structed and has been maintained in operating condition in part through support provided by Wright Air Development Center through a contract with The Ohio State University Research Foundation. The gratings were ruled at the University of Michigan. A Golay detector having a diamond window was made available by Elias Burstein of Naval Research Laboratory. The indium antimonide crystals were produced under a contract between Wright Air Development Center and Battelle Memorial Institute.

PHYSICAL REVIEW VOLUME 101, NUMBER 2 JANUARY 15, 1956

Deformation Potential Theory for *n*-Type Ge†*

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(Received June 29, 1955; revised manuscript received September 21, 1955)

The deformation potential theory has been re-examined for electrons in Ge to take into account the ellipsoidal nature of the energy surfaces, and the effect of shear wave scattering. The coupling between shears and the conduction band energy minima is calculated from Smith's piezoresistance data under the assumption that any changes in mobility due to strain may be neglected. The scattering by shears, which is the dominant mechanism, is strongly anisotropic and cannot be described by a simple relaxation time. We have shown that the distribution function for electrical conductivity has a tensor dependence on the orientation of the electric field. The mobility is calculated assuming several values of E_{1c}, the shift of the conduction band edge with dilation. The calculated values of the mobility are approximately $3\times10^{7}T^{-3/2}$ cm²/v sec. Methods of accounting for discrepancies between the experimental and theoretical values of the mobility and its temperature dependence are discussed.

INTRODUCTION

THE lattice scattering mobility of carriers in nonpolar semiconductors was treated in the deformation potential theory of Bardeen and Shockley.[1] In this theory, scattering by long-wavelength acoustical modes is considered. The electron phonon coupling is the shift in the allowed energy bands due to the compressions and dilations produced by the longitudinal modes. The transverse modes cause no scattering since they produce no dilation.

It is now apparent, from the elastoresistance measurements of Smith,[2] that shifts in the conduction band minima or valleys in *n*-type Ge are caused by shears as well as by dilation. We should expect, therefore, that scattering of electrons will occur that is due to shears produced in the crystal by both longitudinal and transverse waves. In this paper, we wish to recalculate the mobility of electrons in Ge using the deformation potential theory and taking into account the effect of shear wave scattering.

It has been shown by Wannier,[3] and restated by Slater,[4] that in a periodic lattice, with a perturbing potential which varies slowly with position compared to the periodic potential, an electron may be treated essentially as a perturbed free particle with an appropriate effective mass. In the strained coordinate system of the crystal, the deformation potential due to long-wavelength acoustical modes is just such a slowly varying potential. We may therefore use the effective-mass theory to calculate the probability of transitions between momentum states. In such a treatment, any strain-induced changes in the effective mass will be of the order of the strain. Since the electrons are classically distributed, and are close to the conduction band bottom, changes in the effective mass may be ignored.

In principle, the deformation potential theory makes it possible to determine exactly the mobility of carriers in a semiconductor if one knows precisely how the edges of the allowed energy bands shift with strain. In reality, the shift with dilation of the individual band edges is not known; only the sum of shifts of the valence and conduction bands with dilatation has been determined. On the other hand, from the elastoresistance data on Ge, one can calculate uniquely[5] the shift with shear of the conduction band's energy minima. As we shall show, in *n*-type Ge the scattering due to shears is the dominant mechanism, so that one may calculate the mobility to within a small indeterminancy and compare it with the experimental values.

BAND STRUCTURE AND ELASTORESISTANCE IN *n*-TYPE Ge

Bardeen and Shockley assumed in their theory that the surfaces of constant energy in the Brillouin zone

† Submitted in partial fulfillment of the requirements for the Ph.D. degree.

* This research was performed in part at the Chicago Midway Laboratories which are supported by the United States Air Force through the Office of Scientific Research of the Air Research and Development Command.

[1] J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).
[2] C. Smith, Phys. Rev. **94**, 42 (1954).
[3] G. H. Wannier, Phys. Rev. **52**, 191 (1937).
[4] J. C. Slater, Phys. Rev. **76**, 1592 (1949).

