some dependence of the recombination cross section on binding energy, as well as the emission of light as observed by us and by Koenig and Brown.[23]

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Ranges of 7.5- to 52-kev H_2^+, D_2^+, He^+, and Ne^+ Ions in Quartz*

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Experimental values of penetration depths of positive ions in quartz obtained from measurements of reflection coefficient versus wavelength are compared with theoretical predictions. Measurements of the change in refractive index of quartz as a function of the energy dissipated per unit volume are shown to give experimental values for the ratio of energy loss due to displacement collisions per unit thickness to the energy loss due to ionization per unit thickness. The energy loss due to displacement collisions per unit thickness agrees with theoretical predictions. From the experimental values of energy loss due to ionization, it is found that the cross sections for scattering of valence electrons by the field of the incident atoms are an order of magnitude larger than the geometric cross sections.

I. INTRODUCTION

THE penetration in solids of atoms with energies below 50 kev is of current interest in connection with investigation of radiation effects in solids. Most of the information available[1,2] deals with energies above 50 kev and contains very little concerning the penetration of medium weight low-energy atoms such as are formed in solids by fast neutron bombardments. Experimental determination of the ranges of the low-energy atoms of interest here are hampered by the very small penetration distances (10^{-5} cm) involved. However, a variety of techniques have been successfully employed to obtain range information at these low energies.[3–7] In this paper, some recent determinations of ion ranges in quartz[8] are compared with the theoretical predictions.

The theoretical analysis of low-energy atom penetration is limited to approximate methods which are valid over only small energy regions. In general the atoms lose energy both by ionizing atoms of the stopping material and also by making elastic collisions with atoms of the stopping material. The general framework of the theory of penetration of energetic particles is presented by Bohr.[9] More specific discussions of the penetration of low-energy atoms are given by Nielsen[7] and by Seitz and Koehler.[10]

2. THEORY

a. Energy Loss by Elastic Collisions

Following the treatment outlined by Seitz and Koehler,[10] the collision problem can be treated classically as long as

$$b/ƛ \gg 1, \tag{1}$$

where $ƛ=\hbar/\mu V$ and where $b=Z_1Z_2e^2/\frac{1}{2}\mu V^2$ is the classical distance of closest approach in pure Coulomb scattering. Z_1 is the atomic number of the incident atom, V its velocity, and e is the electronic charge. Z_2 is the atomic number of the stationary atom. M_1 and M_2 are the atomic masses of the incident and stationary atoms, respectively, and $\mu=M_1M_2/(M_1+M_2)$ is the reduced mass of the system. In all the cases of interest here, the classical approximation is justified.

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The screening effect of the orbital electrons is taken into account by assuming a potential of the type

$$P(r)=Z_1Z_2e^2r^{-1}\exp(-r/a), \qquad (2)$$

where r is the separation between the two atoms and

$$a=a_h/(Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}})^{\frac{1}{2}}, \qquad (3)$$

where a_h is the Bohr radius of the hydrogen atom. The importance of the screening can be inferred from the size of the parameter ζ where

$$\zeta=b/a. \qquad (4)$$

Values of ζ large compared to unity denote strong screening. The experimental information discussed in this paper gives values of ζ less than unity which denotes weak screening.

Nielsen[7] has shown that for $0.8<\zeta<15$ the potential (2) can be replaced by an inverse square potential. With assumption the energy loss per unit path length by elastic collisions with the screened Coulomb field, $(dE/dx)_c$, is found to be

$$(dE/dx)_c=3.70n_0e^2Z_1Z_2aM_1/(M_1+M_2), \qquad (5)$$

where n_0 is the number of atoms/cc of stopping material.

