is slightly ionic is discussed in reference 5; thus the degeneracy of the optical modes is partly removed. We estimated the longitudinal optical mode to be 290°K by using an expression due to Mott and Fröhlich.[7] It has been assumed that the optical modes do not change with $q$ over the small portion of the zone shown. It is the low-energy acoustical phonons which determine the value of $q(k\theta)$ to be used in the optical selection rule. The acoustical spectrum was determined from elastic constants of InSb.[8]

In Fig. 2(b) are shown two possible valence band structures, one with the maximum along the (1,0,0) axis assuming 21° and 16° phonons giving $q(k\theta)=0.05q_m$, the other with its maximum along the (1,1,1) axis assuming 24° and 12° phonons giving $q(k\theta)=0.09q_m$. It is assumed that the minimum of the conduction band is at the center of the zone (0,0,0), i.e., $\mathbf{k}_f=0$; thus $\mathbf{k}_i=\mathbf{q}(k\theta)$. As discussed in CML and by Parmenter[9] and Dresselhaus,[10] other alternatives are permitted by symmetry considerations.

The valence band energy profiles are shown as parabolas. If this is a valid assumption, and the maximum lies on the (1,1,1) axis, the effective mass for holes is $1.35m_e$. This is not inconsistent with the value $m^*>1.2m_e$ determined from the cyclotron resonance experiment.[11]

This suggested band structure is also consistent with two other experimental facts. Fan and Gobeli[12] recently reaffirmed in a thin sample of InSb that the optical gap is 0.175 ev. The thermal gap at 300°K is 0.160 ev as determined by Breckenridge *et al.*[13]

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# Vacancies and Displacements in a Solid Resulting from Heavy Corpuscular Radiation

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The number of displacements $D(E)$ and the number of vacancies $V(E)$ produced in a monatomic solid as a result of collisions due to an incident ion of initial energy $E$, are obtained as solutions of the equation

$$f(E)=\int_0^E dyK(E,y)\{p(y)[f(y-\alpha)+1-\theta q(E-y)]+[1-p(E-y)q(y)]f(y)\},$$

where $f(E)=D(E)$ or $V(E)$, $p(y)$ denotes the probability that a struck atom is displaced when it has received energy $y$, $q(E-y)$ is the probability that the striking atom replaces it if displacement has occurred, $K(E,y)$ is the scattering kernel, and $\alpha$ is the minimum amount of energy that is assumed to be necessary to displace an atom (it is assumed that the struck atom loses energy $\alpha$ in breaking away from its lattice site). In the equation, $f(E)=0$ for $E<\alpha$, with $\theta=0$ for displacements and $\theta=1$ for vacancies.

This equation is solved for some representative cases of $p(y)$ and $q(y)$. The functions $p(y)$ and $q(y)$ can be chosen to fit experimental estimates of either $D(E)$ or $V(E)$ singly but indicate a fundamental discrepancy of the joint estimates. The discrepancy, if not due to inaccuracy in the interpretation of experimental results, suggests that a mathematical model based on individual collisions is inadequate.

## I. INTRODUCTION

In previous investigations[1,2] the authors have determined the number of displacements $D(E)$ and the number of vacancies $V(E)$ in a monatomic solid produced as a result of collisions due to an incident atom of initial energy $E$. These calculations were based on a simple mathematical model characterized by a displacement energy $\alpha$ of the lattice atoms and the energy distribution of the struck atoms was determined by using the cross sections for collisions with free atoms. Taking $y$ as the energy of the struck atom after the collision, we made the following assumptions:

(A) A displacement is produced whenever $y>\alpha$.

(B) A replacement is produced whenever $y>\alpha$ and $E-y<\alpha$.

Thus, a vacancy is produced whenever $y>\alpha$ and $E-y>\alpha$. The displacement energy $\alpha$ is often taken as about 25 ev.

[1] W. S. Snyder and J. Neufeld, Phys. Rev. **97**, 1637 (1955).
[2] J. Neufeld and W. S. Snyder, Phys. Rev. **99**, 1326 (1955).

The occurrence of replacements while a collision takes place has been suggested by Kinchin and Pease[3] who also calculated the number of replacements and displacements resulting from heavy particle bombardment. The assumption (B) regarding the occurrence of replacements is different from that of Kinchin and Pease who considered a second and smaller threshold energy to permit replacement collisions to occur.

With the above assumptions, the number of displacements and vacancies are roughly determined as follows:

$$D(E)\sim E/2\alpha. \tag{1}$$

$$V(E)\sim E/3\alpha. \tag{2}$$

The above values for $D(E)$ and $V(E)$ do not agree with those experimentally obtained. Unfortunately very few experiments give reliable estimates of $D(E)$ and $V(E)$ and therefore it is difficult[4] to estimate the extent of the discrepancy between the calculated values and the actual values of $D(E)$ and $V(E)$.