[5] Actually there is a very weak dependence upon the dilation effect.

were spherical. We now know from recent cyclotron resonance experiments[6,7] that the conduction band of Ge has eight degenerate minima or valleys oriented along the $\langle 1,1,1\rangle$ directions in the first Brillouin zone. Near each of these minima, the surfaces of constant energy are elongated ellipsoids, the major axes of which are in the $\langle 1,1,1\rangle$ directions.

It will be convenient to associate with each valley a coordinate system, the z axis of which will be identical with the major axis of the family of ellipsoids corresponding to that valley. According to the data of Dexter, Zeiger, and Lax, the effective mass of electrons, expressed in the coordinate system of a valley is

$$m^*=\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_1 & 0 \\ 0 & 0 & m_2 \end{bmatrix}, \tag{1}$$

where $m_1=0.08m$ and $m_2=1.3m$, m being the free-electron mass.

The elastoresistance experiments on Ge[2] have given evidence that another scattering mechanism exists for electrons in Ge, namely shears produced by both longitudinal and transverse waves. Smith found that a shear with respect to the $\langle 1,0,0\rangle$ set of crystal axes in n-type Ge results in a considerable anisotropy of the conductivity. If such an effect were due to a change in the mobility of the electrons, or to the reorientation of the valleys in momentum space, one would expect it to be of the same order of magnitude as the shear, but actually it is about 90 times larger. The explanation of this effect is as follows.[2,8,9] Ordinarily the total conductivity of Ge, resulting from the highly anisotropic conductivity contributions of the eight symmetrically placed and equally populated valleys, is isotropic. This must be true because of the cubic symmetry of Ge. The degenerate states in the conduction band occur far from one another in the first Brillouin zone and have wave functions which are considerably different. The degeneracy is destroyed when the cubic symmetry is removed by a shear, and some states go up in energy, and others down. There is a net transfer of electrons from the valleys whose energy has been raised to those which have been lowered. As a result, the conductivity contributions of the more highly populated valleys predominate over the others, and the total conductivity is no longer isotropic. In this way, a large anisotropy in the conductivity may be produced by a relatively small shear.

We will now calculate the shift of the $[1,1,1]$ oriented valley for a simple shear. This result will be needed in order to determine the mobility of electrons in Ge. Smith found that the shear dependence of the anisotropic part of the conductivity could be expressed in the $\langle 1,0,0\rangle$ crystal axes as

$$-\sigma_{xy}/\sigma=m_{44}\epsilon_{xy}, \tag{2}$$

where σ_{xy} and ϵ_{xy} are elements of the conductivity and strain tensors respectively, and m_{44} is an experimentally determined quantity. Let us now put a pure shear on the crystal and calculate the resulting off diagonal conductivity. Let this shear be

$$\epsilon=\tfrac{1}{2}\begin{bmatrix} 0 & \epsilon_{xy} & 0 \\ \epsilon_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and imagine that the $[1,1,1]$ valley is shifted in energy by ΔE. The $[1,1,\bar{1}]$, $[1,\bar{1},1]$, and $[\bar{1},1,1]$ valleys will also be shifted by ΔE, but the $[\bar{1},1,1]$, $[1,\bar{1},1]$, $[1,1,\bar{1}]$ and $[1,\bar{1},\bar{1}]$ valleys are shifted by $-\Delta E$, since a reversal of direction of the x axis or y axis would correspond to changing the sign of ϵ_{xy}. We may write

$$\Delta E=E_3\epsilon_{xy}, \tag{3}$$

where E_3 is to be determined. For a more general shear, the shift of the $[1,1,1]$ valley is

$$\Delta E=\tfrac{1}{2}E_3\textstyle\sum_{i\neq j}\epsilon_{ij}. \tag{3a}$$

The sum over all the off-diagonal strain components occurs, because each off-diagonal component of the strain will cause the same shift in energy of the valley as will any other off-diagonal component of equal magnitude, due to the symmetry of the $[1,1,1]$ direction with respect to the $\langle 1,0,0\rangle$ crystal axes.

