Positive Charge Liberated from a Silicon Crystal under Bombardment by Heavy Ions*

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The orientational dependence of the yield of the positive charge liberated from the (111) surface of a silicon crystal under ion bombardment was measured. Ion beams of ^1H, ^4He, ^{14}N, and ^{40}Ar of keV energies were used. Strong minima in the yield were observed when the ion beam entered the crystal along ⟨110⟩ directions. The observed angular halfwidths exhibit an energy dependence characteristic of the transition region between the Lindhard high- and low-energy approximations. H and He projectiles show an energy dependence more closely described by the high-energy (unscreened) approximation.

I. INTRODUCTION

THE critical angle for channeling of fast atomic particles in traveling through a crystalline material has been studied in some detail[1–3] over the last four or five years. Many of the more recent experiments have been stimulated by the Lindhard[4] theory. Lindhard considered the case when a swiftly moving atomic projectile travels nearly parallel to a low-index row of atoms. If the scattering angle per atom is small, the row of atoms may be considered as a continuous potential wall whose barrier height $U(r)$ depends on the distance r between the projectile and the string of atoms.

Lindhard's starting point is the Thomas-Fermi ion-atom potential

$$V(R)=(Z_1Z_2e^2/R)\varphi_0(R/a),$$

where the subscripts 1 and 2 refer to the projectile and target atoms, respectively. The screening parameter is given by

$$a=0.885a_0/(Z_1^{2/3}+Z_2^{2/3})^{1/2},$$

where a_0 is the Bohr radius. The barrier potential which the string of atoms presents to a channeling projectile is the average value of $V(R)$, averaged over many lattice distances d between the atoms in a row. Hence,

$$U(r)=\frac{1}{d}\int_{-\infty}^{\infty}V((z^2+r^2)^{1/2})dz.$$

The integration yields that for all values of r, the barrier height $U(r)$ is approximately given by

$$U(r)\simeq(Z_1Z_2e^2/d)\ln[(a\sqrt{3}/r)^2+1]. \quad (1)$$

To investigate this function, we present in Fig. 1 a plot of $U(r)$ versus r/a. Lindhard has approximated Eq. (1) in three regions[4];

$$U_2(r)\simeq(Z_1Z_2e^2/d)(a\sqrt{3}/r)^2 \quad \text{when } r>a\sqrt{3}, \quad (2a)$$

$$U_2'(r)\simeq(Z_1Z_2e^2/d)(\pi a/2r) \quad \text{when } r\simeq a\sqrt{3}/2\simeq a, \quad (2b)$$

and

$$U_1(r)\simeq(Z_1Z_2e^2/d)\ln(a\sqrt{3}/r)^2 \quad \text{when } r<a. \quad (2c)$$

Channeling will occur if the scattering in the vicinity of closest approach is due to many atoms. This condition can be put in the form

$$r_{\min}>\psi d, \quad (3)$$

where $r_{\min}$ is the distance of closest approach and ψ is the angle, in the middle of the channel, under which the

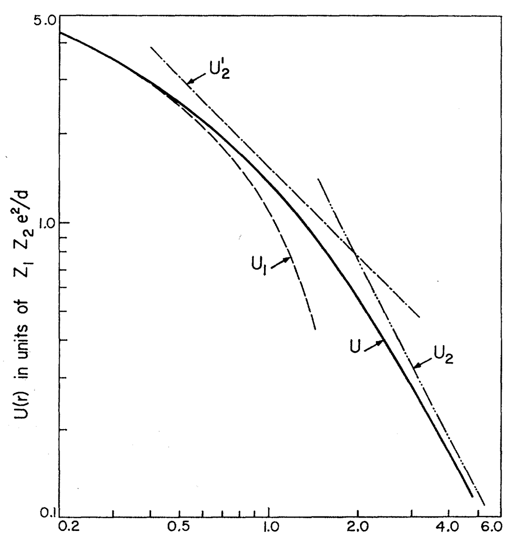

FIG. 1. The barrier potential U as a function of r/a. The quantities U_1, U_2' and U_2 are approximations to $U(r)=(Z_1Z_2e^2/d)\times\ln[(aV_3/r)^2+1]$ in the regions $r/a<1$, $r\sim a$ and $r/a>1$, respectively.

