2.5 at.units) or more. Oen and Robinson's exponential result also exceeds ours, but only by roughly 65%, uniformly over the entire range.

In addition, Lindhard's prediction of average stopping power is given by the formula

$$S = \frac{Z_1^{1/6} \cdot 8\pi \, \hbar \, a_B \, Z_1 Z_2 \, p \, V_1}{(Z_1^{2/3} + Z_2^{2/3})^{3/2}}$$

in energy/unit length, where p is the atomic density of the target ($5 \cdot 10^{22}$/cc for silicon), V_1 the ion velocity and a_B the Bohr radius. For E_0= 1 kev the Lindhard formula gives an average S of 0.041 at.units, which corresponds to our calculated S at $R \approx 2.4$ at.units. This value of R is, as it ought to be, less than the average interatomic distance in silicon, which is about 3 at.units. It is also large enough that the corresponding deflection of the boron ion, based on calculation with a Moliere potential, is only about 2° for 1 kev, and the dominant stopping mechanism is electronic.

Our stopping power calculations for boron in silicon are highly dependent upon the boron shell structure; however, they appear consistent with Lindhard's prediction. When the stopping power is expressed as a function of the nuclear impact parameter R, our predictions, as well as those of Oen and Robinson, fall below those of Firsov by about a factor of two.

There is, unfortunately, no experimental data available at low energies from which to infer effective charge. The work of Brandt and Kitagawa [9] would predict a value of 0.3 for Z_1^*/Z_1 when the boron ion is assumed to have 4 electrons in its cloud. This value agrees with what we calculate (for a nuclear impact parameter of 2.5 at.units) when we concentrate all 4 electrons in the boron (1s) shell. We previously, like Brandt and Kitagawa, have employed a single shell whose exponential function was obtained by a minimization procedure, so it is not surprising to get the same result.

As we include the (2s) shell (that is, when the 4 boron electrons are split between the (1s) and (2s) shells) we obtain the higher value of 0.6 for Z_1^*/Z_1 (when R=2.5). This is due to the fact that the screening effect is less pronounced; electrons from the target may see just the two electrons of the boron (1s) shell. In order to get a value of Z_1^*/Z_1 as small as 0.3 the majority of the target electrons must see the ion dressed with 4 electrons, which requires an R of 6 at.units or greater (unphysically large for boron in silicon).

We have shown here that the quantum shell structure of boron has a strong effect on its stopping power as it moves through a silicon target. Our continuation of these calculations to other ion-target combinations is expected also to show strong shell effects.

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