For weak screening when $\zeta\ll 1$, the interaction is primarily due to the unscreened nuclear Coulomb fields and, as given by Seitz,[10] is

$$(dE/dx)_c=2\pi n_0Z_1^2Z_2^2e^4M_2^{-1}V^{-2}\log(T_m/T_a), \qquad (6)$$

where

$$T_m=4M_1M_2(M_1+M_2)^{-2}E,$$
$$T_a=4Z_1^2Z_2^2R_h^2E^{-1}M_1M_2^{-1}(Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}}),$$

and R_h is the Rydberg constant for hydrogen.

b. Energy Loss by Ionization

The excitation of electrons of the stopping material is relatively improbable when the energy parameter, ϵ given by

$$\epsilon=m_eE/M_1, \qquad (7)$$

of the incident atom is small compared to the first strong excitation potential, I, of the stopping material. m_e is the electron mass. For quartz, $I=6.2$ ev. Although the actual calculation given by Seitz and Koehler[10] for the energy loss per unit path length by ionization applies only to metals, it can be modified to apply to insulators as well. It is convenient to use the coordinate system in which the incident atom is at rest and the stopping material is moving with velocity V. The energy transfer is then due to the scattering of the valence electrons as they move past the atom that is now considered at rest. However, only those collisions are allowed which scatter the electrons to unoccupied states. This means that only collisions where the energy gain exceeds I are allowed. Assuming that the valence electrons are bound in a Coulomb field, their kinetic energy will approximately equal their binding energy[11] and they thus are uniformly distributed in a thin spherical shell in velocity space at a velocity V_0 where

$$V_0=(2I/m)^{\frac{1}{2}}, \qquad (8)$$

and where m is the effective electron mass. The energy transferred to the electrons is on the order of $2mVV_0$ per collision when $V<V_0$. The fraction of allowed collisions $f(\theta)$, due to scattering through an angle θ in the center-of-mass system, is

$$f(\theta)=(4VV_0\sin\tfrac{1}{2}\theta-V_0^2+4V^2\sin^2\tfrac{1}{2}\theta)/8VV_0\sin\tfrac{1}{2}\theta. \qquad (9)$$

The energy loss per unit path length due to electronic collisions, $(dE/dx)_e$, is then given by

$$(dE/dx)_e\simeq\tfrac{1}{2}N_0\sigma\int_0^\pi(2mVV_0)f(\theta)\sin\theta d\theta, \qquad (10)$$

where N_0 is the number of valence electrons/cc and σ is the total scattering cross section for valence electrons in collisions with the field of the incident atom. It follows that

$$(dE/dx)_e\simeq N_0\sigma(2I^{\frac{1}{2}}\epsilon^{\frac{1}{2}}-I). \qquad (11)$$

c. Diffusion Effects

In the above discussions it must be remembered that the quantity x is the distance actually traveled by the ion. For low-energy ions with masses approximately equal to the mass of the stopping atoms, the scattering is isotropic in the center-of-mass system and almost every collision will result in a large deflection and the ion penetration will be determined by diffusion effects. Consequently, the experimental results are expressed in terms of t, the depth beneath the surface. Nielsen[7] has shown how the theory developed for neutron scattering can be used by making only minor changes in notation. By comparing Eqs. (13) and (21) given by Nielsen[7] it is seen that the depth R at which the incident flux falls to one half of its initial value is approximately given by the relation

$$R/x=M_1M_2(M_1+M_2)^{-2}[0.75\xi(1-\langle\cos\varphi\rangle_{\mathrm{av}})]^{-\frac{1}{2}}, \qquad (12)$$

where $\langle\cos\varphi\rangle_{\mathrm{av}}=2M_1/3M_2$, $\xi=1+r(1-r)^{-1}\log r$, and $r=(M_2-M_1)^2/(M_2+M_1)^2$. Equation (12) is applicable only when the number of scattering events is large enough to make the motion of the incident ions random. An approximate idea of the significance of (12) can be obtained by calculating the number of collisions per incident ion, $C(\varphi)$, which result in deflections of more than φ in the laboratory system. This is

$$C(\varphi)=n_0\Delta t\sigma_c(\varphi), \qquad (13)$$

where $\sigma_c(\varphi)$ is the cross section for scattering through an angle of more than φ in the lab system, and Δt is the thickness of stopping material. For small values of ζ where the screening is weak, it follows from Seitz and

[11] E. Fermi and E. Teller, Phys. Rev. **72**, 399 (1947).