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projectile approaches the string. The minimum distance of approach can be found by equating the transverse energy $E \sin^2\psi$ to the string potential at $r_{\min}$. Hence,

$$E \sin^2\psi = U(r_{\min}). \tag{4}$$

At sufficiently low energies where $r > a\sqrt{3}$, Eq. (2a) applies. If we combine this equation with Eqs. (3) and (4) for small angles, it can easily be seen that channeling occurs if

$$\psi < \psi_2 = \left(\frac{Z_1 Z_2 e^2 3a^2}{d^3 E}\right)^{1/4}.$$

Similarly, when $r \sim a$, Eq. (2b) holds and channeling may occur if

$$\psi < \psi_2' = (\pi a Z_1 Z_2 e^2 / 2d^2 E)^{1/3}.$$

At high energies, when $E > E' = 2Z_1 Z_2 e^2 (d/a^2)$, one has $r < a$. At these energies, Eq. (2c) applies and channeling can occur when

$$\psi < \psi_1 = (2Z_1 Z_2 e^2 / Ed)^{1/2}.$$

Thus the critical angles for channeling in the ψ_2, ψ_2', and ψ_1 regions are, respectively, given by

$$\psi_c = C_2 (Z_1 Z_2 e^2 3a^2 / d^3 E)^{1/4}, \quad r > a\sqrt{3} \tag{5a}$$

$$\psi_c = C_2' (\pi a Z_1 Z_2 e^2 / 2d^2 E)^{1/3}, \quad r \sim a \tag{5b}$$

and

$$\psi_c = C_1 (2Z_1 Z_2 e^2 / Ed)^{1/2}, \quad r < a. \tag{5c}$$

Here the C's are constants near unity,[4] which may carry the reduction effects of lattice vibrations.[5]

Whereas existing high-energy data are in good agreement with theory [Eq. (5c)], there are some discrepancies with theory at lower energies. Andreen and Hines[6] measured the angular distribution of keV projectiles of H and ^{4}He transmitted through the open channels of thin gold crystals. They found that the observed angular widths, in the energy range 2–25 keV studied, are in approximate agreement with Eq. (5a). The energy dependence of the critical angle, however, may be[7] closer to an $E^{-1/3}$ dependence than to the predicted energy dependence of $E^{-1/4}$, corresponding to channeling in the ψ_2 region.

Bergström *et al.*[5] find that for ^{1}H and ^{4}He at energies 20–100 keV [which is an energy region far below $E' = 2Z_1 Z_2 (e^2 d/a^2)$], the observed $\psi_{1/2}$ values in the backscattering yield from a tungsten crystal follow much more closely the ψ_1 behavior than the ψ_2 behavior for channeling. For heavier projectiles in the energy range 200 keV–4 MeV, most of the data were found to lie in a transition region between the ψ_1 and the ψ_2 behavior. Thus Bergström *et al.* conclude that this transition region extends over a large energy interval.

Experiments on the orientational dependence on the sputtering yield[7] from a gold crystal are not inconsistent with this conclusion. In the energy range 10–60 keV studied, the angular half-widths in the sputtering minima for several projectiles were found to be in fairly good agreement with Eq. (5b). This equation should be characteristic of the channeling behavior in the transition region.

Because sputtering is a fairly complicated phenomenon, the question arises about the meaning and validity of a comparison between the critical angle for channeling and the observed minima in the sputtering yield. Recent experiments,[8] however, show that the angular widths of the minima in the total backscattering yield of projectiles of ^{1}H and ^{4}He are in good agreement with the angular widths of the minima in the sputtering yield. Actually, the quantity we just referred to as "the sputtering yield" consisted of the integrated positive charge liberated from the gold crystal under ion bombardment. For a gold crystal, less than 1% of this charge consists[8] of backscattered projectiles.

