Energy-Loss Spectra of Channeled Iodine and Oxygen Ions in Gold*

B. R. Appleton, Sheldon Datz, C. D. Moak, and Mark T. Robinson
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830
(Received 2 November 1970)

Energy-loss spectra are reported for 15- and 21.6-MeV ^{127}I ions and for 10-MeV ^{16}O ions transmitted through the {111} and {100} planar channels of thin gold crystals. In agreement with earlier observations on 60-MeV ^{127}I and 3-MeV ^{4}He ions, the stopping power in each case is accurately proportional to the frequency with which the ions oscillate in traversing the channel. From the results of these experiments, it is concluded that the ^{4}He and ^{16}O ions behave in gold planar channels as test charges which sample the electron distribution of the medium. The ^{127}I ions behave nearly as test charges, but for them there is some evidence that the screening of the nuclear charge changes with the position of the ion in the channel.

When beams of positive ions are transmitted through thin gold crystals in directions nearly parallel to the more closely packed atomic planes, considerable structure is observed in the spectrum of the transmitted-ion energies.[1-4] The details of the observed spectra depend upon the distance which the ions travel through the crystal and upon the angular relations between the crystal axes and the directions of the incident beam and of the small-angle transmitted-ion detector. The occurrence of structure in such spectra and its qualitative dependence on the pathlength and the angular variables have been explained[1,3-5] by a model in which the ions execute transverse anharmonic oscillations under the influence of the planes of atoms which border the channel and in which the rate at which an ion loses energy depends upon its distance from the atomic planes. This model is described in detail in the second following paper.[6] In earlier experiments on the energy-loss spectra of 60-MeV ^{127}I ions and 3-MeV ^{4}He ions in the {111} and {100} channels of thin gold crystals,[3] it was found that the stopping power of the ions was proportional to their frequency of oscillation in the planar-channel potential. The experiments reported here were undertaken to determine how generally this relationship might prevail and to study the dependence of the interaction potential on the ion and its energy. Energy-loss spectra have been obtained for 15- and 21.6-MeV ^{127}I ions and for 10-MeV ^{16}O ions traversing the {111} and {100} channels of thin gold crystals. A preliminary account of some of the former data has been reported previously,[4] but recent improvements in the theory of the underlying model[6] require a partial reinterpretation of it.

The experimental technique has been discussed

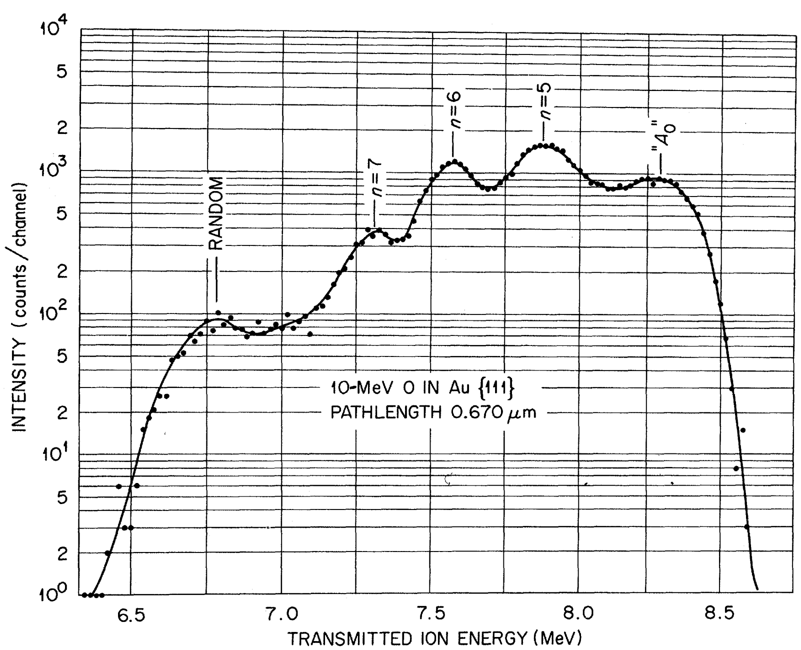

FIG. 1. Energy spectrum observed for 10-MeV ^{16}O ions transmitted through the {111} channel of a 0.670-μm-thick gold crystal.