Harrison and Seitz[5] using the experimental data of Cooper, Koehler, and Marx[6] estimate that the number of vacancies is

$$V(E)\sim E/10\alpha, \tag{3}$$

and, therefore, the calculated values as given by Eq. (2) is too large.

On the other hand, Aronin's[7] experiments indicate that the number of displacements is

$$D(E)\sim 2.5E/\alpha \tag{4}$$

and, therefore, the calculated value as given by Eq. (1) is too small to explain the disordering phenomena. The calculations of Kinchin and Pease agree with Aronin's results but their model does not bring the number of vacancies into line with the results of Harrison and Seitz.

## II. FORMULATION OF THE PROBLEM

In an effort to reduce the discrepancy between the calculated values and the values obtained experimentally, the model characterizing the collisions has been modified.

Let $p(y)$ be the probability that the struck atom having energy $y$ after collision escapes from its lattice site. Also, let $q(z)$ be the conditional probability for the striking atom to replace the struck atom assuming a displacement has occurred and that the striking atom has energy $z$ after the collision. The assumptions (A) and (B) amount to taking $p(y)=I(y/\alpha)$ and $q(z)=1-I(z/\alpha)$, where $I(x)$ is the Heavyside unit step function defined by putting $I(x)=1$ for $x\geqq 1$ and $I(x)=0$ for $x<1$. The modified form of the function $p(y)$ suggested by Sampson, Hurwitz, and Clancy[8] replaced the abrupt threshold energy for displacement to occur by a gradual transition from a low-energy region where displacement is unlikely or impossible of occurrence to a high-energy region where displacement is certain to occur. They argue that a struck atom having little energy is more likely to be deflected back and trapped in the original lattice site than a struck atom receiving more energy. The modified model thus suggests a second parameter $k$ such that if $y>k\alpha$, displacement is certain to occur. Then $p(y)$ is defined by $p(y)=0$ for $y<\alpha$, $p(y)=1$ for $y>k\alpha$, and $p(y)=(y-\alpha)/(k-\alpha)$ for $\alpha<y<k$, so that the probability for displacement increases gradually from zero to one as the energy transmitted to the struck atom increases from $\alpha$ to $k\alpha$.

In the present model, we take $q(z)=1-p(z)$. This amounts to assuming that after the struck atom is displaced, the striking atom with residual energy $z$ has the same probability of remaining at the site as would a struck atom of energy $z$. This probability is one for $y<\alpha$ and decreases linearly to zero in the range $\alpha<y<k\alpha$.

Let an atom of energy $E$ make a first collision and let $K(E,E')dE'$ be the probability that it loses energy $E'$ in $dE'$. There are three possible cases:

(a) No displacement occurs, the probability for this being $dE'K(E,E')[1-p(E')]$.

(b) Displacement occurs but the striking atom replaces the displaced atom. The probability for this to occur is $dE'K(E,E')p(E')q(E-E')$.

(c) Displacement occurs without replacement, the probability for this to occur being

$$dE'K(E,E')p(E')[1-q(E-E')].$$

In case (a), no displacement occurred on the first collision and the atom has energy $E-E'$ after the collision so that the expected number of displaced atoms produced in this way is $dE'K(E,E')[1-p(E')]\times D(E-E')$. In case (b), a displacement has occurred on the first collision and a single atom of energy $E'-\alpha$ is free after the collision. The expected number of displacements resulting from this case is thus $dE'\times K(E,E')p(E')q(E-E')[1+D(E'-\alpha)]$. In case (c), a displacement has occurred and two atoms are free with energies of $E-E'$ and $E'-\alpha$. The expected number of displacements in this case is thus

$$dE'K(E,E')p(E')[1-q(E-E')][1+D(E-E')+D(E'-\alpha)].$$

Since these three cases are mutually exclusive and exhaustive, we may sum them and also sum on $dE'$

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TABLE I. Variation of vacancies and displacements with the probability of replacement.

