TABLE V. Approximate percentage correction to (1) from $C_K$ and $C_L$.

| Incident proton energy (Mev) | $Z=30$ | 50 | 70 | 90 |
|---|---|---|---|---|
| 1 | +4.3[a] | +14[a] | +21[b] | +26[b] |
| 5 | −3.9[a] | − 1.4[a] | + 1.4[a] | + 2.8[b] |
| 10 | −3.0 | − 2.3 | − 0.7[a] | + 0.4[b] |
| 20 | −1.7 | − 2.0 | − 1.5[a] | − 0.9[a] |
| 50 | −0.9 | − 1.2 | − 1.3 | − 1.1[a] |
| 100 | −0.4 | − 0.7 | − 0.8 | − 0.9 |
| 200 | −0.2 | − 0.4 | − 0.5 | − 0.5 |
| 500 | −0.07 | − 0.14 | − 0.2 | − 0.3 |
| 1000 | −0.03 | − 0.06 | − 0.09 | − 0.13 |

[a] For these values $C_K$ is negative (see text).
[b] For these values $C_K$ and $C_L$ are negative (see text).

A comparison of our values of $f_L$ with those obtained by Hönl[10] shows a close check as indeed it should since they were both obtained in the same approximation, i.e., using hydrogen-like wave functions. Like Hönl we observe that for $\theta_L=0.35$ this approximation gives a value of $f_L$ which is much too high. Since the oscillator strength per electron for hydrogen for a transition $2p\rightarrow 1s$ is[13] $-0.139$, we can set an upper limit for $f_L$ of about $1+\frac{3}{4}(0.139)\approx 1.1$. Thus we see that our calculations of $B_L$ and $C_L$ for $\theta_L<0.45$ are not reliable. Lacking a more accurate calculation of an asymptotic formula for this region ($Z<30$), it is reasonable to proceed as follows: Calculate $f_L$ using Hartree wave functions for the desired atom, and then with this $f_L$ and a corresponding $\lambda_L$ from Table IV, write $B_L\simeq 4(1+f_L)\ln(16\eta_L/\lambda_L)$.

## V. SUMMARY OF EFFECT OF *K*- AND *L*-SHELL BINDING CORRECTIONS

In order to summarize the effect of the *K*- and *L*-shell binding corrections, in Table V, we give for various $Z$ and incident proton energies the approximate percentage correction to the simple formula (1) introduced by $C_K$ and $C_L$. Since the first two terms of $B_K$, given by (2), may be written $S_K(\theta_K)\ln\{\eta_K\exp[T_K(\theta_K)/S_K(\theta_K)]\}$, it is apparent that for $\eta_K<\exp[-T_K(\theta_K)/S_K(\theta_K)]$, $C_K$ must assume negative values to prevent $B_K$ from incorrectly becoming negative. A similar situation holds also for $C_L$. Consequently, for low enough energies the $C_K$ and $C_L$ corrections become large and negative.

## ACKNOWLEDGMENTS

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The author is deeply indebted to Professor H. A. Bethe for his valuable guidance and encouragement of this work.

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[13] See Table XVI, H. Bethe, *Handbuch der Physik* (Verlag Julius Springer, Berlin, 1933), Vol. 24, Part 1, p. 443.

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# Transport and Deformation-Potential Theory for Many-Valley Semiconductors with Anisotropic Scattering

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A transport theory which allows for anisotropy in the scattering processes is developed for semiconductors with multiple nondegenerate band edge points. It is found that the main effects of scattering on the distribution function over each ellipsoidal constant-energy surface can be described by a set of three relaxation times, one for each principal direction; these are the principal components of an energy-dependent relaxation-time tensor. This approximate solution can be used if all scattering processes either conserve energy or randomize velocities. Expressions for mobility, Hall effect, low- and high-field magnetoresistance, piezoresistance, and high-frequency dielectric constant are derived in terms of the relaxation-time tensor. For static-field transport properties the effect of anisotropic scattering is merely to weight each component of the effective-mass tensor, as it appears in the usual theory, with the reciprocal of the corresponding component of the relaxation-time tensor.

The deformation-potential method of Bardeen and Shockley is generalized to include scattering by transverse as well as longitudinal acoustic modes. This generalized theory is used to calculate the acoustic contributions to the components of the relaxation-time tensor in terms of the effective masses, elastic constants, and a set of deformation-potential constants. For *n* silicon and *n* germanium, one of the two deformation-potential constants can be obtained from piezoresistance data. The other one can at present only be roughly estimated, e.g., from the anisotropy of magnetoresistance. Insertion of these constants into the theory yields a value for the acoustic mobility of *n* germanium which is in reasonable agreement with observation; a more accurate check of the theory may be possible when better input data are available. For *n* silicon, available data do not suffice for a check of the theory.

## 1. INTRODUCTION

IN the last few years, it has been become clear[1] that most of the well-studied semiconductors have energy band structures greatly different from the simple model which had nearly always been assumed in earlier theoretical work. Whereas this simple model [Fig. 1(a)] assumed a nondegenerate band-edge state with wave vector $\mathbf{K}=0$ and spherical surfaces of constant energy, many or most actual band structures seem to be either of the "many-valley" type [Fig. 1(b)], with several nondegenerate band-edge points $\mathbf{K}^{(i)}$ and ellipsoidal

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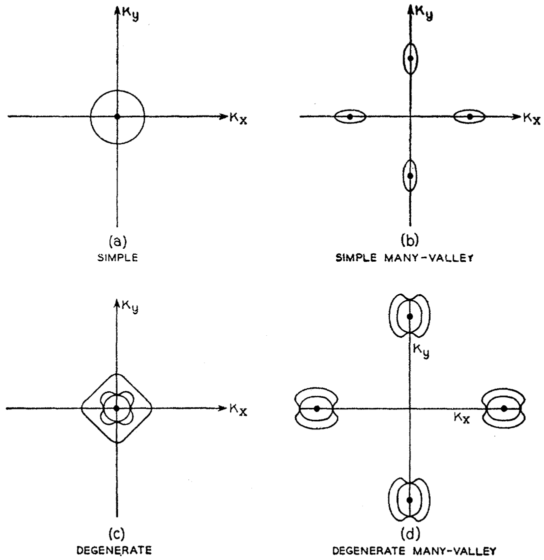
[1] For a brief review of some of the evidence, see C. Kittel, Physica **20**, 829 (1954).

energy surfaces around each, or of the "degenerate" types [Fig. 1(c) or 1(d)], for which the presence of two or more band edge states of the same energy and wave vector causes the energy surfaces to have more complicated shapes. Of these nonsimple models, the many-valley model of Fig. 1(b), which seems to occur for the conduction bands of silicon and germanium, is the easiest to treat theoretically. The transport properties of this model have been discussed in several papers.[2–4] All these papers have assumed that the scattering processes which the electrons or holes undergo can be described by a relaxation time which may depend on energy but which is independent of position over a constant-energy surface. A qualitative study of the adequacy of this assumption[5] has shown that it is probably quite good for the contributions of neutral impurity scattering and intervalley lattice scattering, and in nonpolar crystals for that of optical mode scattering as well. However, the assumption is only sometimes good for scattering by acoustical modes, and it is usually quite poor for ionized impurity scattering.

There is thus a need for a tractable theory of transport phenomena based on less restrictive assumptions regarding the scattering processes. The first of the two objectives of the present paper is to develop such a theory, for the many-valley model. Since a rigorous treatment of the most general type of scattering law would be very difficult, we shall undertake to solve the Boltzmann equation by an approximate method to be described in Sec. 2, which is applicable when all scattering processes either conserve energy or randomize velocity and which should give very good results when the anisotropy of the scattering processes is not too extreme. Instead of a single relaxation time $\tau(\epsilon)$ characterizing all states of energy $\epsilon$, this approach makes use of three relaxation time functions $\tau_1(\epsilon)$, $\tau_2(\epsilon)$, $\tau_3(\epsilon)$, assigned respectively to the three principal directions of the energy surfaces of a valley. These $\tau_\alpha(\epsilon)$ are, of course, explicitly calculable from the scattering probabilities $S(\mathbf{K}\to\mathbf{K}')$. In Sec. 3, we shall apply this method to the calculation of mobility, piezoresistance, Hall effect, magnetoresistance, and high-frequency dielectric constant, describing all of these effects in terms of the three $\tau_\alpha(\epsilon)$.

The second objective of this paper is to generalize the deformation-potential approach of Bardeen and Shockley[6] to the many-valley model, and with it to express the $\tau_\alpha(\epsilon)$ for pure acoustical scattering in terms of constants describing the shifts of the band edge energies with strain. This will be done in Secs. 4 and 5. The calculations, though straightforward in principle, are rather tedious because they involve integrations of anisotropic scattering probabilities over ellipsoidal energy surfaces. In Sec. 6, we shall apply the theory to the quantitative correlation of mobility, piezoresistance, and other data for $n$-type silicon and $n$-type germanium.



(a) SIMPLE

(b) SIMPLE MANY-VALLEY

(c) DEGENERATE

(d) DEGENERATE MANY-VALLEY

FIG. 1. Different types of band structure for a semiconductor, illustrated by the forms of the surfaces of constant energy in wave number space. The band edge points $\mathbf{K}^{(i)}$ are represented by heavy dots.

## 2. SPHERICAL HARMONIC DEVELOPMENT OF THE DISTRIBUTION FUNCTION

Let $f$ be the distribution function for the electrons or holes in $\mathbf{K}$-space, $S(\mathbf{K}-\mathbf{K}')$ the transition probability into unit volume of $\mathbf{K}$-space due to scattering, so that, when nondegenerate statistics apply, the Boltzmann equation is

$$\frac{\partial f(\mathbf{K})}{\partial t}=\left(\frac{\partial f(\mathbf{K})}{\partial t}\right)_{\text{fields}}+\int[f(\mathbf{K}')S(\mathbf{K}'\to\mathbf{K})-f(\mathbf{K})S(\mathbf{K}\to\mathbf{K}')]d\mathbf{K}'. \qquad (1)$$

It is easy to show that the integral in (1) can be greatly simplified if $S$ randomizes velocity in the sense that

$$S(\mathbf{K}\to\mathbf{K}')=S(\mathbf{K}\to\mathbf{K}'^*)=S(\mathbf{K}^*\to\mathbf{K}'), \qquad (2)$$

where $\mathbf{K}^*$ is the state in the same valley as $\mathbf{K}$ but with opposite velocity. For this case, the part $f^-$ of $f$ which is odd under the inversion $\mathbf{K}\rightleftarrows\mathbf{K}^*$ contributes nothing to the integral of the first term. The total contribution of $f^-$ is thus determined by the second term, and is of the form $f^-(\mathbf{K})/\tau(\mathbf{K})$, this being a definition of a relaxation time $\tau(\mathbf{K})$. Since the first-order effect of a small electric field or temperature gradient is to produce a departure from equilibrium which is odd, any scattering law of the type (2) permits easy solution of (1) for all except "hot-electron" phenomena. Here we

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[2] S. Meiboom and B. Abeles, Phys. Rev. **93**, 1121 (1954); B. Abeles and S. Meiboom, Phys. Rev. **95**, 31 (1954).

[3] M. Shibuya, J. Phys. Soc. Japan **9**, 134 (1954); Phys. Rev. **95**, 1385 (1954).

[4] C. Herring, Bell System Tech. J. **34**, 237 (1955).

[5] Reference 4, Appendix A.

[6] J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).

wish to consider the more general case

$$S = S_c + S_r, \tag{3}$$

where the subscripts $r$ and $c$, which we shall use throughout the paper, stand for "randomizing" and "conservative" respectively; $S_r$ satisfies (2), and $S_c$ represents energy-conserving intravalley processes, i.e., processes $\mathbf{K} \rightarrow$ some $\mathbf{K}'$ on the same constant-energy ellipsoid. Thus $S_c$ contains a factor $\delta(\epsilon - \epsilon')$. For such a case, and for infinitesimal electric field, the contribution of $S_r$ to (1) can be described by a relaxation time, while the contribution of $S_c$ possesses the simplifying property that it does not mix the $f$'s of different energy surfaces. Thus the solution of (1) reduces to the solution of a two-dimensional integral equation on each energy ellipsoid.

The form (3) includes most of the situations which occur in semiconductors. Intervalley and optical mode scattering satisfy (2) to a good approximation, because the matrix element is nearly independent of the positions of $\mathbf{K}$ and $\mathbf{K}'$ in their respective valleys.[5] Normal impurity scattering and acoustical mode scattering conserve energy, or nearly so. However, electron-electron collisions, which have a moderate effect when ionized impurity scattering is pronounced,[7] are not describable in this way. The fact that electron-electron collisions mix different energies without randomizing velocities prevents the considerations of this paper from applying with any exactitude to the high carrier concentrations at which degenerate statistics occur. However, it is not hard to generalize the results at each stage so that they are applicable to a hypothetical case where (1) and (3) apply with Fermi statistics, and we shall indicate from time to time how this generalization is to be made.

It is convenient to define new coordinates, in whose space the energy surfaces become spheres, by changes of scale in the three directions corresponding to the principal axes of the ellipsoids:

$$\varphi_\alpha = \hbar(K_\alpha - K_\alpha^{(i)})/(m_\alpha^*)^{\frac{1}{2}}, \tag{4}$$

$$\Delta\epsilon \equiv |\epsilon - \epsilon_b| = \tfrac{1}{2}\varphi^2, \tag{5}$$

where $m_\alpha^*$ is the effective mass in the $\alpha$th principal direction, $\epsilon(\mathbf{K})$ is the energy, and $\epsilon_b = \epsilon(\mathbf{K}^{(i)})$ is the band edge energy. This transformation, besides simplifying the treatment of scattering processes which conserve energy, has the further advantage, which we shall use later, that the changes in time due to a magnetic field become simple rigid rotations in $\boldsymbol{\varphi}$ space.