For the simple shear we are considering, four valleys are shifted up a small amount in energy and four down. The number of excess electrons in the ith valley above the number n_i that were there before the shear is simply

$$\Delta n_i=(\partial f_0/\partial E)\Delta E_i=-n_i(\Delta E_i/kT), \tag{4}$$

where f_0 is the Boltzmann distribution at equilibrium. Since $\sum_i \Delta n_i=0$, the Fermi level of the distribution has remained constant. The excess conductivity contribution of the ith valley is

$$\Delta\sigma_i=-(\Delta E_i/kT)\sigma_i, \tag{5}$$

where σ_i is a tensor which may be written in the coordinate system of the valley as

$$\sigma_i=\begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_1 & 0 \\ 0 & 0 & \sigma_2 \end{bmatrix}. \tag{6}$$

If now we transform the excess conductivity contributions of the eight valleys to the coordinate system of the $\langle 1,0,0\rangle$ crystal axes and sum, we find

$$\sigma_{xy}=\frac{8}{3}(\Delta\sigma_2-\Delta\sigma_1)=\frac{8}{3}\frac{\Delta E}{kT}(\sigma_1-\sigma_2). \tag{7}$$

[6] Dexter, Zeiger, and Lax, Phys. Rev. **95**, 557 (1954).
[7] Dresselhaus, Kip, and Kittel, Phys. Rev. **98**, 368 (1955).
[8] E. N. Adams, Chicago Midway Laboratories Technical Report CML-TN-P8.
[9] C. Herring, Bell System Tech. J. **34**, 237 (1955). A detailed discussion of the various ways in which strain can effect the conductivity of a many valley semiconductor appears in this paper. Also, in an appendix a general expression for the elements of the elastoresistance tensor is derived, using a notation that differs considerably from that used in the present paper.

The normal conductivity without strain is also found by transforming the σ_i's to the crystal axes and summing. This conductivity is isotropic and is given by

$$\sigma=(8/3)\ \mathrm{tr}[\sigma_i]. \tag{8}$$

Using (7) and (8) along with (3) in Eq. (2) we obtain[10]

$$E_3=-\frac{m_{44}kT\ \mathrm{tr}[\sigma_i]}{\sigma_1-\sigma_2}. \tag{9}$$

The value of E_3 which we calculate from the elastoresistance data will depend upon the degree of anisotropy of σ_i.

We will now calculate the conductivity of n-type Ge. We shall consider deformation potential scattering by both shears and dilation produced by acoustical modes. In our theory there will occur two parameters, E_3 and E_{1c}. E_3 is defined by Eq. (3a) and E_{1c} is the shift in the bottom of the conduction band for unit dilation. We may calculate E_3 from Eq. (9) using Smith's elastoresistance data once we know the anisotropy of the conductivity contribution of a valley. However, as we shall see, the anisotropy will depend on the ratio of E_{1c} to E_3, and E_{1c} is not experimentally known. Only E_{1G}, the shift in energy with unit dilation of the gap between the valence and conduction bands, has been determined,[11] and this is approximately -5.5 ev. We shall assume that E_{1c} is of the same sign and order of magnitude as E_{1G}, and shall make conductivity calculations for several values of E_{1c}/E_3 corresponding to this assumption. For each value of this ratio we will obtain different values of E_3, and of the total conductivity.

Our first task will be to calculate the probability for transitions between momentum states in the same valley. Then we will solve the Boltzmann equation for $f(\mathbf{p})$, the electron distribution in an electric field. We may then calculate the conducivity contribution of a single ellipsoid and the total conductivity.

TRANSITION PROBABILITY

For sufficiently long wavelengths, we may treat the crystal as an elastic continuum. Imposing periodic boundary conditions, we may expand the displacement of the continuum as a series of traveling waves:

$$\delta\mathbf{R}=\sum_{\mathbf{k}\lambda}\mathbf{u}_{\mathbf{k}\lambda}[e^{i\mathbf{k}\cdot\mathbf{r}}q_{\mathbf{k}\lambda}(t)+e^{-i\mathbf{k}\cdot\mathbf{r}}q_{\mathbf{k}\lambda}^*(t)], \tag{10}$$

where the sum over the wave number $\mathbf{k}$ includes the allowed values of small $\mathbf{k}$ in the first Brillouin zone. Here $\mathbf{u}_{\mathbf{k}\lambda}$ is a unit polarization vector, and the summation over λ includes a longitudinal mode and two transverse modes for every $\mathbf{k}$ value.