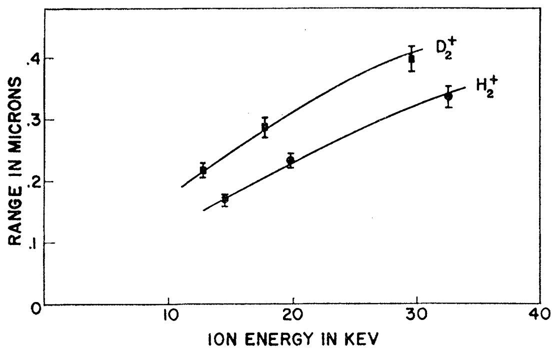

FIG. 1. Range in quartz of H_2^+ and D_2^+ ions as a function of ion energy. The molecular ions split into atomic particles as they enter the solid so that the range for atomic ions of a given energy will be equal to the range of molecular ions of twice the energy.

Koehler,[10] Eqs. (7.2) and (3.6), that

$$\sigma_c=\pi Z_1^2Z_2^2e^4(\sin^{-2}\tfrac{1}{2}\theta-1)/\mu^2V^4, \qquad (14)$$

where $M_2\sin\theta/(M_1+M_2\cos\theta)=\tan\varphi$.

d. Relation of Bombarded Layer Depth to Range

Intuitively, the depth of the layer formed when an ion beam bombards a quartz surface is expected to be related to the range of the ions. The following discussion shows the exact nature of the relationship. The range, R, is defined as the depth at which the flux of ions falls to one half of the incident flux at the surface of the stopping material. The depth, d, of the bombarded layer is obtained by fitting the theoretical curve of reflection coefficient versus wavelength predicted for a layer with uniform refractive index to the experimental points of reflection coefficient versus wavelength. However, the layer is expected to be nonuniform near the end of the range of the particles. For saturation bombardments, the change in refractive index of the bombarded layer as a function of depth, $\Delta n[t]$ is believed to be constant for values of $t<R$ and to monotonically approach zero for values of $t>R$. Analysis of a simple case of a nonuniform layer (curve b in Fig. 2 given by Hines and Arndt[8]) shows that the approximation of fitting the curves for a uniform layer gives a value of d which is numerically equal to $\int_0^\infty\Delta n[t]dt/\Delta n[0]$. In a first approximation this integral relationship is equivalent to defining d by the relation

$$\Delta n[d]=\tfrac{1}{2}\Delta n[0]. \qquad (15)$$

The change in refractive index as a function of depth is due to the fact that the energy liberated per unit volume in displacement collisions, $\mathcal{E}(t)$, is a function of the depth. Thus, it is more accurate to represent the change in refractive index by $\Delta n[\mathcal{E}(t)]$. If $E_c'(t)$ is the energy liberated in displacement collisions per unit thickness of stopping material at a depth t below the surface, (15) can be expressed in the form

$$\Delta n[E_c'(d)F(d)]=\tfrac{1}{2}\Delta n[\langle E_c'\rangle_{av}F(0)]. \qquad (16)$$

$\langle E_c'\rangle_{av}$ is the value of $E_c'(t)$ averaged over the depth d of the bombarded layer. $F(t)$ is the time integrated flux density of the incident beam as a function of t. From Fig. 8 given by Hines and Arndt,[8] it is seen that it is possible to choose a value of incident time integrated flux density, $F_R(t)$, such that

$$\Delta n[\langle E_c'\rangle_{av}\tfrac{1}{2}F_R(0)]=\tfrac{1}{2}\Delta n[\langle E_c'\rangle_{av}F_R(0)]. \qquad (17)$$