To make use of the new coordinates, let the departure of the distribution function from equilibrium be expanded in spherical harmonics in $\boldsymbol{\varphi}$ space:

$$f - f^{(0)} = \sum_{l,m} F_{lm}(\varphi) Y_{lm}(\boldsymbol{\varphi}/\varphi). \tag{6}$$

Since $S_c$ conserves energy, the changes brought about by this type of scattering can be described by equations of the form

$$\left[\frac{\partial F_{lm}(\varphi)}{\partial t}\right]_{S_c} = \sum_{l',m'} (lm|S_c|l'm') F_{l'm'}(\varphi), \tag{7}$$

the coefficients being, of course, functions of $\varphi$. For the other type of scattering postulated in (3), that which randomizes velocity, we have for odd $l$ an analogous equation

$$\left[\frac{\partial F_{lm}(\varphi)}{\partial t}\right]_{S_r} = \sum_{l',m'} (lm|S_r|l'm') F_{l'm'}(\varphi), \tag{8}$$

For infinitesimal electric field, the only case we shall consider, only terms with odd $l$ occur in (6), whether or nor there are magnetic fields or periodic time variations. Thus, the Boltzmann equation (1) reduces to a set of simultaneous equations in the $F_{lm}$ for each value of $\varphi$ (or energy).

Note that if $S_r$ randomizes the final state over an energy surface, instead of merely satisfying (2), the right-hand side of (8) reduces simply to $-F_{lm}(\varphi)/\tau_r(\varphi)$. This is the case for the principal $S_r$-processes, *viz.*, optical mode and intervalley scattering.[5]

All the transport properties mentioned in the introduction can be described in terms of the dependence of the current on the magnetic and electric fields and on time or frequency. The contribution of each energy shell to the current is a linear combination of the coefficients $F_{1m}$ for $l=1$. The central ideal of the present section is to note that if the terms $l' \neq l$ in (7) and (8) are not too large, the $F_{1m}$ can be derived fairly accurately by neglecting the terms $l>1$ in (7) and (8), the error being of the second order in the neglected coefficients. This conclusion follows from a consideration, in physical terms, of the structure of the simultaneous equation system to which we have reduced the Boltzmann equation:

The electric field feeds the $F_{1m}$ from $f^{(0)}$.

The magnetic field, producing a rigid rotation in $\boldsymbol{\varphi}$ space, feeds each $F_{lm}$ only from $F_{lm'}$ of the same $l$, i.e., it does not mix $l$'s.

$S_c + S_r$ feeds each $F_{lm}$ from many $F_{l'm'}$, but, by hypothesis, feeds the $F_{1m}$ more strongly from each other than from the $F_{l'm'}$ with $l'>1$.

Thus, if the coefficients $(1m|S_c+S_r|l'm')$ for $l'>1$ are taken as small quantities of the first order, the $F_{l'm'}$ for $l'=3$, 5—will be of the first order, and their effect on the feeding of the $F_{1m}$ will be of the second order.

A preliminary investigation of scattering processes in semiconductors[5] has shown that the anisotropy of scattering in $\boldsymbol{\varphi}$ space, though often appreciable, is not usually very extreme. Thus, it is reasonable to hope that the approximation just outlined will be a good one in most cases. To make this expectation more

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[7] L. Spitzer, Jr., and R. Härm, Phys. Rev. 89, 977 (1953).

quantitative, we have investigated, in Appendix A, some special scattering functions for which (1) is exactly soluble, and have compared the exact answers with those computed by neglecting terms $l>1$ in (7) or (8). For a given electric field, the current computed in the latter way is always too small; this is a general consequence of the positive-definiteness of the dissipation function. However, the results of Appendix A suggest that the error will usually be only a few percent if the relaxation time $\tau(\mathbf{K})$ of a carrier, or some similar measure of the effectiveness of $S$, does not vary by more than a factor two or so over an energy surface. Some rough estimates[5] have indicated that the anisotropy of the scattering due to acoustic modes is usually, though not always, no worse than this. The range of anisotropy to be expected for impurity scattering is less certain, but clearly slight to moderate amounts of impurity scattering cannot take the over-all scattering function out of the domain of applicability of the present method.

It remains to express the $l=1$ terms of (7) and (8) as integrals of the scattering probability. If the basis for the $F_{1m}$ is chosen to consist of functions transforming as $x$, $y$, $z$, the coefficients $(1m|S|1m')$ become second rank tensors $S_{\alpha\beta}$. If the crystal has two or more symmetry planes through $\mathbf{K}^{(i)}$, as we shall assume, the principal axes of this tensor must coincide with those of the constant-energy ellipsoids. When the coordinate axes are chosen in these principal directions, the sum of (7) and (8) must have the form

$$\left[\frac{\partial F_{1x}(\varphi)}{\partial t}\right]_S=-\frac{F_{1x}(\varphi)}{\tau_x(\varphi)}=-F_{1x}(\varphi)\left(\frac{1}{\tau_{rx}}+\frac{1}{\tau_{cx}}\right),\tag{9}$$

with analogous equations for $y$ and $z$; $\tau_x$, $\tau_y$, $\tau_z$ are the eigenvalues of a relaxation time tensor $\boldsymbol{\tau}$ or $\tau_{\alpha\beta}$ reciprocal to $S_{\alpha\beta}$. The contribution of the velocity-randomizing processes to (9) is given by (1) and (8), with only the second term of (1) contributing; we may calculate it by putting $\varphi_x$ for $f$, since $Y_{1x}\propto\varphi_x$. For Maxwellian statistics, we find

$$\frac{1}{\tau_{rx}(\varphi)}=-\int\varphi_x(\partial f/\partial t)_{S_r}d\Omega_\varphi\bigg/\int\varphi_x f d\Omega_\varphi$$

$$=\int\int\varphi_x^2S_r(\boldsymbol{\varphi}\rightarrow\boldsymbol{\varphi}')d\boldsymbol{\varphi}'d\Omega_\varphi\bigg/\int\varphi_x^2d\Omega_\varphi,\tag{10}$$

where $d\Omega_\varphi$ is the element of solid angle in $\boldsymbol{\varphi}$ space and $S_r(\boldsymbol{\varphi}\rightarrow\boldsymbol{\varphi}')$ is the scattering probability into unit volume of $\boldsymbol{\varphi}$-space. For Fermi statistics, a little algebra shows that the second equation of (10) should be modified by inserting a factor $[1-f^{(0)}(\varphi')]/[1-f^{(0)}(\varphi)]$ in the integrand of the numerator. To get the contribution of the energy-conserving processes, let $S_c$ be equivalent to a scattering probability $\Lambda(\boldsymbol{\varphi}\rightarrow\boldsymbol{\varphi}')$ into solid angle $d\Omega_\varphi'$ at $\boldsymbol{\varphi}'$ on the sphere $\varphi'=\varphi$, i.e., $S_c(\boldsymbol{\varphi}\rightarrow\boldsymbol{\varphi}')=\Lambda\delta(\varphi-\varphi')/\varphi^2$. With $f\rightarrow\varphi_x$ as before, we find, for either statistics,

$$\frac{1}{\tau_{cx}(\varphi)}=-\frac{\displaystyle\int\int\varphi_x(\varphi_x'-\varphi_x)\Lambda(\boldsymbol{\varphi}\rightarrow\boldsymbol{\varphi}')d\Omega_\varphi'd\Omega_\varphi}{\displaystyle\int\varphi_x^2d\Omega_\varphi}.\tag{11}$$

Equations of the same form as (10) and (11) of course hold for $y$ and $z$ also.

The calculations of Secs. 4 to 6 will be devoted to cases where the $\mathbf{K}^{(i)}$ are on threefold or fourfold axes of symmetry, since these are the cases which occur for the conduction bands of silicon and germanium and since they are simpler to treat than band edge points of lower symmetry. The simplicity arises from the fact that the energy surfaces must be ellipsoids of revolution, and the concomitant fact that the three $\tau$'s reduce to two: $\tau_z=\tau_{\parallel}$, $\tau_x=\tau_y=\tau_\perp$. We can show that for such cases the $\Lambda$ in (11) can be replaced by its azimuthal average, defined as

$$\langle\Lambda(\boldsymbol{\varphi}\rightarrow\boldsymbol{\varphi}')\rangle=\text{average on }\alpha\text{ of }\Lambda(D_\alpha\boldsymbol{\varphi}\rightarrow D_\alpha\boldsymbol{\varphi}'),\tag{12}$$

where $D_\alpha$ is the operation of rotation through angle $\alpha$ about the preferred axis of the valley, i.e., about the $z$-direction. This replacement is obviously justified for the integral defining $\tau_{\parallel}^{-1}$; for $\tau_\perp^{-1}$, we need merely note that use of $\Lambda(D_\alpha\boldsymbol{\varphi}\rightarrow D_\alpha\boldsymbol{\varphi}')$ instead of $\Lambda$ amounts to computing $\tau_\perp^{-1}$ with respect to a rotated set of $x,y$ axes, hence must give the same result.

### 3. TRANSPORT PROPERTIES OF MANY-VALLEY SEMICONDUCTORS

We have seen, in Sec. 2, that the Boltzmann equation (1) simplifies greatly when all scattering processes either conserve energy or randomize velocity. Under these conditions scattering does not mix the distributions in different energy shells, at least if we limit attention to departures from equilibrium which are of the first order in the electric field or temperature gradient. Moreover, to this order the rate of change of the distribution due to the electric field or temperature gradient depends only on the equilibrium distribution, while the rate of change in any energy shell due to the magnetic field depends, again, only on the distribution in this energy shell. Therefore, the Boltzmann equation can be solved independently for each energy shell $d\Delta\epsilon$ of each valley $i$ and the resulting current contributions $d\mathbf{j}^{(i)}$ can be added vectorially to give the total current $\mathbf{j}$ corresponding to the given fields. Since all the transport properties mentioned in the introduction are describable in terms of the dependence of $\mathbf{j}$ on the electric and magnetic field vectors, the temperature gradient, and the frequency, the theory of all of these phenomena reduces to the calculation of shell contributions $d\mathbf{j}^{(i)}$. In this section we shall calculate these shell contributions and combine them, in the approximation which describes the scattering by the relaxation time tensor $\boldsymbol{\tau}(\Delta\epsilon)$ whose components are given by (9) to (11). We shall not assume axially symmetrical valleys except in places where the equations are significantly simplified by this assumption.

It turns out, as one might expect, that the calculations using the present assumptions parallel very closely the more familiar ones[2–4] based on the assumption of a single relaxation time for each energy shell. We shall start by proving the theorem that for static electric and magnetic fields the contribution $d\mathbf{j}^{(i)}$ of any energy shell to the current depends on the effective-mass tensor $\mathbf{m}^*$ and the relaxation-time tensor $\boldsymbol{\tau}$ only through the product $\mathbf{m}^{*-1}\cdot\boldsymbol{\tau}$, i.e., involves only the three quotients $\tau_\beta/m_\beta^*$. This follows at once from the Boltzmann equation. The time rate of change of the partial current vector $d\mathbf{j}^{(i)}$ due to the electric field is proportional to the acceleration $\pm e\mathbf{m}^{*-1}\cdot\mathbf{E}$ of the charge carriers, with a factor of proportionality which depends on the energy and the unperturbed distribution function. The contribution of the magnetic field to $\partial d\mathbf{j}^{(i)}/\partial t$ is just $\pm e$ times the sum of the Lorentz accelerations $\pm(e/c)\mathbf{m}^{*-1}\cdot(\mathbf{v}\times\mathbf{H})$ suffered by all the charge carriers in the shell, since the Lorentz acceleration, unlike that due to the electric field, does not displace any velocity vectors across the boundary of the energy shell. However, the sum over the whole shell of $\mathbf{v}\times\mathbf{H}$ is proportional to $d\mathbf{j}^{(i)}\times\mathbf{H}$ so that the combined contribution of the electric and magnetic fields to the time rate of change of current is a linear combination of $\mathbf{m}^{*-1}\cdot\mathbf{E}$ and $\mathbf{m}^{*-1}\cdot(d\mathbf{j}^{(i)}\times\mathbf{H})$. On the other hand the contribution of the scattering processes to the time rate of change of the partial current vector is equal to $-\boldsymbol{\tau}^{-1}\cdot d\mathbf{j}^{(i)}$. Therefore the mass tensor and the relaxation-time tensor occur in the Boltzmann equation only as the product of $\boldsymbol{\tau}$ with $\mathbf{m}^{*-1}$ [see Eqs. (13) and (14) below]. If components are referred to principal axes, the transport properties involving static fields always have the reciprocal of each effective mass, $1/m_\mu^*$, weighted with $\tau_\mu$. However, for transport properties involving alternating electric fields—such as the high-frequency dielectric constant discussed below—the form of the weighting is somewhat different.

Thus we have shown that a simple weighting of mass tensor components by the relaxation-time tensor components holds for the partial current vectors of all the static-field transport phenomena. In general, however, each of the components of the relaxation-time tensor depends on the energy of the shell, so that these components must be included in the Maxwellian average of the partial currents $d\mathbf{j}^{(i)}$. If all of the components of the relaxation-time tensor depend on the energy $\Delta\epsilon$ in the same way then all the static-field transport properties can be obtained from the formulas of the older theory based on isotropic relaxation-time constants[2–4] by the simple prescription given above, i.e., by weighting $m_{\parallel}^{*-1}$ and $m_{\perp}^{*-1}$ with $\tau_{\parallel}$ and $\tau_{\perp}$, respectively. The explicit calculations below confirm this and also show how $\tau_{\perp}$ and $\tau_{\parallel}$ occur in the Maxwellian averages over shells.