Because the velocity of sound in Ge is not isotropic, there is a certain amount of mixing between the longitudinal and transverse modes for directions of propagation away from the $\langle 1,0,0\rangle$, $\langle 1,1,0\rangle$, and $\langle 1,1,1\rangle$ directions. The writer solved the normal modes problem for various other directions and found that the direction of motion of the predominantly longitudinal mode is never more than 8° away from the direction of propagation and that this deviation is generally much smaller. Since it is the square of the wave amplitudes that will enter the transition probability, mixing will cause errors no greater than a few percent, and consequently it will be ignored.

The acoustical modes can be shown to be formally analogous to a group of quantized harmonic oscillators. In such a representation the $q_{\mathbf{k}\lambda}$'s have matrix elements between phonon states. The only nonvanishing elements are[12]

$$(n+1\,|\,q_{\mathbf{k}\lambda}\,|\,n)=\left[\frac{\hbar\omega(n+1)}{2C_{\mathbf{k}\lambda}k^2}\right]^{\frac{1}{2}}e^{i\omega t},$$

and

$$(n-1\,|\,q_{\mathbf{k}\lambda}^*\,|\,n)=\left[\frac{\hbar\omega n}{2C_{\mathbf{k}\lambda}k^2}\right]^{\frac{1}{2}}e^{-i\omega t}, \tag{11}$$

which correspond to the emission or absorption of a phonon respectively. $C_{\mathbf{k}\lambda}$ is the appropriate combination of elastic constants entering into the velocity of propagation of the $\mathbf{k}\lambda$th mode.

The perturbing potential acting upon the carriers is the deformation potential

$$V=E_{1c}\textstyle\sum_i\epsilon_{ii}+\frac{1}{2}E_3\sum_{i\neq j}\epsilon_{ij}, \tag{12}$$

where the first term is the shift in the energy of the conduction band edge because of dilation and the second term is the shift in the [1,1,1] oriented energy minima because of the total shear with respect to the $\langle 1,0,0\rangle$ crystal axes. Because we shall wish to work in the coordinate system of the [1,1,1] valley, we shall transform V to these coordinates. It is easy to show that V becomes

$$V=E_{1c}\textstyle\sum_i\epsilon_{ii}+E_3(2\epsilon_{zz}-\epsilon_{xx}-\epsilon_{yy}). \tag{12a}$$

The strain tensor is given by

$$\epsilon=\nabla\cdot\delta\mathbf{R}=i\sum_{\mathbf{k}\lambda}\mathbf{k}\mathbf{u}_{\mathbf{k}\lambda}[e^{i\mathbf{k}\cdot\mathbf{r}}q_{\mathbf{k}\lambda}-e^{-i\mathbf{k}\cdot\mathbf{r}}q_{\mathbf{k}\lambda}^*], \tag{13}$$

so that the deformation potential becomes

$$V=i\sum_{\mathbf{k}\lambda}F_\lambda(\beta)k[e^{i\mathbf{k}\cdot\mathbf{r}}q_{\mathbf{k}\lambda}-e^{-i\mathbf{k}\cdot\mathbf{r}}q_{\mathbf{k}\lambda}^*], \tag{14}$$

where

$$\begin{aligned}F_1&=E_{1c}+E_3(3\cos^2\beta-1),\\ F_2&=3E_3\cos\beta\sin\beta\cos\gamma,\\ F_3&=3E_3\cos\beta\sin\beta\sin\gamma.\end{aligned} \tag{15}$$

[10] This result would be unchanged if there were four valleys instead of eight.

[11] W. Paul and H. Brooks, Phys. Rev. **94**, 1128 (1954). See references quoted there.

[12] See, for instance, W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, Oxford, 1944), second edition, p. 59.

Here β is the angle between $\mathbf{k}$ and the z axis of the valley, and γ is the angle between $\mathbf{u}_{\mathbf{k}2}$ and the plane determined by the [0,0,1] and [1,1,1] directions. The terms for $\lambda=2,3$ corresponding to the transverse modes have, as they should, no dilation effects.