in detail before.[3] The ion beams were extracted from the Oak Ridge tandem Van de Graaff accelerator, and collimated to <0.05 deg. The targets were {001} Au monocrystals, approximately 0.5 μm thick, prepared and characterized as previously described.[3] By adjustment of the goniometer in which the targets were mounted, either the {100} or the {111} channel could be selected and the pathlength through either channel varied over a considerable range. The energies of the transmitted ions were measured using either an electrostatic analyzer equipped with a position-sensitive detector, a solid-state detector, or a time-of-flight technique.[3] The acceptance angle of the detector was about 0.01 deg; the energy resolution was about ± 0.06 MeV for O ions and about ± 0.10 MeV for I ions. A typical spectrum, obtained for 10-MeV O ions in a {111} channel, is shown in Fig. 1. Since the incident beam and the transmitted-ion detector were collinear, the peaks in the spectra correspond to groups of particles which make integral numbers of oscillations in passing through the crystal.[3,5] It is with the positions of these peaks and of the (extrapolated) high-energy limit of the spectrum that the following analysis is concerned.

The experimental data consist of observations of the energies E of ions of incident energy E_0, transmitted through a pathlength z, in the thin crystal target. From these, it is desired to deduce the frequency with which the ions oscillate in the channel and the stopping power, averaged over the oscillatory motion, but corrected to the incident ion energy. The latter quantity will be termed the mean initial stopping power. Assuming it to vary with energy as E^p, the initial stopping power is[5]

$$\left(\frac{-dE}{dz}\right)_{E=E_0} = \begin{cases} [E_0^p/(1-p)z](E_0^{1-p} - E^{1-p}) , & p \neq 1 \\ (E_0/z) \ln(E_0/E) , & p = 1 \end{cases} \tag{1}$$

and the channel oscillation "frequency" is

$$\omega = \begin{cases} \dfrac{n(1-2p)\,(E_0^{1-p} - E^{1-p})}{z(1-p)\,(E_0^{1/2-p} - E^{1/2-p})} , & p \neq \tfrac{1}{2}, 1 \\[2ex] \dfrac{4n}{z}\, \dfrac{(E_0^{1/2} - E^{1/2})}{\ln(E_0/E)} , & p = \tfrac{1}{2} \\[2ex] \dfrac{n \ln(E_0/E)}{z\,(E^{-1/2} - E_0^{-1/2})} , & p = 1 \end{cases} \tag{2}$$

where n is the (integral) number of oscillations which the ion makes in passing through the channel. Note that ω is not a true frequency, since a factor $(2m)^{1/2}$, m being the mass of the ion, has been omitted from its definition. The values of n may be estimated from the data by noting the difference in pathlength between successive appearances of particular values of the stopping power.[3,5] The wavelengths of the oscillations, though not constant, are approximately $2E_0^{1/2}/\omega$; the values observed in the experiments range from 0.05 to 0.18 μm, depending on the ion, its energy, and its stopping power.

In Fig. 2, the initial stopping power is plotted as a function of channel oscillation frequency for 15-MeV ^{127}I ions in the Au {111} channel and compared with the result obtained earlier[3,5] at 60 MeV. Figures 3 and 4 display the results obtained for 21.6-MeV ^{127}I and 10-MeV ^{16}O ions, respectively, transmitted through Au {111} and {100} channels. As was found earlier for 60-MeV ^{127}I and for 3-MeV ^{4}He, the initial stopping power is proportional to the channel oscillation frequency. This proportionality appears to be general and to apply to planar channeling in gold, irrespective of the ion or of its energy. In every case, the initial stopping power is well represented by the straight line

$$\left(\frac{-dE}{dz}\right)_{E=E_0} = \alpha + \beta\omega \quad , \tag{3}$$

where the parameters α and β and their uncertainties can be evaluated from the data by the method of least squares. The values obtained for these parameters depend rather strongly on the value chosen for the stopping-power energy exponent p. However, according to the theory,[6] as long as Eq. (3) is correct, the curvature of the planar-channel potential is given by