| $k$ | $D(E)$ | $V(E)$ | $D(E)/V(E)$ |
|---|---|---|---|
| 1 | $0.5(E+\alpha)/\alpha$ | $0.333(E+\alpha)/\alpha$ | 1.5 |
| 2 | $0.438(E+\alpha)/\alpha$ | $0.262(E+\alpha)/\alpha$ | 1.67 |
| 3 | $0.365(E+\alpha)/\alpha$ | $0.211(E+\alpha)/\alpha$ | 1.73 |
| 4 | $0.314(E+\alpha)/\alpha$ | $0.178(E+\alpha)/\alpha$ | 1.76 |
| 5 | $0.276(E+\alpha)/\alpha$ | $0.154(E+\alpha)/\alpha$ | 1.79 |
| 6 | $0.247(E+\alpha)/\alpha$ | $0.136(E+\alpha)/\alpha$ | 1.82 |
| 10 | $0.173(E+\alpha)/\alpha$ | $0.0935(E+\alpha)/\alpha$ | 1.855 |
| 15 | $0.127(E+\alpha)/\alpha$ | $0.0674(E+\alpha)/\alpha$ | 1.881 |
| 20 | $0.100(E+\alpha)/\alpha$ | $0.0527(E+\alpha)/\alpha$ | 1.897 |
| 30 | $0.0705(E+\alpha)/\alpha$ | $0.0367(E+\alpha)/\alpha$ | 1.921 |
| 40 | $0.0544(E+\alpha)/\alpha$ | $0.0282(E+\alpha)/\alpha$ | 1.930 |
| 50 | $0.0443(E+\alpha)/\alpha$ | $0.0229(E+\alpha)/\alpha$ | 1.934 |

and thus get the integral equation for $D(E)$:

$$D(E)=\int_0^E dE'K(E,E')\{p(E')[1+q(E-E')\times D(E'-\alpha)+(1-q(E-E'))(D(E'-\alpha)+D(E-E'))]+[1-p(E')]D(E-E')\}, \quad (5)$$

$D(E)=0$ for $E<\alpha$.

A similar analysis of cases yields the following equation for $V(E)$:

$$V(E)=\int_0^E dE'K(E,E')\{p(E')[q(E-E')V(E'-\alpha)+(1-q(E-E'))(1+V(E'-\alpha)+V(E-E'))]+[1-p(E')]V(E-E')\}, \quad (6)$$

$V(E)=0$ for $E<\alpha$.

## III. CALCULATIONS

Equations (5) and (6) are valid for any choice of the kernel $K(E,E')$. The calculations discussed below assume isotropic scattering so that $K(E,E')=1/E$. With the above choices of $K(E,E')$, $p(E)$, and $q(E)=1-p(E)$, the equations were solved numerically on the Oak Ridge digital computer for the range $\alpha\leqq E\leqq 2k\alpha$. For $E>2k\alpha$, the equations simplify considerably. In fact, multiplying both members by $E$ and differentiating, we obtain the very simple differential difference equations

$$ED'(E)=D(E-\alpha), \quad EV'(E)=V(E-\alpha). \quad (7)$$

An exact solution of these equations is given by $D(E)=a(E+\alpha)$, $V(E+\alpha)=b(E+\alpha)$ for any choice of the constants $a$ and $b$. The constants $a$ and $b$ were chosen to match these solutions to the curves computed for $E<2k\alpha$. In fact, it is easy to prove that if $a_1$ and $a_2$ are chosen so that $a_1(E+\alpha)\leqq D(E)\leqq a_2(E+\alpha)$ in the range $(2k-1)\alpha\leqq E\leqq 2k\alpha$, then the inequality remains valid for $E>2k\alpha$. In all cases considered, the values of $a_1$ and $a_2$ could be chosen to be quite close and still verify the desired inequality so that the extension of the solution by this linear function is sufficiently accurate for our purpose. The formula for $D(E)$ is given in Column II of Table I for various values of $k$. The slopes obtained for $V(E)$ were computed in similar fashion, and the formula for $V(E)$ is given in Column III of the table for the same values of $k$.

## IV. CONCLUSIONS

We wish to emphasize the lack of reliable experimental data on $D(E)$ and $V(E)$. Assuming that the experimental estimates given by Harrison and Seitz[5] and by Aronin[7] are correct, the ratio $D(E)/V(E)$ would have the value 25. On the other hand, the ratio $D(E)/V(E)$ obtained from Eqs. (5) and (6) and shown in Column IV of the foregoing table is considerably smaller, and for $k$ varying from 1 to 50 it increases slowly from 1.5 to 1.934. This discrepancy leads to the conclusion that the above calculations do not agree with the results of Harrison and Seitz and those of Aronin. It is easily seen that values of $k$ and $\alpha$ can be chosen to fit the results of either of the above two experimental estimates and, in fact, in a variety of ways.

Although the experimental results are rough, it may be doubted whether the experimental errors are entirely responsible for the discrepancy noted. Rather, it may be possible that a mathematical model not solely concerned with individual and separate collisions is necessary for a satisfactory theory.

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