Let us now calculate the matrix elements for transitions between momentum states in the same valley,

$$(n\pm1,\mathbf{p}'|V|n,\mathbf{p})=i\sum_{\mathbf{k}\lambda}kF_\lambda\left[\frac{\hbar\omega(n+\frac{1}{2}\pm\frac{1}{2})}{2C_{\mathbf{k}\lambda}k^2}\right]^{\frac{1}{2}}\times\int_{\substack{\text{unit}\\\text{volume}}}\exp\left[i\left(\frac{\mathbf{p}-\mathbf{p}'}{\hbar}\pm\mathbf{k}\right)\cdot\mathbf{r}\right]d^3\mathbf{r}. \quad (16)$$

The integral vanishes unless $\mathbf{p}'-\mathbf{p}=\pm\hbar\mathbf{k}$, in which case it is one.

At temperatures for which thermal scattering is dominant and impurity scattering can be neglected, the energy of the scattering phonon is small compared to either the kinetic energy of an electron or kT. We can therefore make the following approximations. First, we can neglect any changes in the energy of an electron which occur in the scattering process and shall consider the electrons to be scattered on a surface of constant energy. Secondly, we can set

$$\hbar\omega n=\frac{\hbar\omega}{\exp(\hbar\omega/kT)-1}\cong kT, \quad (17)$$

thereby considering the modes to be classically excited.

The probability per unit time for transitions between momentum states becomes

$$W(\mathbf{p},\mathbf{p}')=\frac{2\pi}{\hbar}\sum_\lambda F_\lambda^2\frac{kT}{C_{\mathbf{k}\lambda}}\delta(E'(\mathbf{p}')-E(\mathbf{p})). \quad (18)$$

Because the $C_{\mathbf{k}\lambda}$'s are rather complicated functions of the direction of propagation, average values for the longitudinal modes and for the transverse modes were used. C_L represents the simple unweighted average of the three sets of elastic constant entering into the velocities of longitudinal sound waves propagating in the [1,0,0], [1,1,0], and [1,1,1] directions, and C_T is a similar average of the six sets of elastic constants entering into the velocities of transverse waves propagating in these same directions. The $C_{\mathbf{k}\lambda}$'s do not differ from their averages by more than 20%, so that only a slight error is likely to be introduced by this simplification. Values of the elastic constants of Ge are given by Bond, Mason, McSkimin, Olsen, and Teal.[13]

Substituting for the F_λ's and using $\sin^2\beta=1-\cos^2\beta$, we obtain $W(\mathbf{p},\mathbf{p}')$ as a series of even powers of $\cos\beta$,

$$W(\mathbf{p},\mathbf{p}')=\frac{2\pi}{\hbar}\frac{kT}{C_L}\{(E_{1c}-E_3)^2+6[(E_{1c}-E_3)E_3+\tfrac{3}{2}(C_L/C_T)E_3^2]\cos^2\beta+9E_3^2(1-C_L/C_T)\cos^4\beta\}\delta(E'-E). \quad (19)$$

SOLUTION OF BOLTZMANN EQUATION

Let us now calculate $f_1(\mathbf{p})=f(\mathbf{p})-f_0(\mathbf{p})$ from the Boltzmann equation

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}=\int W(\mathbf{p},\mathbf{p}')[f_1(\mathbf{p}')-f_1(\mathbf{p})]\frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}=-e\mathcal{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial E}, \quad (20)$$

where $\mathcal{E}$ is the electric field, $\mathbf{v}$ the velocity, and E the energy. Because of the complicated nature of $W(\mathbf{p},\mathbf{p}')$, which depends upon both $\mathbf{p}$ and $\mathbf{p}'$, a solution for f_1 of the form $f_1=e\tau\mathcal{E}\cdot\mathbf{v}\partial f_0/\partial E$, corresponding to the existence of a relaxation time, does not exist. We can see, however, that for an electric field along any of the axes of the valley, the electron distribution will be deformed in the direction of the field. For example, if $\mathcal{E}=\mathcal{E}_z$ the distribution would deform symmetrically with respect to the z axis and f_1 would be of the form $f_1=e\tau_2\mathcal{E}_z v_z\partial f_0/\partial E$. Here τ_2 may be a function of θ, the angle between $\mathbf{p}$ and the z axis, but cannot be a function of the angle of rotation around the z axis because of the symmetry of the valley. Again, if $\mathcal{E}=\mathcal{E}_x$,