$$y = 2\pi^2(s_0 - \alpha)^2/\beta^2 l = V_2''(0)/l \ , \tag{4}$$

where l is the half-width of the channel, s_0 is the stopping power at the center of the channel, determined experimentally from the high-energy edge of the energy-loss spectrum, $V_2(x)$ is the planar-channel potential, and the primes represent differentiation with respect to x—the displacement of the ion from the center of the channel. It is well to emphasize that the derivation of Eq. (4) involved no significant restrictions on the nature of the potential function. Figure 5 displays plots of the curvature parameter y as a function of p for each combination of ion, energy, and channel. For 3-MeV ^{4}He ions, where the energy is larger than that corresponding to the maximum stopping power in Au, the range $-1<p<0$ was chosen; for 10-MeV ^{16}O, approximately at the energy of the maximum stopping power, the range $-1<p<0.4$ was selected; for 15–60-MeV ^{127}I, where the energies are all well below that of the maximum stopping power, the range $0<p<1$ was taken. As the solid lines in Fig. 5 show, the curvature parameter is independent of p to within $\pm 2\%$ at worst, which is within the experimental uncertainties. This constancy may be contrasted with variations of 10–50% in the values

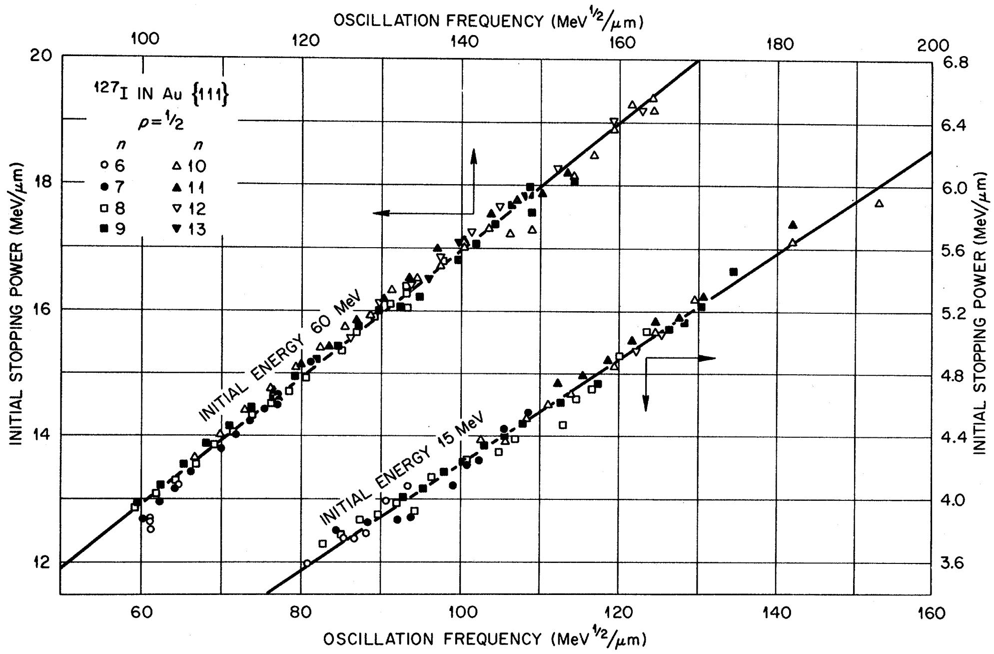

FIG. 2. Initial stopping power as a function of channel oscillation "frequency" for 15- and 60-MeV ^{127}I ions in the {111} channel of gold. The 60-MeV data are from Refs. 3 and 5. The stopping-power energy exponent was assumed to be $\frac{1}{2}$.

of α and β over the same ranges of p.