Since (16) is true for any $F(t)$ including $F_R(t)$, it is seen that

$$F_R(d)=\tfrac{1}{2}[\langle E_c'\rangle_{av}/E_c'(d)]F_R(0). \qquad (18)$$

The distribution of the penetration of the majority of the particles as a function of depth is expected to be a Gaussian function.[1] Thus

$$F(d)=F(0)\tfrac{1}{2}\{1-\mathrm{erf}[(d-R)/\sqrt{2}\Omega]\}, \qquad (19)$$

where R is the mean range and Ω is the root mean square fluctuation in particle penetration. From (19) and (18) it follows that

$$R=d-\sqrt{2}\Omega\ \mathrm{erf}^{-1}\{1-[\langle E_c'\rangle_{av}/E_c'(d)]\}. \qquad (20)$$

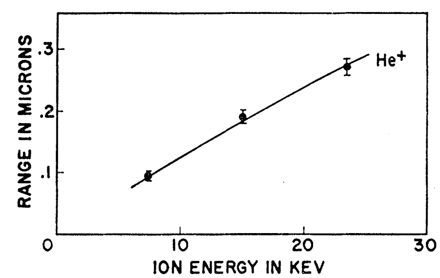

FIG. 2. Range in quartz of He^+ ions as a function of ion energy.

e. Ratio of Ionization Energy Loss to Displacement Energy Loss

For values of the energy parameter such that

$$\epsilon<I/8 \qquad (21)$$

it is expected that practically all of the particle energy loss is due to displacement collisions.[12] Under this condition the energy per unit volume required to produce a given change in refractive index is independent of the bombarding particle. For larger values of ϵ, energy is lost through ionization as well as through displacement collisions. If $E'(t)$ is the total energy loss per unit thickness at a depth t, and $E_e'(t)$ is the energy loss per unit thickness at depth t due to ionization, then

$$\langle E'\rangle_{av}=\langle E_c'\rangle_{av}+\langle E_e'\rangle_{av}, \qquad (22)$$

and

$$F_{50\%}E/d=F_{50\%}\langle E_c'\rangle_{av}+F_{50\%}\langle E_e'\rangle_{av}, \qquad (23)$$

where $F_{50\%}$ is the time integrated flux density of ions required to produce 50% of the saturation change in

[12] F. Seitz, Discussions Faraday Soc. 5, 271 (1949).

TABLE I. A comparison of experimental and theoretical values for the energy loss due to displacement collisions per unit thickness of quartz, E_c'; the energy loss due to ionization per unit thickness of quartz, E_e'; and the total energy loss per unit thickness of quartz E'. The calculated values of the ratio, ζ, of the collision diameter to the screening constant; the ratio, $b/\lambda\!\!\!^-$, of the collision diameter to the incident atom wavelength/2π; and the energy parameter, $\epsilon = m_e E/M_1$, are also included. The averages for $\langle E_e'\rangle_{av}/\langle E_c'\rangle_{av}$ are taken over the depth of the bombarded quartz layer.

Atom	Energy kev	ϵ ev	ζ	$b/\lambda\!\!\!^-$	$\langle E_e'\rangle_{av}/\langle E_c'\rangle_{av}$	E' Mev/cm	E_e' Mev/cm	E_e' theory Mev/cm	E_c' Mev/cm	E_c' theory Mev/cm
H	11.8	6.41	0.0601	28.9	45 ±5.5	539± 62	527± 61	49.3	11.7± 1.9	12.4
D	10.6	2.90	0.0730	43.2	10.1 ±1.3	464± 65	422± 59	17.5	41.8± 7.6	26.6
He	15.5	2.12	0.122	101	3.1 ±0.5	885± 74	668± 61	12.9	216 ± 32	128
Ne	45.0	1.23	0.368	673	0.45±0.13	6240±1900	1940±700	0	4300 ±1330	6060

Δn. The averages are taken over the depth, d, of the bombarded layer. For $F_{50\%}\langle E_c\rangle_{av}$ the value of 7.8×10^{23} ev/cc found by averaging the values of $F_{50\%}E/d$ for A^+ ion bombardment given by Hines and Arndt[8] is used because for A^+ ion bombardment the energy parameter is small enough to neglect ionization. Thus the ratio of ionization energy loss to displacement energy loss can be found from (23) to be

$$\langle E_e'\rangle_{av}/\langle E_c'\rangle_{av} = [(F_{50\%}E/d)/7.8\times10^{23}]-1. \qquad (24)$$