$$f_1=e\tau_1\mathcal{E}_x v_x\partial f_0/\partial E,$$

where τ_1 is in general a function of θ. For an arbitrary electric field, the distribution function will be of the form

$$f_1=e\mathcal{E}\cdot\tau\cdot\mathbf{v}\partial f_0/\partial E, \quad (21)$$

where τ is a tensor given by

$$\tau=\begin{bmatrix}\tau_\perp & 0 & 0\\ 0 & \tau_1 & 0\\ 0 & 0 & \tau_2\end{bmatrix}.$$

Let us first consider the case for which $\mathcal{E}=\mathcal{E}_z$ and substitute the corresponding f_1 into the Boltzmann equation. After canceling out the common factors we obtain

$$p_z=\int W(\mathbf{p},\mathbf{p}')[\tau_2(\mathbf{p})p_z-\tau_2(\mathbf{p}')p_z']\frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}. \quad (22)$$

To facilitate the integration over $d^3\mathbf{p}'$, we shall next make a change of variables which project the ellipsoids of constant energy onto spheres. This transformation is

$$\mathbf{p}=\alpha^{-\frac{1}{2}}\cdot\mathbf{P},\quad \mathbf{v}=m^{-1}\alpha^{\frac{1}{2}}\cdot\mathbf{P}, \quad (23)$$

[13] Bond, Mason, McSkimin, Olsen, and Teal, Phys. Rev. 78, 176 (1950).

where

$$\alpha=\frac{m}{m^*}=\begin{bmatrix}\alpha_1 & 0 & 0\\ 0 & \alpha_1 & 0\\ 0 & 0 & \alpha_2\end{bmatrix}.$$

Also

$$\cos^2\beta=\frac{\alpha_1}{\alpha_2}\frac{\cos^2\beta'}{1+(\alpha_1/\alpha_2-1)\cos^2\beta'},$$

where

$$\cos^2\beta'=(P_z-P_z')^2/(\mathbf{P}-\mathbf{P}')^2.$$

Our transformed integral equation is

$$P_z=\int W(\mathbf{P},\mathbf{P}')[\tau_2(\mathbf{P})P_z-\tau_2(\mathbf{P}')P_z']\frac{d^3\mathbf{P}'}{(2\hbar\pi)^3(\det\alpha)^{\frac{1}{2}}}.$$

A similar equation containing τ_1 and P_x can be obtained from the case in which $\mathcal{E}=\mathcal{E}_x$.

The transformed tensor τ will be dependent upon the direction of $\mathbf{P}$ through the polar angle $\theta(\mathbf{P})$. Since $W(\mathbf{P},\mathbf{P}')$ is symmetric about the equatorial plane of the energy surfaces, τ must also be symmetric. Therefore, we may expand the elements of τ in series of even Legendre polynomials of $\cos\theta$. A trial solution for τ equivalent to the first two terms of each series and of the form

$$\tau_1=\tau_0(A_0+A_1\cos^2\theta),\quad \tau_2=\tau_0(B_0+B_1\cos^2\theta),\quad (24)$$

was then attempted.

The integrals over the surface of constant energy may be performed exactly. These integrals will be functions of the parameters A_i and B_i. The two integral equations can now be expressed as

$$P_x=A_0g_0+A_1g_1,\quad P_z=B_0h_0+B_1h_1,\quad (25)$$

where the g_i's and h_i's are functions of $\theta(\mathbf{P})$ and were tabulated for 11 values of $\theta(\mathbf{P})$ between 0° and 180°. By trial and error the A_i's and B_i's were adjusted until the closest simultaneous fit of the equation was achieved. Using this method, the integral equation (20) was satisfied to within a few percent over the full range of $\theta(\mathbf{P})$.