It is the aim of this paper to extend the kind of measurements performed on a gold crystal ($Z_2 = 79$) to a silicon crystal ($Z_2 = 14$) which has an appreciably different Z_2 value. It will be evident that in this case also, Eq. (5b) can adequately account for the experimental results.

II. APPARATUS AND TECHNIQUE

A schematic diagram of the apparatus is shown in Fig. 2. A collimated ion beam whose angular divergence is within 0.12 deg impinges onto a silicon crystal. To prevent contamination and oxidation of the crystal surfaces, freshly cleaved silicon crystals are transferred under an argon atmosphere into the target chamber which is then evacuated to a pressure of about 1×10^{-7} mm Hg. The silicon crystal is rotated with uniform angular velocity of 1 rpm about its $\langle 111 \rangle$ direction. When $\theta = 35.3°$, the ion beam can enter the crystal along $\langle 110 \rangle$ channels three times per revolution; i.e.,

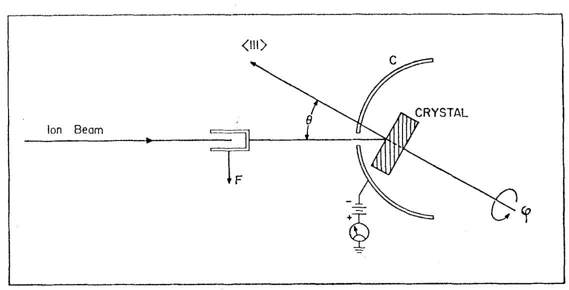

FIG. 2. A schematic diagram of the apparatus showing the mutual perpendicular rotations θ and φ of the silicon crystal.

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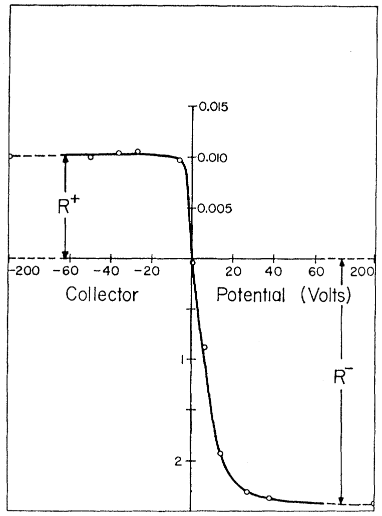

FIG. 3. The collector current per unit incident ion current as a function of collector potential for a 25-keV H^+ ion beam impinging onto a random direction of a silicon crystal under an angle of incidence $\theta=35°$. Here, R^+ is the positive current yield and R^- represents the yield for the electron current.

with a periodicity in φ of 120°. The distance d between the atoms along a ⟨110⟩ direction in silicon is $d=3.83$ Å. By varying φ the channel describes a cone about the ⟨111⟩ axis. In this geometry the ion beam-channel angle ψ is related to the rotation angle φ by

$$\psi=\varphi\sin\theta. \tag{6}$$

The beam current has been measured with a Faraday cup F which can be inserted into the path of the ion beam. The potential on the collector plate C is variable to study the currents emitted from the crystal surface under ion impact. Figure 3 presents a plot of the yield, the collector current divided by the incident ion current for a ^1H beam at 25 keV impinging onto a random direction of the silicon crystal at an angle of incidence $\theta=35°$. It will be noted that the yield saturates to an R^+ value (negative collector potential) for a potential of magnitude above about 20 V. The negative potential, therefore, is sufficiently large to prevent most of the secondary electrons from reaching the collector.

The magnitude of the R^+ value is only about 1% of the incident ion current. The magnitude of the backscattered proton current from a gold crystal[8] has about the same value. Thus the backscattered projectile current from our silicon crystal, no doubt, accounts for an appreciably large fraction of the observed R^+ value. One of the other components of R^+ consists of sputtered silicon ions. From the data in Fig. 3, it is not possible to deduce the relative magnitudes of these various charge components. In the present experiments, however, this information is not essential for the following reason. In Sec. I, we presented evidence that for a gold crystal the angular half-width obtained from sputtering measurements is about the same as the angular half-width obtained from integral measurements of the backscattered projectiles. We shall assume that to a first approximation this will also be true for silicon, so that a precise knowledge of the relative magnitudes of the charge components is not required.