A similar analysis may be applied to some data obtained at a single pathlength, 0.495 μm, using ^{127}I ions of 15, 21.6, 29.4, 38.4, 48.6, and 60 MeV, that is, at equal intervals in velocity. Here, instead of $(-dE/dz)_{E=E_0}$, its product with E_0^{-p} is used, since this is independent of energy if p is constant. Straight lines analogous to Eq. (3) are obtained and the resulting curvature parameters are shown as functions of p by the dashed lines in Fig. 5. It is tempting to use the intersections of dashed and solid lines to establish the energy dependence of p, but this would be inconsistent with the necessary assumption of the constancy of p which underlies the analysis. It is concluded, in contrast to our earlier suggestion,[4] that the value of p cannot be established

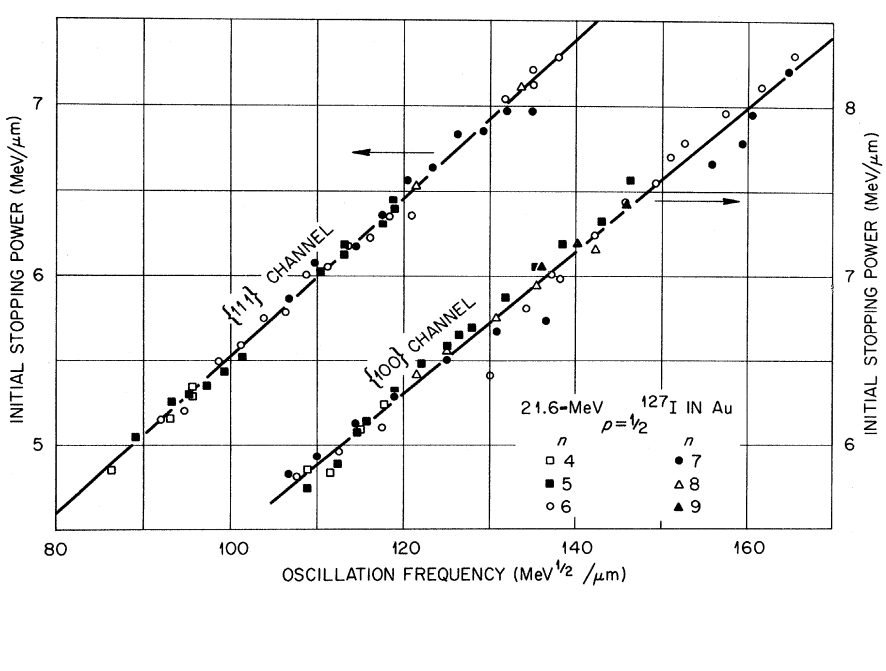

FIG. 3. Initial stopping power as a function of channel oscillation "frequency" for 21.6-MeV ^{127}I ions in the {111} and {100} channels of gold. The stopping-power energy exponent was assumed to be $\frac{1}{2}$.

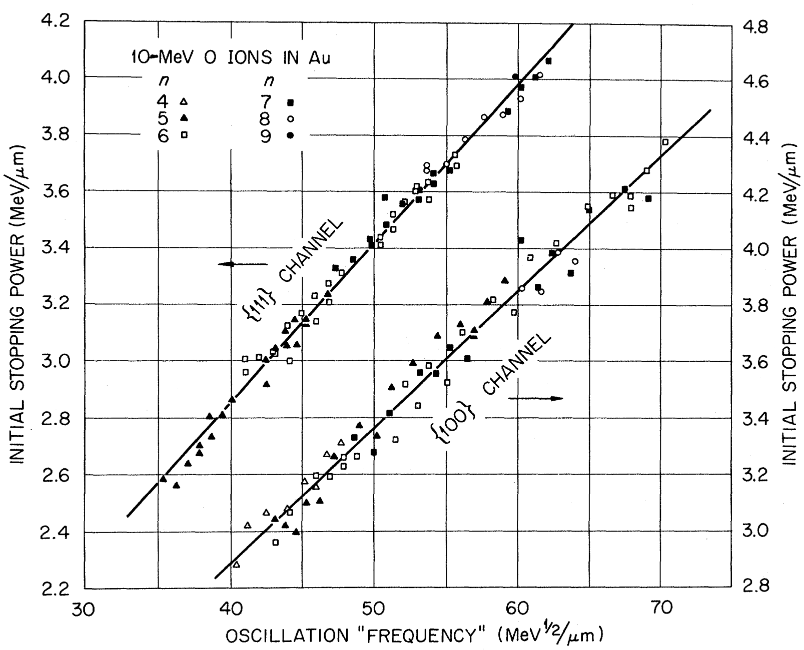

FIG. 4. Initial stopping power as a function of channel oscillation "frequency" for 10-MeV ^{16}O ions in the {111} and {100} channels of gold. The stopping-power energy exponent was assumed to be 0.