Three solutions of the Boltzmann equation were made for three values of the ratio E_{1c}/E_3. τ is therefore given by (21) and (24), where

$$\tau_0=\frac{\pi\hbar^4C_L(\det\alpha)^{\frac{1}{2}}}{m(2mE)^{\frac{1}{2}}kTE_3^2},\quad (26)$$

and where the constants entering into τ_1 and τ_2 are given in Table I along with the accuracy with which it was possible to satisfy Eq. (20).

TABLE I. Solutions of the Boltzmann equation for the parameters in elements of the tensor τ [Eqs. (21) and (24)]; and the accuracy to within which the Boltzmann equation was satisfied by these solutions.

E_{1c}/E_3	A_0	A_1	B_0	B_1	Acc.
−0.5	0.226	0.012	0.312	0.034	1%
−1	0.220	0.066	0.428	0.110	2%
−1.5	0.190	0.096	0.532	0.228	4%

TABLE II. Directional dependence of σ_i, E_3 and E_{1c} (in ev), and μ and μ_d (in cm²/v sec).

E_{1c}/E_3	Γ_1	Γ_2	E_3	E_{1c}	$\mu T^{3/2}$	μ(300°K)	μ_d(300°K)
−0.5	2.86	0.256	5.48	−2.74	3.48×10^7	6700	115 000
−1	2.91	0.380	5.84	−5.84	3.18×10^7	6100	25 400
−1.5	2.62	0.515	6.52	−9.78	2.37×10^7	4550	9 400

RESULTS FOR MOBILITY

Knowing f_1, we shall calculate the conductivity contribution of a single valley. The contribution to the total current is

$$\mathbf{j}_i=\sigma_i\cdot\mathcal{E}=-e\int\mathbf{v}f_1\frac{d^3\mathbf{p}}{(2\pi\hbar)^3},\quad (27)$$

where f_1 is given by (21). Making the change of variables (23), we obtain

$$\sigma_i=\frac{e^2}{m^2kT}\alpha\cdot\int\mathbf{PP}\cdot\tau(\mathbf{P})f_0\frac{d^3\mathbf{P}}{(2\pi\hbar)^3(\det\alpha)^{\frac{1}{2}}},\quad (28)$$

$$\sigma_i=\frac{2}{3}\frac{(2\pi)^{\frac{1}{2}}n_ie^2\hbar^4C_L(\det\alpha)^{\frac{1}{2}}}{m^{5/2}(kT)^{3/2}E_3^2}\Gamma,\quad (29)$$

where

$$\Gamma=\begin{bmatrix}\Gamma_i & 0 & 0\\ 0 & \Gamma_1 & 0\\ 0 & 0 & \Gamma_2\end{bmatrix},$$

and where

$$\Gamma_1=\alpha_1(A_0+\tfrac{1}{5}A_1),\quad \Gamma_2=\alpha_2(B_0+\tfrac{3}{5}B)_1.$$

We can see that the conductivity contribution of a single valley has a directional dependence which depends upon both the tensor form of the effective mass and also upon the directional dependence of f_1, which in turn reflects the highly anisotropic scattering probability.

The total conductivity is isotropic, as is the mobility, which is given by

$$\mu=\frac{2}{3}\frac{(2\pi)^{\frac{1}{2}}e\hbar^4C_L(\det\alpha)^{\frac{1}{2}}}{m^{5/2}(kT)^{3/2}E_3^2}\times\tfrac{1}{3}\,\mathrm{tr}[\Gamma],\quad (30)$$

or

$$\mu=17.5\times10^7T^{-3/2}E_3^{-2}\,\mathrm{tr}[\Gamma]\ \mathrm{cm}^2/\mathrm{v\ sec},$$

where E_3 is in electron volts.

Knowing the directional dependence of the conductivity contribution of a single valley, we may go back to the elastoresistance theory and calculate E_3. Using E_3 we may then calculate μ. These quantities are presented in Table II, again for the three values of E_{1c}/E_3. For the purposes of comparison, we have also listed μ_d, the mobility which would arise if only dilational scattering were present. We have used the same values of E_{1c} to calculate μ_d as were used in calculating the corresponding values of μ. From Table II we can

see that, except for very large values of E_{1c}, scattering by shears is the dominant mechanism.