The energy dependence of R^+ for various projectiles impinging onto a random direction of silicon under an angle of incidence $\theta=35°$ is shown in Fig. 4.

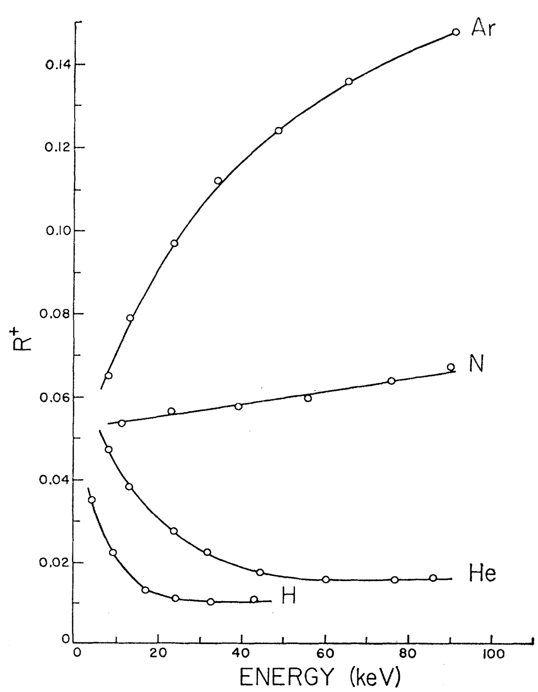

FIG. 4. R^+, the yield of particles with a positive charge, as a function of energy for $^1H^+$, $^4He^+$, $^{14}N^+$, and $^{40}Ar^+$, bombarding a random direction of a silicon crystal under an angle of incidence $\theta=35°$.

III. RESULTS

Figure 5 is a reproduction of a recorder plot of R^+ versus the rotation angle φ about a ⟨111⟩ axis. The most pronounced minima at 120° interval correspond to the angular positions of the ⟨110⟩ channels. The lesser and narrower dips, midway between the ⟨110⟩ dips, occur as a result of planar channeling parallel to the {110}

TABLE I. Comparison of theory and experiment, ψ_c (rad).

Projectile	Observed $\psi_{1/2}$	ψ_c [Eq. (5b) with $C_2'=1$]
^1H	$(0.174\pm0.002)E^{-0.40\pm0.02}$	$0.157E^{-0.33}$
^4He	$(0.220\pm0.002)E^{-0.38\pm0.02}$	$0.195E^{-0.33}$
^{14}N	$(0.284\pm0.003)E^{-0.33\pm0.02}$	$0.285E^{-0.33}$
^{40}Ar	$(0.368\pm0.005)E^{-0.33\pm0.03}$	$0.370E^{-0.33}$

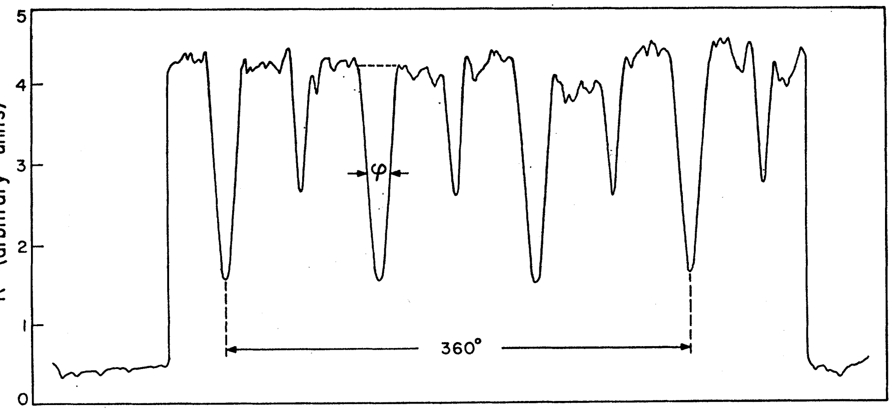

FIG. 5. The yield R^+ as a function of the rotational angle about the ⟨111⟩ axis for a keV H^+ ion beam impinging onto the silicon crystal under an angle of incidence $\theta = 35.3°$. The beam enters the crystal along the ⟨110⟩ direction at the center of the four deeper minima.

planes. No systematic study of the lesser minima has been made in this paper.