The remarks that have been made above enable us to write down at once the Boltzmann equation for the current contribution $d\mathbf{j}^{(i)}$ of an energy shell of any particular energy $\Delta\epsilon$ relative to the band edge. Let us choose a right-handed coordinate system oriented along the principal axes of the valley, and let $\delta_{\alpha\beta\gamma}=1$ if $\alpha\beta\gamma$ is an even permutation of 123, $-1$ if an odd permutation, zero if any two of these indices are the same. With the upper sign for electrons, the lower for holes, the transport equation is

$$\frac{\partial dj_\alpha^{(i)}}{\partial t}=\frac{2\Delta\epsilon}{3kT}\frac{e^2E_\alpha dn^{(i)}}{m_\alpha^*}\mp\frac{e}{c}\frac{\sum_{\beta,\gamma}\delta_{\alpha\beta\gamma}H_\gamma dj_\beta^{(i)}}{m_\alpha^*}-\frac{dj_\alpha^{(i)}}{\tau_\alpha},\tag{13}$$

where $dn^{(i)}$ is the equilibrium number of carriers in the energy shell in question, per unit volume of crystal. For static-field problems, the left of (13) is to be set equal to zero; the three equations (13) then involve, as we have already noted, only the combinations of $\tau_\alpha/m_\alpha^*$. For any $\mathbf{H}$, these can be solved as simultaneous equations for the $dj_\alpha^{(i)}$. Although for large magnetic fields $H$ a solution of (13) by determinants is the most convenient, an iterative solution is simplest for small $H$. Writing (13), with left side zero, in the form

$$0=\frac{2\Delta\epsilon}{3kT}\frac{e^2\tau_\alpha E_\alpha dn^{(i)}}{m_\alpha^*}-\sum_\beta(\delta_{\alpha\beta}\pm O_{\alpha\beta})dj_\beta^{(i)},$$

where

$$O_{\alpha\beta}=(e\tau_\alpha/m_\alpha^*c)\textstyle\sum_\gamma\delta_{\alpha\beta\gamma}H_\gamma,\tag{14}$$

we can express the solution in terms of the series for the reciprocal of the tensor $(1\pm O)$:

$$dj_\beta^{(i)}=\frac{2\Delta\epsilon}{3kT}\sum_\alpha\frac{e^2\tau_\alpha E_\alpha dn^{(i)}}{m_\alpha^*}\times(\delta_{\alpha\beta}\mp O_{\beta\alpha}+\textstyle\sum_\gamma O_{\beta\gamma}O_{\gamma\alpha}\cdots).\tag{15}$$

### Mobility

The leading term of (15) gives the conductivity $\sigma_0$ at $H=0$, or equivalently the mobility $\mu$. The contribution of the $i$th valley to the conductivity tensor can be expressed as $n^{(i)}e\mu_{\alpha\beta}^{(i)}$, where $n^{(i)}=\int dn^{(i)}$ is the concentration of carriers in states of the $i$th valley, and where $\mu_{\alpha\beta}^{(i)}$ is diagonal relative to the axes of the $i$th valley. From (15), we find

$$\mu_{\alpha\alpha}^{(i)}=\frac{e}{m_\alpha^*}\frac{\langle\Delta\epsilon\tau_\alpha\rangle}{\langle\Delta\epsilon\rangle},\tag{16}$$

where the angular brackets represent Maxwellian averages, $\langle\Delta\epsilon\rangle=\frac{3}{2}kT$, etc. For a cubic crystal the average of (16) over the different valleys is the same as the average over $\alpha$ in a single valley, so we have for the total mobility

$$\mu=\frac{\sigma_0}{ne}=\mathbf{E}\cdot\sum_i\int d\mathbf{j}^{(i)}\bigg/neE^2=\frac{e}{3\langle\Delta\epsilon\rangle}\sum_\alpha\frac{\langle\Delta\epsilon\tau_\alpha\rangle}{m_\alpha^*},\tag{17}$$

where $n=\sum n^{(i)}$.

### Hall Effect

The $O_{\beta\alpha}$ term in (15) gives the low-field Hall conductivity; the contribution of the $i$th valley to this is

$$\sigma_{\alpha\beta\gamma}{}^{(i)}\equiv\frac{\partial^2 j_\alpha{}^{(i)}}{\partial E_\beta\partial H_\gamma}=\mp\frac{e^3n^{(i)}}{c}\frac{\langle\Delta\epsilon\tau_\alpha\tau_\beta\rangle}{\langle\Delta\epsilon\rangle}\frac{\delta_{\alpha\beta\gamma}}{m_\alpha^*m_\beta^*}.\tag{18}$$

Summing this on valleys gives the total $\sigma_{\alpha\beta\gamma}$, equal to $\mp(\sigma_0\mu_H/c)\delta_{\alpha\beta\gamma}$, where $\mu_H$ is the Hall mobility. For a cubic crystal with axially symmetrical valleys, we find

$$\frac{\mu_H}{\mu}=\frac{3\langle\Delta\epsilon\rangle\left(\dfrac{2\langle\Delta\epsilon\tau_\parallel\tau_\perp\rangle}{m_\parallel^*m_\perp^*}+\dfrac{\langle\Delta\epsilon\tau_\perp{}^2\rangle}{m_\perp^{*2}}\right)}{\left(\dfrac{\langle\Delta\epsilon\tau_\parallel\rangle}{m_\parallel^*}+\dfrac{2\langle\Delta\epsilon\tau_\perp\rangle}{m_\perp^*}\right)^2}.\tag{19}$$

### Low-Field Magnetoresistance

In a similar way, the third term of (15) gives the low-field magnetoresistance, or more properly, magnetoconductivity. We find for the contribution of the $i$th valley, in the principal axis system of this valley,

$$\sigma_{\alpha\beta\gamma\delta}{}^{(i)}\equiv\frac{1}{2}\frac{\partial^3 j_\alpha{}^{(i)}}{\partial E_\beta\partial H_\gamma\partial H_\delta}$$

$$=\frac{e^4n^{(i)}}{c^2}\sum_\lambda\frac{\langle\Delta\epsilon\tau_\alpha\tau_\beta\tau_\lambda\rangle}{\langle\Delta\epsilon\rangle}\frac{(\delta_{\lambda\gamma\beta}\delta_{\lambda\alpha\delta}+\delta_{\lambda\delta\beta}\delta_{\lambda\alpha\gamma})}{2m_\alpha^*m_\beta^*m_\lambda^*}.\tag{20}$$

The total magnetoconductivity tensor is again obtained by summing on valleys. For axially symmetrical valleys, the results all come out in the form

$$\sigma_{\alpha\beta\gamma\delta}\equiv\frac{1}{2}\frac{\partial^3 j_\alpha}{\partial E_\beta\partial H_\gamma\partial H_\delta}=\frac{ne^4}{c^2\langle\Delta\epsilon\rangle}\left[g_{30}\frac{\langle\Delta\epsilon\tau_\perp{}^3\rangle}{m_\perp^{*3}}\right.$$

$$\left.+g_{21}\frac{\langle\Delta\epsilon\tau_\perp{}^2\tau_\parallel\rangle}{m_\perp^{*2}m_\parallel^*}+g_{12}\frac{\langle\Delta\epsilon\tau_\perp\tau_\parallel{}^2\rangle}{m_\perp^*m_\parallel^{*2}}\right],\tag{21}$$

where $n$ is the total density of carriers and the coefficients $g_{pq}$ depend on $\alpha\beta\gamma\delta$. Table I gives values of the $g_{pq}$ and relates the $\sigma_{\alpha\beta\gamma\delta}$ to the magnetoresistance constants $\bar{b}$, $\bar{c}$, $\bar{d}$ introduced by Seitz,[8,9] and defined by

$$\left(\frac{\Delta\rho}{\rho_0}\right)_j^H=\bar{b}H^2+\bar{c}\frac{(\mathbf{j}\cdot\mathbf{H})^2}{j^2}+\frac{\bar{d}(j_x{}^2H_x{}^2+j_y{}^2H_y{}^2+j_z{}^2H_z{}^2)}{j^2},\tag{22}$$

where $\Delta\rho=\rho-\rho_0$ is the change in resistivity $\rho$ of a specimen, due to a small field $\mathbf{H}$, for a given direction of $\mathbf{j}$. We have put bars over the letters in an effort to avoid confusion between the magnetoresistance constant $\bar{c}$ and the velocity of light.

TABLE I. Low-field magnetoconductivity components for cubic crystals with axially symmetrical valleys, referred to the crystal axes. Tabulated quantities are the coefficients $g_{30}$, $g_{21}$, $g_{12}$, respectively, in Eq. (21) for $\sigma_{\alpha\beta\gamma\delta}$.

| Component, referred to crystal axes | Type of Valleys (direction of a $\mathbf{K}^{(i)}$) 100 | 111 |
|---|---|---|
| $\sigma_{\alpha\alpha\alpha\alpha}=-\sigma_0(\bar{b}+\bar{c}+\bar{d})$<br>$=-\sigma_0(\Delta\rho/\rho_0H^2)_{100}{}^{100}$ | 0, 0, 0 | −2/9, 4/9, −2/9 |
| $\sigma_{\alpha\alpha\beta\beta}=-\sigma_0\bar{b}-\sigma_0(\mu_H/c)^2$<br>$=-\sigma_0(\Delta\rho/\rho_0H^2)_{100}{}^{010}$<br>$-\sigma_0(\mu_H/c)^2$ | $-\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}$ | −2/9, −5/9, −2/9 |
| $\sigma_{\alpha\beta\alpha\beta}=-\frac{1}{2}\sigma_0\bar{c}+\frac{1}{2}\sigma_0(\mu_H/c)^2$ | $0, \frac{1}{2}, 0$ | 1/9, 5/18, 1/9 |

### High-Field Magnetoresistance

For large magnetic fields it is, as we have remarked, simplest to solve the Boltzmann equation (13) or (14) by determinants. The conductivity tensor which relates the sum of all the current contributions $d\mathbf{j}^{(i)}$ to the electric field comes out in the form of a Maxwellian average of a quotient with a numerator of the third degree and a denominator of the second degree in the components of $\mathbf{m}^{*-1}\cdot\boldsymbol{\tau}$. As $H\rightarrow\infty$, the limiting value of the resistivity transverse to the magnetic field turns out to involve terms of order 1, $1/H$, and $1/H^2$ in the conductivity tensor, and for the most general dependence of $\tau_\parallel$ and $\tau_\perp$ on energy this limiting form is too complicated to be worth writing down. We shall therefore be content to give, for general forms of $\tau_\parallel(\Delta\epsilon)$, $\tau_\perp(\Delta\epsilon)$, only the limiting form of the conductivity tensor as $H\rightarrow\infty$; this suffices to determine the limiting longitudinal magnetoresistance, though not the transverse. A simple calculation gives for the contribution of the $i$th valley to this limiting conductivity tensor

$$\sigma_{\alpha\beta}{}^{(i)}(H\rightarrow\infty)=e^2n^{(i)}\frac{H_\alpha H_\beta}{\langle\Delta\epsilon\rangle}$$

$$\times\left\langle\frac{\Delta\epsilon}{H_1{}^2m_1{}^*/\tau_1+H_2{}^2m_2{}^*/\tau_2+H_3{}^2m_3{}^*/\tau_3}\right\rangle,\tag{23}$$

where $H_1$, $H_2$, $H_3$ are the components of $\mathbf{H}$ along the principal axes of valley $i$. This is the generalization of Eq. (75) of reference 4.

When $\tau_\parallel$ and $\tau_\perp$ are each proportional to $\Delta\epsilon^{-\frac{1}{2}}$, as for the ideal case of acoustic lattice scattering, the complete high-field magnetoresistance can of course be taken from the work of Abeles and Meiboom[2] or that of Shibuya,[3] with the replacement of $m_\parallel^*/m_\perp^*$ by $m_\parallel^*\tau_\perp/m_\perp^*\tau_\parallel$

The limiting Hall constant as $H\rightarrow\infty$ turns out to be simply $1/nec$, just as in the simpler theory.[2–4] The lack

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[8] F. Seitz, Phys. Rev. **79**, 372 (1950).

[9] G. L. Pearson and H. Suhl, Phys. Rev. **83**, 768 (1950).

of dependence on $\tau_{\parallel}$ and $\tau_{\perp}$ is of course to be expected in view of the lack of dependence on $m_{\parallel}^*$ and $m_{\perp}^*$.

### Piezoresistance

It was pointed out in reference 4 that for a many-valley semiconductor two effects predominate over all others in producing a change of resistance with strain of the sort observed by Smith[10] for silicon and germanium. The first of these is the change in the populations of different valleys due to the different shifts in the energies of band edge points differently situated with respect to an anisotropic strain. This "electron transfer effect" gives a contribution to the piezoresistance which is proportional to the anisotropy of the conductivity tensor for a single valley and inversely proportional to the absolute temperature. The second effect, which is important only when intervalley scattering is appreciable, is the effect of strain on the relaxation times, due to increase or decrease in the energies of the valleys containing possible final states for intervalley scattering. These two effects, and other effects of much smaller magnitude, give additive contributions to the electroresistance tensor. The latter is defined for a cubic crystal as

$$m_{\alpha\beta\gamma\delta}\equiv-\sigma^{-1}\partial\sigma_{\alpha\beta}/\partial u_{\gamma\delta}, \tag{24}$$

where $u_{\gamma\delta}$ is the strain tensor and $\sigma_{\alpha\beta}$ is the conductivity tensor, which in the absence of strain has the form of $\sigma\delta_{\alpha\beta}$.