It is also possible to estimate the ratio $E_c'(d)/\langle E_c'\rangle_{av}$ by using the experimental observation from Figs. 1, 2, and 3 that the range versus energy curves are approximately linear. This means that $E'(t)$ is constant and that

$$\langle E'\rangle_{av} \simeq E_c'(d) \qquad (25)$$

because $E_e'(d)$ is small when the ions are near the end of their range and moving slowly. It follows from (22), (24), and (25) that

$$E_c'(d)/\langle E_c'\rangle_{av} \simeq (F_{50\%}E/d)/7.8\times10^{23}. \qquad (26)$$

3. DISCUSSION

The experimental penetration depths found by Hines and Arndt[8] for H_2^+, D_2^+, He^+, and Ne^+, ions in quartz are presented in Figs. 1, 2, and 3. The data for penetration of A^+, Kr^+, and Xe^+ ions in quartz are not included here because the depth of the altered quartz layer may be partly or completely due to the primary Si and O knockons created by the heavy atoms and may bear little relationship to the penetration of the heavy atoms themselves.

It must be remembered that the ions are penetrating a layer of damaged quartz whose density is close to that of vitreous silica (2.20 g/cc). Thus a density of 2.20 g/cc is used in the range calculations rather than the density of quartz (2.65 g/cc).

Although the incident atoms are positively charged, the cross sections for charge exchange are very large and the beam quickly reaches a charged state independent of the original charge. In particular, Allison[13] states that thicknesses of 10^{-8} g/cc (0.1% of the penetrations discussed here) are sufficient to produce charge equilibrium. Also, the charge-equilibrated state is predominantly neutral. 70% of the charge-equilibrated beam of 10-kev hydrogen emerging from a silicon monoxide film is neutral and 96% of a 16-kev helium beam in neon gas is neutral. Consequently, the particles of interest here can be considered neutral during most of the time they are moving through the solid.

The molecular ions are expected to split as they penetrate the first surface layers of atoms with the subsequent atomic particles following independent paths. The energy will be shared equally between the two atomic particles because they have equal velocities and masses. Fogel *et al.*[14] find that the energy distribution and charge state of the beam emerging from an Al foil for an incident beam of 32-kev H_2^+ ions is the same as it is for an incident beam of H^+ ions with half the energy of the molecular ions. Here, all calculations for molecular beams are carried out assuming the penetrating particles are neutral atomic particles with one half the energy of the incident molecular ion.

The relationship of bombarded layer depth to range is given by (20) and (26). Using the experimental values of $F_{50\%}E/d$ given by Hines and Arndt,[8] it is seen that the difference between the range and the penetration depth varies from 0.60Ω for 7.5-kev He^+ ions to 2.34Ω for 32.6-kev H_2^+ ions. Although no theory exists for calculating Ω in this energy range, it is expected to be small and can be neglected because most of the energy is lost by ionization and the average energy loss per ionization event is only 10^{-3} of the total energy. Some

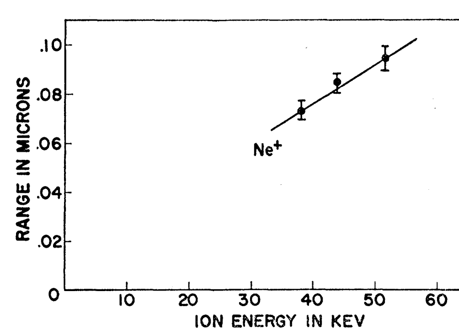

FIG. 3. Range in quartz of Ne^+ ions as a function of ion energy.

[13] S. K. Allison, Revs. Modern Phys. **30**, 1137 (1958).

[14] I. M. Fogel, B. G. Safronov, and L. I. Krupnik, J. Exptl. Theoret. Phys. (U.S.S.R.) **28**, 711 (1955) [translation: Soviet Phys.—JETP **1**, 546 (1955)].

straggling is also to be expected from nuclear Coulomb scattering, but, as shown below, only a minor fraction of the incident atoms are scattered through large angles.