by these data. However, since the curvature parameters evaluated at constant initial energy are independent of p, this failure is unimportant.

The experimental curvature parameters are listed in Table I for each combination of ion, energy, and channel, using both the present data and those reported before.[3] The values are in no way dependent on assumptions about the potential function. The values of y are strongly dependent upon the ion and its energy, showing that the planar-channel potential must also depend on these variables. However, the ratio of the values for the two channels appears to be essentially independent of the ion and its energy. If the interaction potential between the channeled ion and the individual lattice atoms is of the screened Coulomb type, the curvature parameter is[6]

$$y = -8\pi\rho Z_1 Z_2 e^2 b\ \phi'(bl)\ , \qquad (5)$$

where ρ is the atomic density of the target, Z_1e and Z_2e are the (effective) nuclear charges of the two particles, $\phi(br)$ is the screening function, and b is a constant. The ratio of the values for two channels determines the value of the screening constant, b. The constancy of the ratio y_{111}/y_{100} in Table I implies the similar constancy of b, which is thus shown to be a property of the gold crystal. Physically, the implication is that the nuclear charge of the ion is always screened by the same number of electrons, whatever its position in the channel. As it approaches a target atom, it never gets so close that this screening is reduced significantly. Thus, it acts always as a simple charged particle which does not much perturb the medium. That is, all three ions may be considered as test charges. The strong variation of the experimental curvature parameters with the ion and its energy results from changes in the magnitude of the ionic charge with these variables.

TABLE I. Curvature parameters observed for ions moving in the planar channels of gold crystals.

Ion	Energy (MeV)	Curvature parameter (eV/Å^3) y_{111}	y_{100}	Ratio y_{111}/y_{100}	Screening constant b[a] (Å^{-1})
^{4}He	3	64.0±2.8	108.1±5.8	0.592±0.041	3.32±0.44
^{16}O	10	154.4±8.9	253±29	0.610±0.078	3.12±0.82
^{127}I	15	837±48	...	...	...
	21.6	915±53	1600±114	0.572±0.053	3.55±0.58
	60	1288±50	2077±92	0.620±0.037	3.03±0.37
			Weighted mean:	0.604±0.017	3.22±0.18

[a]For a hyperbolic cosine planar-channel potential $b = [\ln(y_{111}/y_{100})]/(l_{100} - l_{111})$. For Au, $l_{100} = 1.0197$ Å and $l_{111} = 1.1774$ Å.