Let us choose a coordinate system, e.g., the crystal axes, which is the same for all the valleys, and let $\sigma_{\alpha\beta}^{(i)}=n^{(i)}e\mu_{\alpha\beta}^{(i)}$ be the conductivity tensor of the $i$th valley relative to these axes. Then, if we neglect all contributions to the elastoresistance other than the two just mentioned, we can write

$$m_{\alpha\beta\gamma\delta}=\frac{1}{\sigma}\sum_{i,j}\frac{\partial\sigma_{\alpha\beta}^{(i)}}{\partial\epsilon^{(j)}}\frac{\partial\epsilon^{(j)}}{\partial u_{\gamma\delta}}, \tag{25}$$

where $\epsilon^{(j)}$ is the energy of the $j$th band-edge point. The quantities $\partial\epsilon^{(j)}/\partial u_{\delta\gamma}$ will be referred to as "deformation potential constants," as they play the central role in the generalization of the Bardeen-Shockley deformation-potential theory of mobility, which we shall discuss in the next section. When the valleys lie on symmetry axes in the Brillouin zone, their symmetry makes it possible to describe all the deformation-potential constants in terms of two or three independent ones. Table II shows one way of doing this. The independent constants $\Xi_d$, $\Xi_u$ for valleys on (100) or (111) axes have been chosen so that $\Xi_d$ represents the shift due to a dilatation in the two directions normal to the axis, while $\Xi_u$ represents that due to a uniaxial shear compounded out of a stretch along the axis and a contraction in the two normal directions; the notation agrees with that of reference 4. The meaning of $\Xi_d$ and $\Xi_u$ for (110) valleys is similar, but now a third constant $\Xi_p$ must be introduced, describing the shift due to a shear in the (001) plane containing the valley axis.

TABLE II. Symmetry restrictions on the deformation potentials for some simple types of valleys in a cubic semiconductor.

| Type of valley (direction of $\mathbf{K}^{(i)}$) → | 100 | 111 | 110 |
|---|---|---|---|
| $\Xi_1=\partial\epsilon^{(i)}/\partial u_{xx}$ | $\Xi_d+\Xi_u$ | $\Xi_d+\frac{1}{3}\Xi_u$ | $\Xi_d+\Xi_u-\frac{1}{2}\Xi_p$ |
| $\Xi_2=\partial\epsilon^{(i)}/\partial u_{yy}$ | $\Xi_d$ | $\Xi_d+\frac{1}{3}\Xi_u$ | $\Xi_d+\Xi_u-\frac{1}{2}\Xi_p$ |
| $\Xi_3=\partial\epsilon^{(i)}/\partial u_{zz}$ | $\Xi_d$ | $\Xi_d+\frac{1}{3}\Xi_u$ | $\Xi_d-\Xi_u+\Xi_p$ |
| $\Xi_4=\partial\epsilon^{(i)}/\partial u_{yz}$ | 0 | $\frac{1}{3}\Xi_u$ | 0 |
| $\Xi_5=\partial\epsilon^{(i)}/\partial u_{xz}$ | 0 | $\frac{1}{3}\Xi_u$ | 0 |
| $\Xi_6=\partial\epsilon^{(i)}/\partial u_{xy}$ | 0 | $\frac{1}{3}\Xi_u$ | $\frac{1}{2}\Xi_p$ |

Now consider the first factor on the right of (25). Since $n^{(i)}$ is proportional to $\exp(-|\epsilon^{(i)}-\epsilon_F|/kT)$ and since in the extrinsic range the variation of the Fermi level $\epsilon_F$ with strain is the average of that of all the $\epsilon^{(i)}$, we have in the present approximation

$$\begin{aligned}\frac{1}{\sigma}\frac{\partial\sigma_{\alpha\beta}^{(i)}}{\partial\epsilon^{(j)}}&=\frac{1}{n\mu}\cdot\frac{\partial(n^{(i)}\mu_{\alpha\beta}^{(i)})}{\partial\epsilon^{(j)}}\\&=\pm\frac{1}{kT}\frac{\mu_{\alpha\beta}^{(i)}}{\mu}\left(\frac{\delta_{ij}}{N_v}-\frac{1}{N_v^2}\right)\\&\qquad-\frac{e}{N_v\mu}\left(\frac{\mathbf{m}^{(i)-1}}{\langle\Delta\epsilon\rangle}\cdot\left\langle\Delta\epsilon\frac{\partial\boldsymbol{\tau}^{(i)}}{\partial\epsilon^{(j)}}\right\rangle\right)_{\alpha\beta},\end{aligned} \tag{26}$$

where $N_v$ is the number of valleys and where ± is + for $n$ type, − for $p$ type, if the $\epsilon^{(j)}$ are understood to be electron energies in all cases. The first term on the right of (26) represents the electron transfer effect, the second the effect of strain on intervalley scattering. It is a simple matter of algebra to combine (25), (26), and Table II and obtain explicit formulas for the elastoresistance constants. The results for the electron transfer contribution, which predominates at low temperatures, are given in Eqs. (27) to (34) below, for the case of a cubic semiconductor. They are expressed in terms of the principal mobilities (16) of a valley and the over-all mobility (17); for the (110) valleys the subscript $p$ is used for the direction normal to the valley axis and in the same (001) type plane as the latter, and the subscript $n$ for the direction normal to this plane. The upper sign is again for electrons, the lower for holes. Valleys centered on (100) axes:

$$\text{Contrib. to } m_{11}\equiv m_{1111}=\pm\frac{2}{9}\frac{\Xi_u}{kT}\left(\frac{\mu_{\parallel}^{(i)}-\mu_{\perp}^{(i)}}{\mu}\right), \tag{27}$$

$$\text{Contrib. to } m_{12}\equiv m_{1122}=\mp\frac{1}{9}\frac{\Xi_u}{kT}\left(\frac{\mu_{\parallel}^{(i)}-\mu_{\perp}^{(i)}}{\mu}\right), \tag{28}$$

$$\text{Contrib. to } m_{44}\equiv m_{1212}=0. \tag{29}$$

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[10] C. S. Smith, Phys. Rev. 94, 42 (1954).

Valleys centered on (111) axes:

$$\text{Contrib. to } m_{11}=\text{that to } m_{12}=0, \tag{30}$$

$$\text{Contrib. to } m_{44}=\pm\frac{1}{9}\frac{\Xi_u}{kT}\left(\frac{\mu_{\parallel}{}^{(i)}-\mu_{\perp}{}^{(i)}}{\mu}\right). \tag{31}$$

Valleys centered on (110) axes:

$\pm$Contrib. to $m_{11}$

$$=\left(\frac{2}{9}\frac{\Xi_u}{kT}-\frac{1}{6}\frac{\Xi_p}{kT}\right)\left(\frac{\mu_{\parallel}{}^{(i)}-\mu_{\perp p}{}^{(i)}}{\mu}\right)$$
$$+\left(-\frac{4}{9}\frac{\Xi_u}{kT}+\frac{1}{3}\frac{\Xi_p}{kT}\right)\left(\frac{\mu_{\perp n}{}^{(i)}-\mu_{\perp p}{}^{(i)}}{\mu}\right), \tag{32}$$

$\pm$Contrib. to $m_{12}$

$$=\left(-\frac{1}{9}\frac{\Xi_u}{kT}-\frac{1}{12}\frac{\Xi_p}{kT}\right)\left(\frac{\mu_{\parallel}{}^{(i)}-\mu_{\perp p}{}^{(i)}}{\mu}\right)$$
$$+\left(\frac{2}{9}\frac{\Xi_u}{kT}-\frac{1}{6}\frac{\Xi_p}{kT}\right)\left(\frac{\mu_{\perp n}{}^{(i)}-\mu_{\perp p}{}^{(i)}}{\mu}\right)$$

$$\pm\text{Contrib. to } m_{44}=\frac{1}{12}\frac{\Xi_p}{kT}\left(\frac{\mu_{\parallel}{}^{(i)}-\mu_{\perp p}{}^{(i)}}{\mu}\right). \tag{33}$$

The corresponding explicit expressions for the contribution of the intervalley scattering effect cannot be put in such a simple form, and will not be given here.

The contributions to the elastoresistance from the various minor effects enumerated in reference 4 all can be shown to be nearly independent of temperature over any range where the relaxation times $\tau_\alpha(\Delta\epsilon)$ have the form $f_\alpha(\Delta\epsilon)g(T)$, e.g., over the range in which acoustic lattice scattering predominates. Over such a range a plot of any component of elastoresistance against $1/T$ should give a straight line with an intercept measuring the influence of these minor effects and a slope measuring the product of a $\Xi$ by the anisotropy of $\boldsymbol{\mu}^{(i)}$. Whereas in the theory of reference 4 this anisotropy was that of the reciprocal effective mass tensor $\mathbf{m}^{*-1}$, in the present theory it is that of $\mathbf{m}^{*-1}\cdot\boldsymbol{\tau}$. However, if $\mathbf{m}^*$ is very anisotropic, the sensitivity to the anisotropy of $\boldsymbol{\tau}$ is slight. We shall use these results in Sec. 6 below, when we attempt to calculate the mobilities of electrons in silicon and germanium.

## High-Frequency Dielectric Constant

When an alternating electric field is applied to an assembly of carriers the response becomes limited, at high frequency, by the inertia of the carriers.[11] The solution of the transport equation proceeds exactly as the solution of the static-field problems above except that now the left side of (13) has the form $i\omega dj_\alpha{}^{(i)}$. This causes the transport equation to contain, besides terms in $\mathbf{m}^{*-1}\cdot\boldsymbol{\tau}$, a term in $\boldsymbol{\tau}$ alone. We find, for the frequency-dependent complex conductivity of a cubic crystal,

$$\sigma(\omega)=\frac{ne^2}{3\langle\Delta\epsilon\rangle}\sum_\alpha\frac{1}{m_\alpha{}^*}\left(\frac{\Delta\epsilon\tau_\alpha}{1+i\omega\tau_\alpha}\right), \tag{35}$$

where the summation is over the three principal directions of a valley. The departure of the dielectric constant from the dielectric constant of the crystal without its free carriers is given by

$$\kappa_0-\kappa(\omega)=-(4\pi/\omega)\,\mathrm{Im}\,\sigma(\omega), \tag{36}$$

where $\mathrm{Im}\,\sigma(\omega)$ is the imaginary part of (35). By expanding the denominators in (35)—a nonconvergent procedure which is nevertheless justified as far as the first two terms—we can express (36) in terms of the carrier density $n$ and Maxwellian averages of powers of the relaxation times:

$$\kappa_0-\kappa(\omega)=\frac{4\pi}{3}ne^2\left[\sum_\alpha\frac{\langle\Delta\epsilon\tau_\alpha{}^2\rangle}{m_\alpha{}^*\langle\Delta\epsilon\rangle}-\omega^2\sum_\alpha\frac{\langle\Delta\epsilon\tau_\alpha{}^4\rangle}{m_\alpha{}^*\langle\Delta\epsilon\rangle}+\cdots\right]. \tag{37}$$

In the simpler type of theory with isotropic relaxation time[4] it was possible to eliminate $\tau$ from the leading terms of this by using the analog of (19) for the Hall mobility $\mu_H$. The leading term of (37) then took the form $4\pi n\mu\mu_H m^{(I)}/B$, where $(m^{(I)})^{-1}=\frac{1}{3}\sum_\alpha m_\alpha{}^{*-1}$ and $B$ was a function of the mass ratios, usually only a little less than unity. The leading term in the present version of (37) can be put in the same form if $m^{(I)}/B$ is replaced by

$$m^{(\kappa)}=\left[\sum_\alpha\frac{\langle\Delta\epsilon\tau_\alpha{}^2\rangle}{m_\alpha{}^*}\right]\left[\frac{\langle\Delta\epsilon\tau_1\tau_2\rangle}{m_1{}^*m_2{}^*}+\frac{\langle\Delta\epsilon\tau_2\tau_3\rangle}{m_1{}^*m_3{}^*}+\frac{\langle\Delta\epsilon\tau_3\tau_1\rangle}{m_3{}^*m_1{}^*}\right]^{-1}. \tag{38}$$

While a rather large anisotropy of $\boldsymbol{\tau}$ is required to make this differ radically from its value $m^{(I)}/B$ for isotropic $\tau$, it is noteworthy that (38) can in principle become larger than the largest of the $m_\alpha{}^*$.

Note that the expression (37), unlike the expressions in earlier parts of this section, does not have each of the reciprocal masses weighted by the corresponding component of the relaxation-time tensor.

## Effect of Fermi Degeneracy

It was pointed out in the preceding two sections that under certain conditions the methods developed in those sections and used here could also be applied to cases involving Fermi statistics. Except for the piezoresistance equations, all of the foregoing formulas can be generalized to Fermi statistics, when these conditions are fulfilled, by replacing $dn^{(i)}/kT$ in (13) and subsequent equations with the sum over a shell of $-\partial f^{(0)}/\partial\Delta\epsilon$ and by performing the averages over shells (angular brackets) with the weighting factor $\partial f^{(0)}/\partial\epsilon$ instead of

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[11] T. S. Benedict and W. Shockley, Phys. Rev. 89, 1152 (1953).

the Maxwellian factor. In the piezoresistance equations (26)–(34) the only change needed is to replace $1/kT$ by $\pm\partial\ \ln n^{(i)}/\partial\epsilon_F$. This has the effect of making the piezoresistance considerably smaller for degenerate than for nondegenerate material.