Table I presents experimental average values of E' obtained by subtracting the lowest and highest energy points given in Figs. 1, 2, and 3 for each ion. These are compared with theoretical values of E_c' and E_e'. The values of $\langle E_e'\rangle_{av}/\langle E_c'\rangle_{av}$ are found using (24) and the experimental values of $F_{50\%}E/d$ given by Hines and Arndt[8] for the middle bombardment energies. Since both E' and $\langle E_e'\rangle_{av}/\langle E_c'\rangle_{av}$ are known, approximate experimental values for $E_c'(E_m)$ and $E_e'(E_m)$ can be found by assuming that

$$\langle E_e'\rangle_{av}/\langle E_c'\rangle_{av} \simeq E_e'(E_m)/E_c'(E_m), \qquad (27)$$

where E_m is the mean energy of the two points used to calculate the experimental values of E'. Since $E_e'(t)$ vanishes at the end of the range, the value of $E_e'(E_m)/E_c'(E_m)$ is larger than $\langle E_e'\rangle_{av}/\langle E_c'\rangle_{av}$. For 45-kev Ne atoms, E_c' is calculated by dividing (5) by (12). The value of $\zeta=0.368$ is outside the region where (5) is valid, however, the agreement between calculated and observed values of E_c' is satisfactory. For the light ions the diffusion factor is not pertinent since the nuclear scattering cross section is low. From (13) and (14), the fraction of incident atoms scattered through lab angles in excess of 45° can be calculated for the thickness involved for the experimental values given in Table I. The fractions are 0.074 for 11.8-kev H atoms, 0.099 for 10.6-kev D atoms, and 0.183 for 15.5-kev He atoms. Since $\zeta \ll 1$ for the H, D, and He incident atoms, the weak screening formula (6) is used to calculate E_c'. For 11.8-kev H atoms the agreement between experimental and theoretical values of E_c' is within the range of experimental error. For 10.6-kev D atoms and 15.5-kev He atoms the experimental values of E_c' are significantly larger than predicted. However, the assumption (27) overestimates the value of E_c'. If ionization energy loss predominates and varies approximately linearly with particle energy, assumption (27) would overestimate E_c' by a factor close to two. Thus it appears that the experimental values of E_c' for 10.6-kev D atoms and 15.5-kev He atoms do agree with theory within the validity of the analysis of the experimental data.

For the ionization energy loss the experimental values are an order of magnitude greater than the theoretical values calculated from (11) if the cross section for scattering of valence electrons by the field of the incident atom is taken equal to the geometric cross section, $\sigma_0=\pi a_h^2 Z_1^{\frac{2}{3}}$, of the incident atom. This result is not sensitive to the assumption (27) because ionization accounts for most of the energy loss for 11.8-kev H atoms, 10.6-kev D atoms, and 15.5-kev He atoms. Consequently it appears that the scattering cross section is considerably larger than the geometric cross section. Comparing the experimental results with (11), the ratios for σ/σ_0 are seen to be 11 ± 1 for 11.8-kev H atoms, 24 ± 3 for 10.6-kev D atoms, and 52 ± 5 for 15.5-kev He atoms. For 45-kev Ne atoms, (11) predicts zero ionization energy loss. Experimentally, some ionization energy loss is observed but it is of doubtful significance since it is only 2.8 times the experimental error.

4. CONCLUSIONS

The experimental value for energy loss per unit path length due to displacement collisions for 45-kev Ne atoms in quartz is consistent with Bohr's theory when the diffusion nature of the Ne atom motion is taken into account. For 11.8-kev H atoms, 10.6-kev D atoms, and 15.5-kev He atoms the energy loss per unit path length due to displacement collisions is consistent with the theory of weakly screened nuclear collisions. The energy loss of 11.8-kev H atoms, 10.6 D atoms, and 15.5-kev He atoms is mainly due to ionization and the cross sections for ionization of the valence electrons by the moving atoms are found to be an order of magnitude larger than the geometric cross sections.