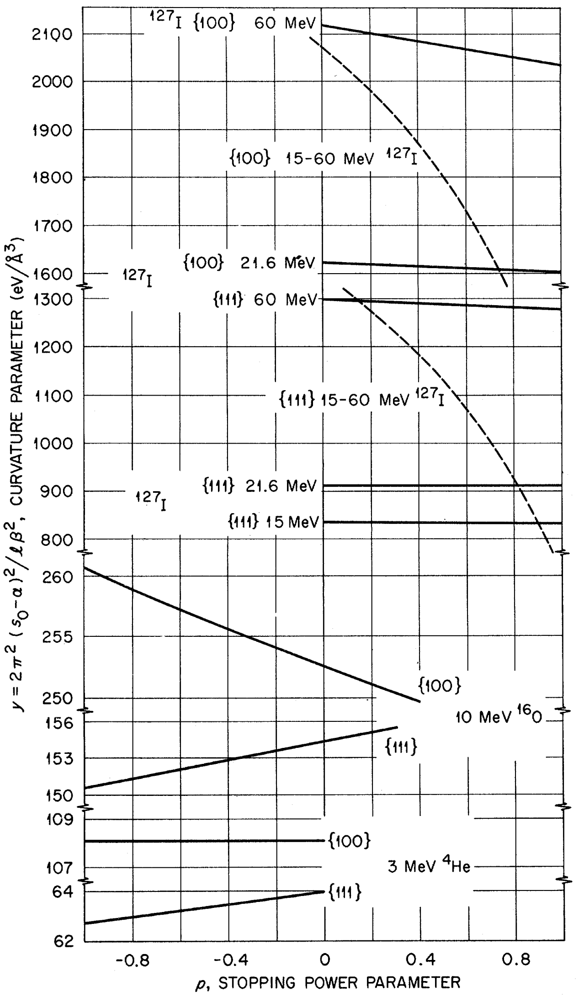

FIG. 5. Dependence of the experimental curvature parameters on the stopping-power energy exponent for several ions in the {111} and {100} channels of gold. The ^{4}He and 60-MeV ^{127}I data are from Refs. 3 and 5. Note the frequent changes of scale on the ordinate.

In the last column of Table I, screening constants are listed on the assumption that the screening function is

$$\phi(br) = 0.35e^{-br} , \qquad (6)$$

that is, the long-range term of the Molière potential.[7] The use of this screening function, which yields $V_2(x) \sim \cosh bx$, has been justified previously.[5] Its limitations will be discussed in detail elsewhere.[6] Accepting the mean screening constant of Table I, the empirical values of the charge product Z_1Z_2 may be deduced. These are listed in Table II. If the ions are indeed acting as test charges, then the ionic charge would be $q_1 = Z_1Z_2/79$, values of which are also shown in Table II. These may be compared with the equilibrium charge states observed for ^{127}I ions[8] and ^{16}O ions[9]; for ^{4}He, the α-particle charge is expected. For the two light ions, q_1 is about 30% less than expected, while for I, it is about 40% greater at each energy. Any simple alteration in the screening function, say by adjusting the numerical factor in Eq. (6), that improves the agreement in the former case will increase the discrepancy in the latter, and vice versa. Nevertheless, the values of q_1 obtained in this way are close enough to expectation to be encouraging for the viewpoint on which the analysis was based. If the screening of the gold nucleus by its electrons follows the Thomas-Fermi model,[10] and the Molière approximation[7] to the Thomas-Fermi screening function is employed, the expected value of b is 2.748 Å^{-1}. The empirical value 3.22 Å^{-1} is somewhat larger, but the discrepancy is not serious.

According to the interpretation outlined above, the three ions—^{4}He, ^{16}O, and ^{127}I—all behave as test charges which sample the electron distribution in the gold channels. This seems an entirely plausible and reasonable result for the two light ions. The ^{4}He ion is almost certainly a bare nucleus throughout its trajectory and the ^{16}O ions carry on the average only two or three electrons. However, the conclusion must be regarded as approximate for the ^{127}I ions, which carry some 30–40 electrons. The degree of approximation may be seen from the fact that the values of q_1 for ^{127}I are greater than the observed ionic charges, whereas they are lower for the two light ions. It seems likely that this effect is due to changes in the screening of the iodine nucleus as it approaches a gold atom. It would be interesting to examine the behavior of

TABLE II. Empirical charge products and ionic charges for ions moving in the planar channels of gold crystals.

Ion	Energy (MeV)	Charge product Z_1Z_2 {111}	{100}	Ionic charge $q_1=Z_1Z_2/79$	Equilibrium ionic charge[a]
^{4}He	3	118 ± 19	120 ± 17	1.5 ± 0.2	2
^{16}O	10	285 ± 47	281 ± 48	3.6 ± 0.6	5.5
^{127}I	15	1540 ± 260	⋯	19 ± 3	13
	21.6	1690 ± 280	1770 ± 260	22 ± 3	15
	60	2370 ± 380	2300 ± 310	29 ± 4	22

[a]From Refs. 8 and 9.

other ions in gold in this regard, but especially to examine the behavior of light ions in a variety of other target substances.