### 4. DEFORMATION-POTENTIAL THEORY

Having thus formulated the theory of transport in terms of a set of principal relaxation times, we turn now to the task of evaluating these relaxation times explicitly for the case of scattering by lattice vibrations of the acoustic range. To do this we shall apply the deformation potential method[6] to calculate the scattering probability $\Lambda(\varphi\rightarrow\varphi')$ between two elements of a constant-energy surface, and hence to evaluate (11). The fundamental idea of the deformation potential approach is that the matrix element $\mathbf{K}\rightarrow\mathbf{K}\pm\mathbf{q}$ for absorption or emission of an acoustic phonon of wave vector $\mathbf{q}$ is practically equal to the $\mathbf{q}$th Fourier coefficient of the function $\delta\epsilon^{(i)}(\mathbf{r})$, defined as the shift of the band edge energy $\epsilon^{(i)}$ which would be produced by a homogeneous strain of magnitude equal to the local strain at point $\mathbf{r}$ due to the mode $\mathbf{q}$. The justification given by Bardeen and Shockley[6] for this assumption can be generalized to include scattering by transverse as well as longitudinal acoustic modes; one can also show that the validity of the method is not impaired by polarization of the filled-band electrons by the presence of the free carrier. Moreover, it is easily shown that electrostatic fields on the scale of the wavelength of the lattice mode usually have a negligible effect, even for a polar semiconductor, unless the crystal is piezoelectric. We shall not undertake to discuss these points here, however, but shall merely take the deformation potential method for granted.

TABLE III. Polarization factors, defined by (42), for normal modes in symmetry directions of a cubic crystal. Values for the symmetry directions not listed are obtainable by permuting the indices of $\mathbf{q}$ and the $f$'s.

| Direction of $\mathbf{q}$ | Branch | $f_1=f_{xx}$ | $f_2=f_{xy}$ | $f_3=f_{zz}$ | $f_4=f_{yz}$ | $f_5=f_{zx}$ | $f_6=f_{xy}$ |
|---|---|---|---|---|---|---|---|
| 100 | long. | 1 | 0 | 0 | 0 | 0 | 0 |
| | trans. 1 | 0 | 0 | 0 | 0 | 0 | 1 |
| | trans. 2 | 0 | 0 | 0 | 0 | 1 | 0 |
| 111 | long. | 1 | 1 | 1 | 2 | 2 | 2 |
| | trans. 1 | 1 | −1 | 0 | −1 | 1 | 0 |
| | trans. 2 | 1 | 1 | −2 | −1 | −1 | 2 |
| $1\bar{1}1$ | long. | 1 | 1 | 1 | −2 | 2 | −2 |
| | trans. 1 | 1 | −1 | 0 | 1 | 1 | 0 |
| | trans. 2 | 1 | 1 | −2 | 1 | −1 | −2 |
| 110 | long. | 1 | 1 | 0 | 0 | 0 | 2 |
| | trans. 1 | 0 | 0 | 0 | 1 | 1 | 0 |
| | trans. 2 | 1 | −1 | 0 | 0 | 0 | 0 |
| $1\bar{1}0$ | long. | 1 | 1 | 0 | 0 | 0 | −2 |
| | trans. 1 | 0 | 0 | 0 | −1 | 1 | 0 |
| | trans. 2 | 1 | −1 | 0 | 0 | 0 | 0 |

We shall assume, as we must if we are to use (11), that the energy of the phonon which a charge carrier absorbs or emits is negligible compared with the energy of the carrier; this is valid for nearly all carriers at any but the very lowest temperatures. With this assumption we can lump absorption and emission together; let $|M|^2$ be the sum of the squared matrix element over absorption and emission. Let $\varphi$ be the projected wave vector defined by (4), related by (5) to the energy $\Delta\epsilon$ relative to the band edge, and let $N_1$ be the number of quantum states of a given spin per unit volume of $\varphi$-space. Then we have for acoustic scattering

$$\Lambda(\varphi\rightarrow\varphi')=(2\pi/\hbar)\sum|M|^2\varphi^2(d\varphi/d\epsilon)N_1 \\ =C\sum|M|^2\Delta\epsilon^{\frac{1}{2}}, \quad (39)$$

say, where the summation is over the three acoustic branches. Combining (39) with (4) and (5) we get for

TABLE IV. Contributions of the longitudinal and transverse branches to the squared matrix element for scattering, for symmetry directions of the phonon wave vector $q$ in a cubic crystal. The values of $|M(\mathbf{q},\alpha)|^2$ are obtained from the table entries by multiplication with $kT/V$. The number of equivalent directions of each type is indicated in parentheses. The quantity $c^*=c_{11}-c_{12}-2c_{44}$ measures the elastic anisotropy of the crystal.

| Type of valley (direction of $\mathbf{K}^{(i)}$) | Direction of $\mathbf{q}$ | Longitudinal | Transverse 1 | Transverse 2 |
|---|---|---|---|---|
| 100 | 100(2) | $\dfrac{(\Xi_d+\Xi_u)^2}{c_{12}+2c_{44}+c^*}$ | 0 | 0 |
| | 110(8) | $\dfrac{(\Xi_d+\frac{1}{2}\Xi_u)^2}{c_{12}+2c_{44}+\frac{1}{2}c^*}$ | 0 | $\dfrac{\frac{1}{4}\Xi_u^2}{c_{44}+\frac{1}{2}c^*}$ |
| | 111(8) | $\dfrac{(\Xi_d+\frac{1}{3}\Xi_u)^2}{c_{12}+2c_{44}+\frac{1}{3}c^*}$ | $\dfrac{\frac{1}{6}\Xi_u^2}{c_{44}+\frac{1}{3}c^*}$ | $\dfrac{(1/18)\Xi_u^2}{c_{44}+\frac{1}{3}c^*}$ |
| | 011(4) | $\dfrac{\Xi_d^2}{c_{12}+2c_{44}+\frac{1}{2}c^*}$ | 0 | 0 |
| | 001(4) | $\dfrac{\Xi_d^2}{c_{12}+2c_{44}+c^*}$ | 0 | 0 |
| 111 | 111(2) | $\dfrac{(\Xi_d+\Xi_u)^2}{c_{12}+2c_{44}+\frac{1}{3}c^*}$ | 0 | 0 |
| | 110(6) | $\dfrac{(\Xi_d+\frac{2}{3}\Xi_u)^2}{c_{12}+2c_{44}+\frac{1}{2}c^*}$ | $\dfrac{(2/9)\Xi_u^2}{c_{44}}$ | 0 |
| | 100(6) | $\dfrac{(\Xi_d+\frac{1}{3}\Xi_u)^2}{c_{12}+2c_{44}+c^*}$ | $\dfrac{\frac{1}{9}\Xi_u^2}{c_{44}}$ | $\dfrac{\frac{1}{9}\Xi_u^2}{c_{44}}$ |
| | $1\bar{1}1$(6) | $\dfrac{(\Xi_d+\frac{1}{9}\Xi_u)^2}{c_{12}+2c_{44}+\frac{1}{3}c^*}$ | $\dfrac{(2/27)\Xi_u^2}{c_{44}+\frac{1}{3}c^*}$ | $\dfrac{(2/81)\Xi_u^2}{c_{44}+\frac{1}{3}c^*}$ |
| | $1\bar{1}0$(6) | $\dfrac{\Xi_d^2}{c_{12}+2c_{44}+\frac{1}{2}c^*}$ | 0 | 0 |

TABLE V. Approximate dependence of the azimuthal average of the squared matrix element for scattering on the angle $\theta$ between **q** and $\mathbf{K}^{(i)}$, the symmetry axis of the valley. The quantity $c^*=c_{11}-c_{12}-2c_{44}$ measures the elastic anisotropy.

| Type of valley (direction of $\mathbf{K}^{(i)}$) | Squared matrix element | Value |
|---|---|---|
| 100 | $\langle \lvert M(\mathbf{q},l)\rvert^2\rangle$ | $\dfrac{(\Xi_d+\cos^2\theta\,\Xi_u)^2}{c_{12}+2c_{44}+\frac{3}{5}c^*}\left[1-\dfrac{c^*(0.15-1.50\cos^2\theta+1.75\cos^4\theta)}{c_{12}+2c_{44}+\frac{3}{5}c^*}\right]\dfrac{kT}{V}$ |
| | $\langle \lvert M(\mathbf{q},t_1)\rvert^2+\lvert M(\mathbf{q},t_2)\rvert^2\rangle$ | $\Xi_u^2\cos^2\theta(1-\cos^2\theta)\left[\dfrac{3}{c_{44}+\frac{1}{3}c^*}-\dfrac{2}{c_{44}+\frac{1}{2}c^*}+6\cos^2\theta\left(\dfrac{1}{c_{44}+\frac{1}{2}c^*}-\dfrac{1}{c_{44}+\frac{1}{3}c^*}\right)\right]\dfrac{kT}{V}$ |
| 111 | $\langle \lvert M(\mathbf{q},l)\rvert^2\rangle$ | $\dfrac{(\Xi_d+\cos^2\theta\,\Xi_u)^2}{c_{12}+2c_{44}+\frac{3}{5}c^*}\left[1+\dfrac{\frac{2}{3}c^*(0.15-1.50\cos^2\theta+1.75\cos^4\theta)}{c_{12}+2c_{44}+\frac{3}{5}c^*}\right]\dfrac{kT}{V}$ |
| | $\langle \lvert M(\mathbf{q},t_1)\rvert^2+\lvert M(\mathbf{q},t_2)\rvert^2\rangle$ | $\Xi_u^2\cos^2\theta(1-\cos^2\theta)\left[\dfrac{0.375}{c_{44}}+\dfrac{0.625}{c_{44}+\frac{1}{3}c^*}+\dfrac{9}{8}\cos^2\theta\left(\dfrac{1}{c_{44}}-\dfrac{1}{c_{44}+\frac{1}{3}c^*}\right)\right]\dfrac{kT}{V}$ |

the coefficient $C$, for a crystal of volume $V$,

$$C=(m_1^*m_2^*m_3^*)^{\frac{1}{2}}V/2^{\frac{3}{2}}\pi^2\hbar^4. \tag{40}$$

When the energy shifts $\delta\epsilon^{(i)}$ at the band-edge points are expressed as linear combinations of the strains $u_s$, the $|M|^2$ for each branch $\alpha$ of the vibrational spectrum becomes a linear combination of products $u_r(\mathbf{q},\alpha)u_s(\mathbf{q},\alpha)$ of Fourier coefficients of the strains. Our task in this section will be to evaluate the thermal averages of these quadratic expressions, in terms of elastic constants and temperatures.

In the preceding section (Table II), we have already made use of the deformation-potential constants $\Xi_s$ ($s=1$ to 6), defined by

$$\delta\epsilon^{(i)}=\sum_{s=1}^{6}\Xi_s^{(i)}u_s, \tag{41}$$

where $\delta\epsilon^{(i)}$ is the shift of the energy at the band edge point $\mathbf{K}^{(i)}$ due to a strain with components $u_s$ indexed in the usual manner and referred to the crystallographic axes. Since the constants going with one valley $i$ of a many-valley semiconductor are derivable by a symmetry transformation from those going with any other valley $j$, we shall henceforth assume that we are working with a particular valley $i$, and omit the suffix $i$ from $\Xi_s^{(i)}$. The coefficient of $u_r(\mathbf{q},\alpha)u_s(\mathbf{q},\alpha)$ in $|M|^2$ is thus $\Xi_r\Xi_s$. To evaluate the thermal average $\langle u_r(\mathbf{q},\alpha)u_s(\mathbf{q},\alpha)\rangle$, let us suppose that

$$u_r(\mathbf{q},\alpha)\propto f_r(\mathbf{q},\alpha), \tag{42}$$

with a factor of proportionality independent of $r$. The $f_r$ are thus simply unnormalized factors describing the state of polarization of the mode $\mathbf{q}$, $\alpha$, factors which can be determined from the theory of elastic waves, or, if $\mathbf{q}$ is in a symmetry direction, from symmetry alone. Since the $\mathbf{q}$'s of interest to us are in the equipartition range, the mean elastic potential energy of the mode $\mathbf{q},\alpha$ is

$$\tfrac{1}{2}V\sum_{r,s}c_{rs}\langle u_r(\mathbf{q},\alpha)u_s(\mathbf{q},\alpha)\rangle=\tfrac{1}{2}kT, \tag{43}$$

where the $c_{rs}$ are the elastic constants and $V$ as before is the volume of the crystal. This equation can be used to determine the proportionality factor in (43). Thus, finally,

$$|M(\mathbf{q},\alpha)|^2=(kT/V)\sum_{r,s}\Xi_r\Xi_sf_rf_s/\sum_{r,s}c_{rs}f_rf_s. \tag{44}$$

We shall be concerned in the following with valleys on (100) or (111) axes in the Brillouin zone of a cubic crystal. For these cases symmetry allows all the $\Xi_r$ to be expressed in terms of two constants $\Xi_d$, $\Xi_u$, as shown in Table II and discussed in the preceding section. Note that the band edge shift $E_1$ per unit change of volume, introduced by Bardeen and Shockley,[6] is given by

$$E_1=\Xi_d+\tfrac{1}{3}\Xi_u. \tag{45}$$

Table III gives values of the polarization factors $f_r(\mathbf{q},\alpha)$, for wave vectors $\mathbf{q}$ in symmetry directions. From these two tables, and (44), we can construct the $|M(\mathbf{q},\alpha)|^2$ for any $\mathbf{q}$ in a symmetry direction. This matrix element of course has the symmetry of the valley in its dependence on the direction of $\mathbf{q}$, and it is independent of the magnitude of $\mathbf{q}$ for any given direction. Table IV gives the results.

To evaluate the relaxation-time integrals (11) we of course need to know $\sum_\alpha|M|^2$ for all directions of $\mathbf{q}$. Moreover, it is useful to keep separate the contributions $|M(\mathbf{q},l)|^2$ of the longitudinal modes and $|M(\mathbf{q},t_1)|^2+|M(\mathbf{q},t_2)|^2$ of the transverse modes, since in one field of application, the phonon contribution to the thermoelectric power,[12] scattering by longitudinal modes has much more effect than an equal amount of scattering by transverse modes. Methods of interpolating these contributions for directions not along symmetry axes are described in Appendix B, and the results are given in Table V. The quantity tabulated is the azimuthal average of the contribution to the squared matrix element, i.e., the average over all directions of $\mathbf{q}$ obtainable by rotating a given $\mathbf{q}$ about the symmetry

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[12] C. Herring, Phys. Rev. 96, 1163 (1954).