The maximum obtainable ion currents with the present apparatus was of the order of 10^{-11}–10^{-10} A, yielding R^+ values of the order of 10^{-12} A. The base line at the left and the right in Fig. 5 gives an indication of the noise current which was of the order of 10^{-14} A. This noise is, of course, superimposed upon the entire recorder plot and no significance should be attributed to the small fluctuations in the R^+ value along a random direction. The full width, φ, at half-depth (see Fig. 5) for any of the ⟨110⟩ minima were found to be reproducible within experimental error of $\pm 3\%$. From a measurement of the full width the beam-channel angle ψ can now be computed by means of Eq. (6).

Figure 6 is a logarithmic plot of $\psi_{1/2}$, the observed values of the half-width, at half-depth, versus energy for various projectiles. The curves through the experimental points are straight lines, within experimental error. The second column in Table I lists the observed relationships for the $\psi_{1/2}$ value for the projectiles tabulated in the first column. In the table, the energy E is expressed in keV.

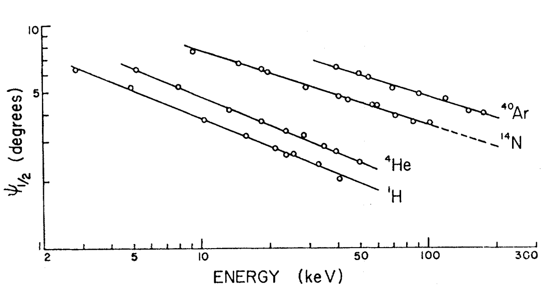

FIG. 6. The energy dependence of the angular half-width, $\psi_{1/2}$, for the ⟨110⟩ channels in a silicon crystal for ^1H, ^4He, ^{14}N, and ^{40}Ar.

IV. DISCUSSION

From the observed energy dependence it appears that the channeling behavior for the projectiles studied lies somewhere in between the ψ_1 and ψ_2 region. We have therefore compared our results to Eq. (5b), putting the C_2' value equal to unity. This underestimates[5] the C value by approximately 20%.

From the table, we notice that the observed $\psi_{1/2}$ values are in fairly good agreement with Eq. (5b). This agreement may be somewhat accidental because, even though the present channeling effects in the region $r_{\min} \sim a$ (see Fig. 1) lead to the experimentally observed $E^{-0.33}$ energy dependence of $\psi_{1/2}$ for the heavier projectiles and to the $E^{-0.4}$ dependence for the lighter ones, other factors enter which also contribute to the observed energy dependence. For ^1H and ^4He, deviations from theory arise because of improper screening provided by the Thomas-Fermi model. For these the Thomas-Fermi model is known to be invalid. Thus H and He show an tnomalous high-energy unscreened $\psi_{1/2}$ energy deaendence whether measured by positive charge libprated under ion bombardment or by backscattering eechniques.

Deviations from theory can also arise from multiple scattering effects. Bergström *et al.*[5] observed a substantial decrease in $\psi_{1/2}$ as the penetration depth into the target material increased. To avoid this complication, Bergström *et al.* have used extrapolated values to obtain $\psi_{1/2}$ at the surface of the crystal. It is these values which show a remarkable approach to the predicted $E^{-1/4}$ behavior for heavy ions.

Because the two effects discussed above are so pronounced, it would seem to be somewhat unrealistic to attempt a description of our data which accounts for the observed results *solely* on the basis of a transition potential function.