The authors are grateful to T. S. Noggle for preparing the thin gold crystals used in these experiments.

*Research sponsored by the U. S. Atomic Energy Commission under contract with Union Carbide Corporation.

[1]H. O. Lutz, S. Datz, C. D. Moak, and T. S. Noggle, Phys. Rev. Letters 17, 285 (1966).

[2]W. M. Gibson, J. B. Rasmussen, P. Ambrosius-Olesen, and C. J. Andreen, Can. J. Phys. 46, 551 (1968).

[3]S. Datz, C. D. Moak, T. S. Noggle, B. R. Appleton, and H. O. Lutz, Phys. Rev. 179, 315 (1969).

[4]S. Datz, C. D. Moak, B. R. Appleton, M. T. Robinson, and O. S. Oen, in *Atomic Collision Phenomena in Solids*, edited by D. W. Palmer, M. W. Thompson, and P. D. Townsend (North-Holland, Amsterdam, 1970), p. 374.

[5]M. T. Robinson, Phys. Rev. 179, 327 (1969).

[6]M. T. Robinson, second following paper, Phys. Rev. B 4, 1461 (1971).

[7]G. Molière, Z. Naturforsch. 2a, 133 (1947).

[8]C. D. Moak, H. O. Lutz, L. B. Bridwell, L. C. Northcliffe, and S. Datz, Phys. Rev. 176, 427 (1968).

[9]F. W. Martin, B. R. Appleton, L. B. Bridwell, M. D. Brown, S. Datz, and C. D. Moak (unpublished).

[10]P. Gombas, in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1956), Vol. 36, p. 109.

PHYSICAL REVIEW B VOLUME 4, NUMBER 5 1 SEPTEMBER 1971

Oscillation Frequencies of Protons in Planar Channels of Silicon*

F. H. Eisen
North American Rockwell Science Center, Thousand Oaks, California 91360

and

Mark T. Robinson
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

(Received 2 November 1970)

Measurements of the angular distributions and energy losses of 0.4-MeV protons transmitted through planar channels in thin silicon crystals have been used to relate the stopping power of the ions to the frequencies with which they oscillate in traversing the channels. In agreement with analogous experiments for several ions in gold, the stopping power is found to be accurately proportional to the channel oscillation frequency. The interaction between the proton and the silicon atoms is in reasonable agreement with expectations based on a Thomas-Fermi model.

A recent series of experiments on the energy-loss spectra of several ions transmitted through planar channels in thin gold crystals was interpreted in terms of a model in which the ions execute transverse anharmonic oscillations under the influence of the planes of atoms bordering the channel and in which an ion loses energy at a rate which is a function of its displacement from the atomic planes.[1-4] In these experiments, the incident beam and the small-acceptance-angle detector were colinear so that the well-resolved peaks in the energy spectra of the transmitted ions corresponded to particles which made an integral number of oscillations in passing through the crystal. An important result of the gold experiments[4] was that in every case the stopping power of the ion was accurately proportional to its channel oscillation frequency, an observation which could be made the basis of a quantitative application of the model.[2,3] It is therefore of considerable interest to know whether this linear relationship between stopping power and oscillation frequency applies to any target other than gold. Its general applicability would establish a remarkable connection between the stopping power of an ion and its interaction potential with the atoms of the target.

The energy spectra of protons transmitted through the planar channels of thin silicon crystals do not contain resolved peaks, so that the experimental procedure used for heavier ions in gold is inapplicable. Nevertheless, an alternative procedure, based on the same physical model, can circumvent this limitation. The basis of the experimental technique may be understood by reference to Fig. 1. Ions of initial energy E_0 are incident on the target at a small angle ψ_0 from the plane that defines the channel. In passing through the channel, the ions oscillate under the influence of the bordering planes with amplitude x_m and wavelength λ. After traveling a distance z, the ions leave the crystal with reduced energy E and at an angle ψ from the channel plane. As illustrated in Fig. 1, there are always two trajectories with the same amplitude, distinguished by having entered the crystal on opposite sides of the channel center and equidistant from it. According to the model,[2,3] these two trajectories will have the same wavelength