TABLE VI. Coefficients in the expressions (49), (50) for the principal relaxation times, for a cubic semiconductor, in terms of the integrals $I_n$, $J_n$, defined in the text. The abbreviations $c^*=c_{11}-c_{12}-2c_{44}$ and $c_l=c_{12}+2c_{44}+\frac{3}{5}c^*$ have been used.

| Type of valley (direction of $\mathbf{K}^{(i)}$) → | 100 | 111 |
|---|---|---|
| $\xi_{\parallel}$ | $I_0+(c^*/c_l)(-0.15I_0+1.5I_1-1.75I_2)$ | $I_0+(c^*/c_l)(0.10I_0-I_1+1.17I_2)$ |
| $\eta_{\parallel}$ | $2I_1+(c^*/c_l)(-0.3I_1+3I_2-3.5I_3)$ | $2I_1+(c^*/c_l)(0.2I_1-2I_2+2.33I_3)$ |
| $\zeta_{\parallel}$ | $I_2+\dfrac{c_l(c_{44}+\frac{5}{6}c^*)}{(c_{44}+\frac{1}{2}c^*)(c_{44}+\frac{1}{3}c^*)}(I_1-I_2)+(c^*/c_l)(-0.15I_2+1.5I_3$ $-1.75I_4)-\dfrac{c^*c_l}{(c_{44}+\frac{1}{2}c^*)(c_{44}+\frac{1}{3}c^*)}(I_2-I_3)$ | $I_2+\dfrac{c_l(c_{44}+\frac{1}{8}c^*)}{c_{44}(c_{44}+\frac{1}{3}c^*)}(I_1-I_2)+(c^*/c_l)(0.10I_2-I_3+1.17I_4)$ $+\dfrac{3}{8}\dfrac{c^*c_l}{c_{44}(c_{44}+\frac{1}{3}c^*)}(I_2-I_3)$ |
| $\xi_{\perp}, \eta_{\perp}, \zeta_{\perp}$ | same as for parallel cases above but with $\frac{1}{2}J_n$ replacing each $I_n$. | |

axis of the valley; according to (12) only this average is needed for the evaluation of (11).

Several features of the table entries are worth noting. All the entries are polynomials in $\cos^2\theta$, where $\theta$ is the angle between $q$ and the symmetry axis of the valley. For vanishing elastic anisotropy $c^*$, these become quadratic forms in $\cos^2\theta$; the last term in the square brackets of each of the four rows of the table represents a small anisotropy correction and contributes terms cubic or quartic in $\cos^2\theta$. The physical origin of the effect of elastic anisotropy is, of course, the effect of this anisotropy in making the rms strain amplitude of modes of a given branch dependent on the direction of $\mathbf{q}$ relative to the crystal axes. Another feature to be noted is that the contributions of the transverse modes involve only the shearing deformation potential $\Xi_u$, and are independent of $\Xi_d$ (or $E_1$). This is to be expected, since in the approximation we have used in Appendix B the transverse modes involve only shearing deformations. For a similar reason, the contribution of the transverse modes vanishes when $\mathbf{q}$ is along the symmetry axis or normal to it: for these directions of $\mathbf{q}$ the shear in a transverse mode (assumed to be exactly transverse) always has an orientation which is forbidden by symmetry to produce a first-order shift in the energy of the center of the valley. Thus the maximum contribution of the transverse modes to the scattering comes from values of $\theta$ near 45° and 135°.

The contributions of the longitudinal and transverse modes to the azimuthal average $\langle\Lambda\rangle$, which we need to use in (11), can now be obtained by inserting the corresponding entries of Table V in place of $\sum|M|^2$ in (39), and using (40).

## 5. EVALUATION OF THE RELAXATION TIMES FOR ACOUSTIC SCATTERING

In this section, we shall outline the tedious but straightforward evaluation of the relaxation time integrals (11) from (39), (40), and Table V.

The integration in the numerator of (11) is over solid angles $d\Omega'$ and $d\Omega$, or equivalently over polar angles $\beta'$, $\beta$ and azimuthal angles $\alpha'$, $\alpha$, defined relative to the symmetry axis of the valley. We have seen that the scattering probability $\Lambda$ on a constant-energy surface can be replaced by its azimuthal average $\langle\Lambda\rangle$, so that the integrand for $1/\tau_{\parallel}$ depends only on $(\alpha'-\alpha)$, while

TABLE VII. Values of the integrals $I_n$, $J_n$ defined in the text, as functions of the ratio $r=m_{\perp}^*/m_{\parallel}^*$.

| | $r<1$ | $r=1$ | $r>1$ |
|---|---|---|---|
| $I_0$ | $4/3$ | $4/3$ | $4/3$ |
| $I_1$ | $\dfrac{4r^{\frac{3}{2}}}{(1-r)^{5/2}}\arcsin(1-r)^{\frac{1}{2}}+\dfrac{4(1-4r)}{3(1-r)^2}$ | $4/5$ | $\dfrac{4r^{\frac{3}{2}}}{(r-1)^{5/2}}\operatorname{arcsinh}(r-1)^{\frac{1}{2}}+\dfrac{4(1-4r)}{3(r-1)^2}$ |
| $I_2$ | $\dfrac{10r^{\frac{3}{2}}}{(1-r)^{7/2}}\arcsin(1-r)^{\frac{1}{2}}+\dfrac{2(2-14r-3r^2)}{3(1-r)^3}$ | $4/7$ | $-\dfrac{10r^{\frac{3}{2}}}{(r-1)^{7/2}}\operatorname{arcsinh}(r-1)^{\frac{1}{2}}-\dfrac{2(2-14r-3r^2)}{3(r-1)^3}$ |
| $J_0$ | $8/3$ | $8/3$ | $8/3$ |
| $J_1$ | $-\dfrac{4r^{\frac{1}{2}}}{(1-r)^{5/2}}\arcsin(1-r)^{\frac{1}{2}}+\dfrac{(8+4r)}{3(1-r)^2}$ | $8/15$ | $-\dfrac{4r^{\frac{1}{2}}}{(r-1)^{5/2}}\operatorname{arcsinh}(r-1)^{\frac{1}{2}}+\dfrac{(8+4r)}{3(r-1)^2}$ |
| $J_2$ | $-\dfrac{2r^{\frac{1}{2}}(3+2r)}{(1-r)^{\frac{7}{2}}}\arcsin(1-r)^{\frac{1}{2}}+\dfrac{(8+22r)}{3(1-r)^3}$ | $8/35$ | $\dfrac{2r^{\frac{1}{2}}(3+2r)}{(r-1)^{\frac{7}{2}}}\operatorname{arcsinh}(r-1)^{\frac{1}{2}}-\dfrac{(8+22r)}{3(r-1)^2}$ |

that for $1/\tau_\perp$ can be averaged for $\alpha'$ for fixed $(\alpha'-\alpha)$. Thus we can reduce the two integrals to

$$\frac{1}{\tau_{\parallel}}=3\pi\int_{-1}^{1}\int_{-1}^{1}\cos\beta(\cos\beta-\cos\beta')\langle\langle\Lambda\rangle\rangle d(\cos\beta')d(\cos\beta) \tag{46}$$

and

$$\frac{1}{\tau_\perp}=\frac{3\pi}{2}\int_{-1}^{1}\int_{-1}^{1}(\sin^2\beta\langle\langle\Lambda\rangle\rangle-\sin\beta'\sin\beta\langle\cos(\alpha'-\alpha)\langle\Lambda\rangle\rangle)\times d(\cos\beta')d(\cos\beta), \tag{47}$$

respectively, where the outermost angular bracket means an average over $(\alpha'-\alpha)$, the inner one being, as before, an average on $\alpha'$ for fixed $(\alpha'-\alpha)$.

According to (39) and Table V, $\langle\Lambda\rangle$ is a polynomial in $\cos^2\theta$, where $\theta$, the polar angle of the wave vector $\mathbf{q}=\pm(\mathbf{K}'-\mathbf{K})$, is a function of $\beta$, $\beta'$, and $(\alpha'-\alpha)$. Using the transformation (4) from $\mathbf{K}$-space to $\varphi$ space, we find explicitly:

$$\cos^2\theta=\frac{(\cos\beta'-\cos\beta)^2}{(\cos\beta'-\cos\beta)^2+(m_\perp^*/m_\parallel^*)[\sin^2\beta'+\sin^2\beta-2\sin\beta'\sin\beta\cos(\alpha'-\alpha)]}. \tag{48}$$

Let us denote by $I_n$ the value of the double integral in (46) when the $n$th power of (48), $\cos^{2n}\theta$, is inserted in place of $\langle\Lambda\rangle$. Similarly, let $J_n$ be the value of the double integral in (47) for the same substitution. Then from (46), (47), (39), and Table V we obtain

$$1/\tau_\parallel=(3\pi CkT\Delta\epsilon^{\frac{1}{2}}/Vc_l)[\xi_\parallel\Xi_d^2+\eta_\parallel\Xi_d\Xi_u+\zeta_\parallel\Xi_u^2], \tag{49}$$

$$1/\tau_\perp=(3\pi CkT\Delta\epsilon^{\frac{1}{2}}/Vc_l)[\xi_\perp\Xi_d^2+\eta_\perp\Xi_d\Xi_u+\zeta_\perp\Xi_u^2], \tag{50}$$

where

$$c_l=c_{12}+2c_{44}+\tfrac{3}{5}c^* \tag{51}$$

is the average elastic constant for longitudinal waves, already encountered in Table V, where the quantity $C$ is given by (40), and where the dimensionless coefficients $\xi_\parallel$, $\eta_\parallel$, etc., are as given in Table VI. The expressions for these coefficients consist of two groups of terms, a major group involving only the $I_n$, $J_n$ for $n=0$, 1, 2, and a group containing the elastic anisotropy $c^*$ in the numerator and involving integrals for $n=3$ or 4. The latter group arises from the last terms in the square brackets of Table V. As we shall see, these terms are fairly small compared with those of the first group.

The integrals $I_n$, $J_n$, though very complicated, can be evaluated analytically.[13] Table VII gives the results for $n=0$, 1, 2, in terms of the mass ratio $r=m_\perp^*/m_\parallel^*$. Figures 2 and 3 show both these exactly calculated integrals and some estimates, believed to be fairly accurate, of the integrals for $n=3$ and 4. The latter were obtained from exact values at $r=0$, 1, and $\infty$ and the trends of the exact integrals for the lower values of $n$. Since the integrals for $n=3$ and 4 occur only in the small terms of Table VI proportional to the elastic anisotropy, it is not necessary to know them as accurately as those for $n=0$, 1, 2.

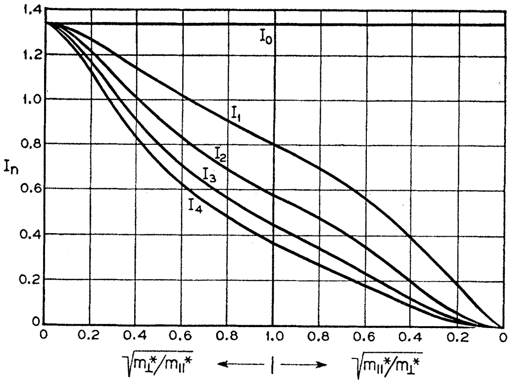

FIG. 2. Values of the integrals $I_n$ as functions of the square root of the mass ratio. Note the change of abscissa at mass ratio unity.

The tables and figures just referred to contain all the information necessary for the calculation of the mobility and other transport properties for the case of pure acoustic scattering. Since the formulas contain quite a number of parameters (masses, elastic constants, deformation potentials), no concise chart can be constructed which will cover the results for all possible cases. However, one can get a fair idea of what to expect in any actual case from sample calculations made for a typical set of ratios of the elastic constants. Such sample calculations of the mobility are given in Fig. 4. The ordinate measures the acoustic mobility $\mu_A$, i.e., the mobility which would be observed in a crystal free of impurities and imperfections, at temperatures low enough for intervalley and optical mode scattering to be negligible. The abscissa is the ratio of the two deformation potential constants defined in Table II; of these two, $\Xi_u$ can be determined with fair accuracy from piezoresistance measurements, as the combination of Eqs. (27) to (31) with (16) and (17) shows.

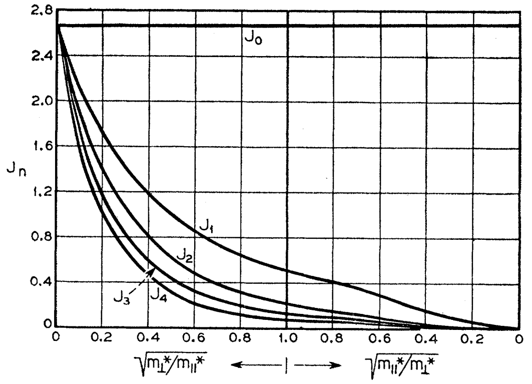

FIG. 3. Values of the integrals $J_n$ as functions of the square root of the mass ratio. Note the change of abscissa at mass ratio unity.

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[13] We are greatly indebted to Dr. M. C. Gray for pointing out that this can be done, and for the explicit evaluations.