The accuracy of these results depends on the approximations used in the calculations. The combined error for ignoring the mixing of the various modes of propagation, and for using average velocities of propagation for the longitudinal and transverse modes, should not exceed 5%. Another maximum error of about 5% could arise from our neglect of any strain induced changes of the mobility in the elastoresistance theory. The errors involved in ignoring the energy of the scattering phonon and in considering the long-wavelength acoustical modes to be classically excited should be negligible. Also, the writer estimates that the error incurred in the solution of the Boltzmann equation would not affect the values of the mobility by more than 5%. Therefore, we should expect the calculated values of the mobility to be accurate within 15%. It is also worth mentioning, that if the effective mass data of Dresselhaus, Kip, and Kittel[7] were used, instead of that given by Dexter, Zeiger, and Lax,[6] the calculated values of the mobility would be smaller by approximately 10 to 15%.

DISCUSSION OF RESULTS

The theoretical temperature dependence of the lattice scattering mobility for intravalley scattering is $T^{-3/2}$. This differs slightly from the experimental temperature dependence[14] in n-type Ge of $T^{-1.66}$, which is known to hold between 80 and 300°K. Also, the experimental value of the mobility at 300°K is 3800 cm/volt sec, and this value is somewhat lower than the calculated values which range between 4550 and 6700 cm^2/v sec.

We may reduce the calculated values of μ by approximately 12% to correspond to what we would have calculated if we had used the more recent effective mass data of Dresselhaus, Kip, and Kittel.[7] One now finds that the calculated value of μ at 300°K for $E_{1c}/E_3 = -1.5$ is 4000 cm^2/v sec, in good agreement with experiment. For this case E_{1c} is approximately -10 ev, a value almost twice that of E_{1G}. However, we have not obtained the correct temperature dependence of the mobility, and in order to do this we shall have to invoke some other mechanism, which will further reduce the mobility at 300°K, for this case, to significantly less than the experimental values. It is therefore not likely that $-E_{1c}$ is as large as 10 ev.

A higher temperature dependence of the lattice scattering mobility than $T^{-3/2}$ can be obtained in several ways. First, if there were a bending over of the energy surfaces away from the energy minima, we would obtain a higher dependence.[15] The reason for this is as follows: The bending over of the energy surfaces corresponds to an increasing effective mass away from the energy minima. At higher temperatures, the electron distribution is more spread out around the energy minima and therefore on the average has a higher effective mass than at lower temperatures. Since the lattice scattering mobility is inversely proportional to the 5/2 power of the effective mass, it will show an increased temperature dependence.

Another possible mechanism sufficient to give a higher temperature dependence is scattering by high-energy phonons, that is intervalley or optical-mode scattering. Herring[9] has shown how such scattering would modify the ordinary magnitude and temperature dependence of the mobility for various phonon temperatures and strengths of this additional scattering. Measurements of Keyes[16] show that the intervalley scattering is small at room temperatures. Therefore, one might also expect the optical modes to contribute only slightly to the total scattering. However, it is only necessary that the intervalley and optical mode scattering be approximately 25% of the total scattering at 300°K in order to explain the observed temperature dependence. In this case, one must assume a high-energy phonon temperature of approximately 300°K, but this is entirely possible since the Debye temperature of Ge is 290°K.[17]

If either high-energy phonon scattering or a "temperature-dependent" effective mass were responsible for the $T^{-1.66}$ temperature dependence of the mobility in Ge, we would expect the mobility at 300°K to be reduced by at least 25% from the theoretical lattice scattering values. If in addition we reduce the calculated mobility values to correspond to the most recent effective mass data,[7] we obtain $\mu = 4400$ and 4000 cm^2/v sec for the cases in which $E_{1c}/E_3 = -0.5$ and -1 respectively. Either value is in good agreement with experiment. In view of the small dependence of μ on E_{1c}, it is not possible to say which value of E_{1c} is more nearly correct.

ACKNOWLEDGMENTS

I wish to thank Dr. E. N. Adams for suggesting this problem and for valuable discussion and encouragement. I also wish to thank Dr. Morrel H. Cohen for his very helpful criticism and advice.

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