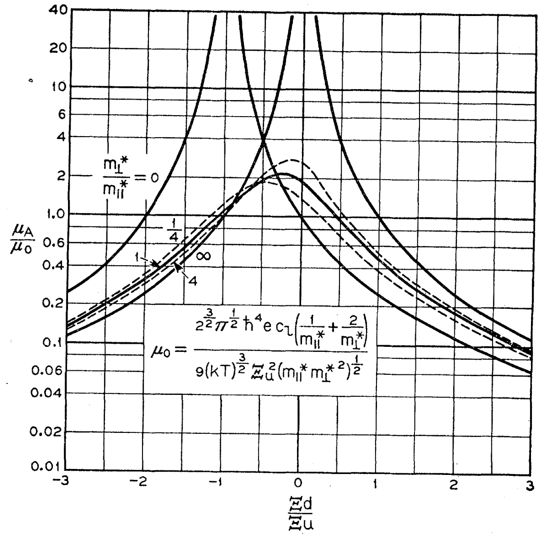

FIG. 4. Dependence of the low-temperature lattice (acoustic) mobility $\mu_A$ on the mass ratio and the ratio $\Xi_d/\Xi_u$ of the two deformation-potential constants, as calculated from the expressions of Tables VI and VII with $c^*=0$, $c_l/c_{44}=3$. The curves apply equally well to valleys centered on (100) or (111) axes.

All the curves of course go down as $\Xi_d^{-2}$ for large $|\Xi_d|$; more interesting are the peaks in the range $-1\leq\Xi_d/\Xi_u<0$. For mass ratio zero the peak is infinite, arising from the fact that for $\Xi_d=-\Xi_u$ the matrix element for scattering in a direction parallel to the valley axis vanishes (see the first and sixth rows of Table IV). Similarly, an infinite peak again occurs, at $\Xi_d=0$, for mass ratio infinity, since for this value the matrix element vanishes for scattering in a direction perpendicular to the valley axis. For intermediate values of the mass ratio, $\mu$ cannot become infinite, since it involves averages over all directions of scattering, and the matrix elements for different directions will not vanish simultaneously; only a finite peak remains. Note that the curves for mass ratios $\frac{1}{4}$ and 4 lie much closer to that for mass ratio 1 than to those for 0 or ∞.

## 6. APPLICATION TO *n*-TYPE GERMANIUM AND SILICON

As we have just noted, calculation of $\tau_{\parallel}$, $\tau_{\perp}$, $\mu_A$, etc., requires as inputs the effective masses, elastic constants, and deformation potentials. For germanium and silicon the masses are fairly accurately known from cyclotron resonance experiments; in this section, we shall adopt the values given by Dresselhaus, Kip, and Kittel.[14] The elastic constants were taken as the liquid air values of Fine[15] (Ge) and McSkimin[16] (Si). The deformation constant $\Xi_u$ corresponding to uniaxial shear is, as we have remarked, almost specified if the largest of the piezoresistance constants is known. Recent piezoresistance measurements,[17] made on *n* type germanium and silicon over a wide range of temperature, show a term in $1/T$ to be dominant as long as only lattice scattering is important; from these data and Eqs. (27), (28), and (31) we shall adopt values, given in the following, for $\Xi_u(\mu_{\parallel}^{(i)}-\mu_{\perp}^{(i)})/\mu$. However, the other deformation potential constant $\Xi_d$, or equivalently the $E_1$ given by (45), can at present only be determined indirectly. Sources of information for this second constant include magnetoresistance data, which under ideal conditions yield the ratio $\tau_{\parallel}m_{\perp}^*/\tau_{\perp}m_{\parallel}^*$, and data on the phonon contribution to the thermoelectric power at temperatures in the boundary scattering range,[18] which tell something about the relative amounts of scattering by longitudinal and transverse modes.[12] Another eventual source of information will materialize when the theory of mobility is worked out for holes in germanium and silicon, since the $E_1$ values for electrons and holes must combine to give the observed change of energy gap with volume. However, as we shall see, none of these sources currently provides a very good value of $\Xi_d$ or $E_1$, so we shall present the results of our calculations in the form of curves showing the dependence on $\Xi_d$ of $\mu_A$, $\tau_{\parallel}/\tau_{\perp}$, and the ratio of scattering by longitudinal modes to total acoustic scattering. These curves will show to what accuracy the presently available data on the various phenomena can be fitted by a single choice of our one remaining adjustable constant $\Xi_d$, or equivalently, how well one can predict the mobility from any given present or future data on the other effects.

The calculated mobilities $\mu_A$ due to acoustic scattering alone can be compared directly with observed mobilities $\mu$ only if there exists a temperature which is high enough for impurity scattering to be unimportant, yet low enough for intervalley and optical mode scattering to be negligible, and not so high as to make it risky to assume applicability of the cyclotron masses. The temperature 100°K, which seems to satisfy these criteria for the best *n* germanium samples, was chosen for the

TABLE VIII. Data used in calculating Figs. 5 and 6. Sources are as described in text.

| | Ge | Si |
|---|---|---|
| $m_{\parallel}^*/m$ | 1.58 | 0.97 |
| $m_{\perp}^*/m$ | 0.082 | 0.19 |
| $(m_{\perp}^*/m_{\parallel}^*)^{\frac{1}{2}}$ | 0.228 | 0.442 |
| $c_{12}$ | $0.53\times10^{12}$ dynes/cm$^2$ | $0.801\times10^{12}$ dynes/cm$^2$ |
| $c_{44}$ | $0.680\times10^{12}$ | $0.650\times10^{12}$ |
| $c^*$ | $-0.534\times10^{12}$ | $-0.426\times10^{12}$ |
| $c_l$ | $1.573\times10^{12}$ | $1.845\times10^{12}$ |
| $m_{11}$ | $\cdots$ | $-(19\,000/T)+$const. |
| $m_{44}$ | $-(29\,600/T)+$const. | $\cdots$ |

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[14] Dresselhaus, Kip, and Kittel, Phys. Rev. **98**, 368 (1955).

[15] M. E. Fine, J. Appl. Phys. **24**, 338 (1953). Our calculations were completed before we noticed that there is a small but perceptible difference between these values and the presumably more accurate ones of reference 16. Use of the latter would increase the $\mu_A$'s of Fig. 5 by a few percent.

[16] H. J. McSkimin, J. Appl. Phys. **24**, 988 (1953).

[17] Morin, Geballe, and Herring (to be published).

[18] T. H. Geballe and G. W. Hull, Phys. Rev. **94**, 1134 (1954).

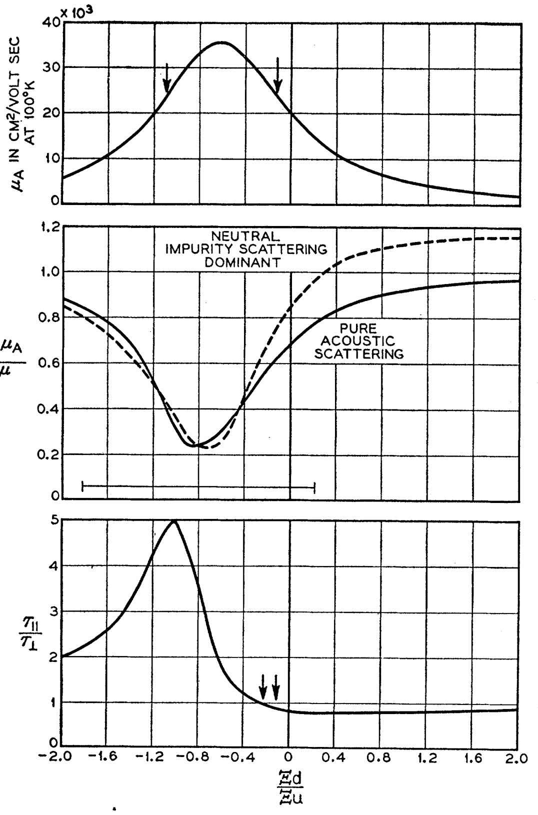

FIG. 5. Some experimentally important quantities for $n$ germanium, plotted against the ratio $\Xi_d/\Xi_u$ of the two deformation potential constants. Top curve: mobility $\mu_A$ at 100°K due to scattering by acoustic modes only. The arrows show the abscissae corresponding to the observed mobility in very pure materials. Middle curves: ratio of the rate of loss of crystal momentum to longitudinal acoustic modes, in an actual crystal, to the rate of loss to all acoustic modes in a perfect crystal. The horizontal line shows roughly the range of abscissae compatible with Geballe's thermoelectric measurements. Bottom curve: ratio of the two relaxation times. The arrows show values obtained from preliminary magnetoresistance measurements by Morin on two very pure specimens.

plots; however, there do not yet seem to be any data on $n$ silicon which satisfy the two scattering criteria.

Table VIII gives the data upon which the calculations were based, and Figs. 5 and 6 give the results for $n$ germanium and $n$ silicon respectively. The way in which the calculations were made is illustrated by the discussions for germanium and silicon which follow. The limitations of the present method, as discussed in Sec. 2 and Appendix A, are such that the calculated $\mu_A$ should always be too small. However, the error should be slight if $\tau_\parallel/\tau_\perp$ is near unity, and should be serious, if at all, only for rather large values of $\tau_\parallel/\tau_\perp$, say $>2$.

## $n$-Type Germanium

The $I_n$ and $J_n$ corresponding to the proper mass ratio were read off the curves of Figs. 2 and 3, and used with Table VI to evaluate the bracketed quantities in the expressions (49) and (50) for the two relaxation times. These were found to be, respectively,

$$[\parallel] = \Xi_u^2[1.24(\Xi_d/\Xi_u)^2 + 2.32(\Xi_d/\Xi_u) + 1.22], \tag{52}$$

$$[\perp] = \Xi_u^2[1.31(\Xi_d/\Xi_u)^2 + 1.61(\Xi_d/\Xi_u) + 1.01]. \tag{53}$$

The ratio of these is the $\tau_\parallel/\tau_\perp$ plotted in Fig. 5. To get $\Xi_u$ from the observed piezoresistance constant $m_{44}$, (16) and (17) were used to write (31) in the form

$$m_{44} = -\frac{1}{3}\frac{\Xi_u}{kT}\left[\frac{(\tau_\parallel m_\perp^*/\tau_\parallel m_\perp^*) - 1}{(\tau_\parallel m_\perp^*/\tau_\parallel m_\perp^*) + 2}\right]. \tag{54}$$

For any assumed $\Xi_d/\Xi_u$, the $\tau_\parallel/\tau_\perp$ just computed were used in this to compute $\Xi_u$ and hence to evaluate (52) and (53), and from these the $\tau$'s and $\mu_A$. The value of $\Xi_u$ corresponding to $\tau_\parallel/\tau_\perp = 1$ (close to the "observed" value) was found to be $+16.7$ ev; the extremes of variation of $\Xi_u$ for different values of $\Xi_d/\Xi_u$ were from 1.02 to 0.7 times this.

## $n$-Type Silicon

By the same method, the bracketed quantities in (49) and (50) were found for this case to be

$$[\parallel] = \Xi_u^2[1.39(\Xi_d/\Xi_u)^2 + 2.34(\Xi_d/\Xi_u) + 1.67], \tag{55}$$

$$[\perp] = \Xi_u^2[1.33(\Xi_d/\Xi_u)^2 + 1.15(\Xi_d/\Xi_u) + 1.18]. \tag{56}$$

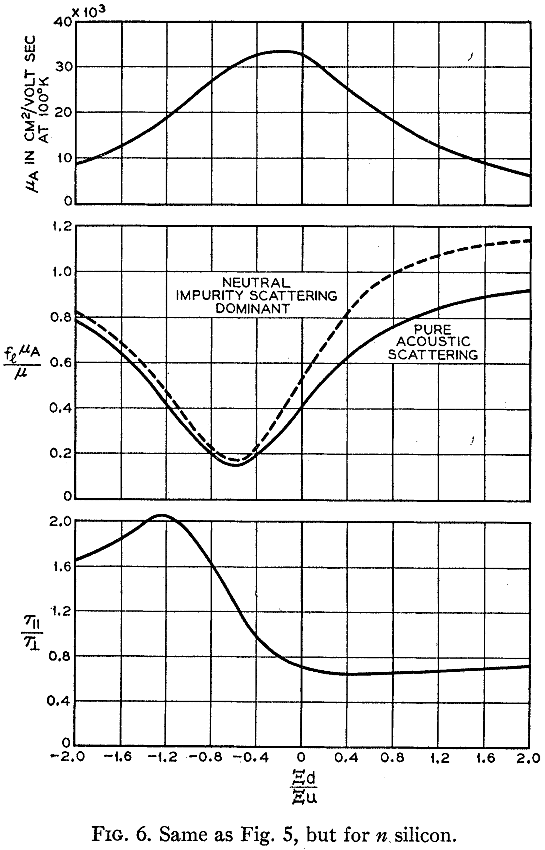

FIG. 6. Same as Fig. 5, but for $n$ silicon.

In place of (54) we used, from (27),

$$m_{11} = -\frac{2}{3}\frac{\Xi_u}{kT}\left[\frac{(\tau_{\parallel}m_{\perp}^*/\tau_{\perp}m_{\parallel}^*)-1}{(\tau_{\parallel}m_{\perp}^*/\tau_{\perp}m_{\parallel}^*)+2}\right]. \tag{57}$$

This gave $\Xi_u = -7.0$ ev for $\tau_{\parallel}/\tau_{\perp}=1$; the extremes for different $\Xi_d/\Xi_u$ were from 1.12 to 0.68 times this. The resulting $\mu_A$ and $\tau_{\parallel}/\tau_{\perp}$ are shown in Fig. 6.

We shall now discuss some of the ways of getting information on the proper value of $\Xi_d/\Xi_u$ to use in Figs. 5 and 6.

### Longitudinal *versus* Total Scattering

The phonon contribution to the thermoelectric power[12] of an extrinsic semiconductor of low carrier concentration has the general form

$$Q_p = \mp \bar{c} f \bar{\tau}/\mu T, \tag{58}$$

where $\bar{\tau}$ is a suitably averaged relaxation time for the participating phonons, $\bar{c}$ an average sound velocity, $\mu$ is the mobility of the current carriers, and $f$ is the fraction of their crystal momentum which in a conduction process is delivered to phonons, as opposed to impurities, etc. The upper sign is for $n$ type, the lower for $p$. A more refined formula is obtained by summing expressions of the form (58) for different groups of phonons, each group having its own $\bar{c}$, $\bar{\tau}$, and $f$. Now it can be shown[19] that, at the long wavelengths which are of interest here, phonons of the longitudinal branch suffer much less scattering by other phonons than those of the transverse branches. If this difference were sufficiently extreme, there would be a range of temperature in which the $\bar{\tau}$ of longitudinal phonons would be determined by boundary scattering and the $\bar{\tau}$ of the transverse phonons would be much smaller and determined by phonon-phonon scattering. In this range $Q_p$ would be determined by $\mu$, the dimensions of the specimen, and the fraction $f_l$ of the carriers' crystal momentum which is delivered to longitudinal phonons. While this idealized state of affairs may not be fully realized, it probably comes close enough to make possible the extraction from thermoelectric data of at least a rough value of $f_l/\mu$, or more conveniently, of the dimensionless quantity $f_l\mu_A/\mu$.

For the case of pure lattice scattering, $\mu=\mu_A$ at the low temperature where $Q_p$ is boundary-limited, and the calculation of $f_l$ can be made easily by breaking up the entries of Table VI into longitudinal and transverse contributions corresponding to the entries of Table V. When impurity scattering is dominant both $f_l$ and $\mu$ will be reduced, and their ratio will be different, since the carriers will be differently distributed in wave number space. However, for any assumed scattering law it is a straightforward matter to compute the steady-state distribution in an electric field, and using the transition probabilities (39) to calculate the rate of loss of crystal momentum to longitudinal phonons. This calculation was carried out for the case $\tau_{\parallel}=\tau_{\perp}=$ constant, corresponding to neutral impurity scattering. The middle sections of Figs. 5 and 6 show the results along with those for pure lattice scattering. No curves are given for the important case of scattering dominated by ionized impurities, however, because it is not yet known what anisotropy should be assumed for ionized impurity scattering.

Experimental data with which to compare these curves are not yet very adequate. If the reciprocal relaxation time of transverse phonons is assumed negligible at 20° K for the $n$ germanium specimen $E$ of the Geballe-Hull paper,[18] and if the longitudinal phonons are assumed diffusely scattered at the boundaries of the specimen and there only, $f_l\mu_A/\mu$ comes out to be 0.76. Relaxation of the former assumption would lower this value, as would any departure from diffuse reflection. Thus to the accuracy of the data we can say that $f_l\mu_A/\mu < 0.76$ unless there was appreciable scattering of phonons by interior imperfections, an occurrence which seems unlikely in the light of the sensitivity of this and similar specimens to changes in size at higher temperatures.

Comparable data on $n$ silicon are not available, as the data of Geballe and Hull[20] for this material do not extend to low enough temperatures to be dominated by boundary scattering.

### Magnetoresistance

If magnetoresistance and Hall effect could be measured under conditions of pure acoustic scattering, $\tau_{\parallel}/\tau_T$ could easily be determined from the values of the low-field ratios $\sigma_{\alpha\beta\gamma\delta}/\sigma_0\mu_H{}^2$, using (21), (17), and (19) or the equivalent equations of the single-$\tau$ theory[2–4] with $m_{\perp}^*/m_{\parallel}^*$ replaced by $w=\tau_{\parallel}m_{\perp}^*/\tau_{\perp}m_{\parallel}^*$. For $n$ germanium, for example, we would have

$$\frac{\sigma_{\alpha\alpha\beta\beta}}{\sigma_{\alpha\alpha\alpha\alpha}} = \frac{(\Delta\rho/\rho H^2)_{100}{}^{010} + (\mu_H/c)^2}{(\Delta\rho/\rho H^2)_{100}{}^{100}} = \frac{1+(5/2)w+w^2}{(w-1)^2}. \tag{59}$$

Alternatively, one could obtain $w$ from the high-field magnetoresistance; for $n$ germanium, for example, we find from (23) or from references 2 and 3

$$H\rightarrow\infty \parallel (100), \quad \rho_{\parallel}/\rho_0 \rightarrow (2+w)(1+2w)/9w. \tag{60}$$

Unfortunately, measured magnetoresistance values seem often to be appreciably perturbed by distortions of current geometry near the ends of the specimens, and at low fields the magnetoresistance is rather sensitive to small amounts of impurity scattering. For these reasons, we do not believe that one can trust to better than ±25% or so the values of $\tau_{\parallel}/\tau_{\perp}$ deducible from measurements such as those of Pearson and Suhl.[9] Morin has commenced some experiments designed to obtain magnetoresistance constants more characteristic

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[19] C. Herring, Phys. Rev. **95**, 954 (1954).

[20] T. H. Geballe and G. W. Hall, Phys. Rev. **98**, 940 (1955).

of ideal conditions, and has supplied us with some preliminary results.[21] These show fair agreement with the 77° high-field magnetoresistance results of reference 9, which give[2] $w \approx 0.05$. At low fields, Morin finds a dependence of the left of (59) on impurity content which is of the expected order of magnitude; if his best specimens can be assumed nearly unaffected by impurity scattering at 78°K, they too give $w=0.05$, or $\tau_{\|}/\tau_{\perp}=1.0$.

For silicon, the available information is less complete. The low-field magnetoresistance data of Pearson and Herring[22] give $w=1/4.6$, or $\tau_{\|}/\tau_{\perp}=1.1$, at liquid air temperature. However, this value may be appreciably in error, as the specimens used must have had appreciable impurity scattering.

### Intervalley Scattering in *n* Germanium

Although our main concern in this paper is with acoustic scattering, it is worth while to add a comment on the apparent smallness of intervalley scattering in *n* germanium, as indicated by the fact that the exponent $p$ in $\mu \propto T^{-p}$ exceeds $\frac{3}{2}$ by only 10% or so.[23] Since there are two atoms per unit cell, there are six branches to the vibrational spectrum of the lattice, and it is at first sight surprising that all of these branches should give small contributions to intervalley scattering. However, a consideration of the symmetry restrictions imposed by the space group of the crystal shows that while part of the smallness is fortuitous, part is not. If, as seems likely theoretically, the band-edge points $\mathbf{K}^{(i)}$ occur at the centers of the hexagonal faces of the Brillouin zone (points $L$ in the notation of Bouckaert, Smoluchowski, and Wigner[24]), the intervalley phonons must have wave vectors $\mathbf{K}^{(j)}-\mathbf{K}^{(i)}$ which end at the centers of the square faces (points $X$). If $D_X{}^{(p)}$ is the representation of the full space group to which the phonon belongs, and $D_L{}^{(e)}$ that to which the electronic band-edge state belongs, the intervalley matrix element connecting two band-edge states can differ from zero only if $D_X{}^{(p)} \times D_L{}^{(e)}$ contains $D_L{}^{(e)}$. If this matrix element vanishes, then phonons of the branch in question can take $\mathbf{K}^{(i)}+\Delta\mathbf{K}^{(i)}$ to $\mathbf{K}^{(j)}+\Delta\mathbf{K}^{(j)}$ only with a matrix element which is of order $\Delta K^{(i)}$ or $\Delta K^{(j)}$, hence very small. Calculation shows that when $D_L{}^{(e)}$ arises from the representation $L_1$ of the group of the wave vector, (in the notation of Bouckaert *et al.*[24]) and $D_X{}^{(e)}$ arises from $X_3$ (in the notation of Herring[25]), then the matrix element in question vanishes. Since $L_1$ is believed to be the symmetry type of the electronic band edge state, and $X_3$ is that of the two lowest branches of the frequency spectrum, this eliminates intervalley scattering by the two branches which might normally be expected to make the biggest contribution.

We may note finally that if the electronic band edge point were in the interior of the Brillouin zone, instead of on its boundary, no such selection rule would obtain.

## CONCLUSIONS

We have seen that for *n* germanium the deformation-potential constant $\Xi_u$ has a value of the order of 17 ev. If $\Xi_d$ were, say, of equal magnitude, the volume deformation-potential constant $E_1$ would, by (45), be about 23 ev. Such a value is unlikely, since the shift $E_{1G}$ of the energy gap with dilatation is only about 5 ev.[6] To reconcile such figures one would have to assume a high $E_1$ for the valence band, and this would probably imply a rather lower hole mobility than is observed. This sort of argument greatly limits the possible choices of abscissa in Fig. 5; for example, if we wish $|E_1|$ to be $\lesssim 10$ ev, we must take $\Xi_d/\Xi_u$ between about $+0.3$ and $-0.9$. Happily, it turns out that the value $-0.14$ indicated by the observed mobility[23] lies within this range, is close to the value $-0.23$ corresponding to the magnetoresistance estimate $\tau_{\|}/\tau_{\perp} \approx 1$, and lies in the range indicated as compatible with thermoelectric evidence on $f_l\mu_A/\mu$. Thus, we have been reasonably successful in finding a value of our single adjustable constant which will fit all the different types of observations. If this calculation is regarded as an attempt to predict the mobility from other data, Fig. 5 indicates that this could have been done with fair confidence to within ±50%; better magnetoresistance data may soon narrow these limits. It is a fortunate accident that for *n* germanium the use of an isotropic relaxation time, as in references 2 to 4, seems to be very nearly justified; things might easily have turned out very differently. This fact implies that the underestimation of the mobility, characteristic of our method, is slight for this case.

For silicon not only are there less data to fix $\Xi_d/\Xi_u$, but even the experimental value of $\mu_A$ seems quite uncertain. A lower limit of $\mu_A(100°)$ is provided by the $\mu(100°)$ of specimen 130 measured by Morin and Maita,[26] which was 9000 cm²/volt sec. However, this was undoubtedly affected by impurity scattering, and a considerably larger $\mu_A$ is not excluded. Figure 6 suggests either that $\mu_A$ is in fact considerably larger, or else that magnetoresistance measurements with more perfect specimens than those of reference 22 would show an anisotropy considerably different from that reported there.

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[21] F. J. Morin (unpublished).

[22] G. L. Pearson and C. Herring, Physica **20**, 175 (1954).

[23] F. J. Morin, Phys. Rev. **93**, 62 (1954).

[24] Bouckaert, Smoluchowski, and Wigner, Phys. Rev. **50**, 58 (1936).

[25] C. Herring, J. Franklin Inst. **233**, 525 (1942).

[26] F. J. Morin and J. P. Maita, Phys. Rev. **96**, 28 (1954).

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## APPENDIX A. TESTS OF THE ACCURACY OF THE APPROXIMATION BASED ON THE RELAXATION-TIME TENSOR

Let there be given some scattering functions $S_r$ and $S_c = \Lambda(\varphi,\varphi')\delta(\varphi'-\varphi)/\varphi^2$ on a constant-energy surface. Let $d\mathbf{j}$ be the contribution to the current from a thin energy shell around this surface, in the presence of an electric field $\mathbf{E}$. We shall compare $d\mathbf{j}$, for a number of calculable cases, with the approximate current $d\mathbf{j}^*$ calculable from the approximation described in Sec. 2, i.e., from (15) and (11). We shall consider only scattering with axial symmetry.

The most obvious class of cases for which the transport equation (1) is soluble is of course the class for which a velocity-dependent scalar relaxation time $\tau$ exists. With axial symmetry $\tau$ can depend only on $\beta$, the angle between $\boldsymbol{\varphi}$ and the symmetry axis, and the transport equation reduces to

$$(\partial f/\partial t)_{\text{fields}} = [f - f^{(0)}]/\tau(\beta). \tag{A1}$$

For such cases, (11) reduces to

$$1/\tau_{\parallel} = 3\langle\cos^2\beta/\tau(\beta)\rangle_S, \tag{A2}$$

$$1/\tau_{\perp} = \tfrac{3}{2}\langle\sin^2\beta/\tau(\beta)\rangle_S, \tag{A3}$$

where the average with a subscript $S$ is over the surface of a sphere in $\boldsymbol{\varphi}$ space. The ratio of approximate to exact currents for fields in the parallel direction is thus

$$dj_{\parallel}^*/dj_{\parallel} = \tfrac{1}{3}\tau_{\parallel}/\langle\tau(\beta)\cos^2\beta\rangle_S, \tag{A4}$$

$$dj_{\perp}^*/dj_{\perp} = \tfrac{1}{3}\tau_{\perp}/\tfrac{1}{2}\langle\tau(\beta)\sin^2\beta\rangle_S. \tag{A5}$$

Table IX gives values of (A4) and (A5) calculated for a few relaxation times of the form

$$1/\tau(\beta) = (1 + A\cos^2\beta + B\cos^4\beta)/\tau_0. \tag{A6}$$

It will be seen that the approximate values are very good when the maximum and minimum values of $\tau(\beta)$ are within a factor two or three of each other, but that they get worse as the anisotropy increases. The last two lines of the table represent singular cases for which the true current is infinite for one of the directions of $\mathbf{E}$; as this infinity is not reproduced in the approximate calculation, the ratio of approximate to true values is zero.

TABLE IX. Comparison of approximate current $d\mathbf{j}^*$ with exact current $d\mathbf{j}$ for some cases describable by a simple relaxation time $\tau(\beta)$.

| $\tau_0/\tau(\beta)$ | $\tau(0)/\tau(\pi/2)$ | $\tau_{\parallel}/\tau_{\perp}$ | $dj_{\parallel}^*/dj_{\parallel}$ | $dj_{\perp}^*/dj_{\perp}$ |
|---|---|---|---|---|
| $1+\cos^2\beta$ | 0.50 | 0.75 | 0.970 | 0.974 |
| $1+\cos^4\beta$ | 0.50 | 0.76 | 0.958 | 0.995 |
| $1-\frac{1}{2}\cos^2\beta$ | 2.00 | 1.29 | 0.92 | 0.98 |
| $1+2\cos^2\beta$ | 0.33 | 0.64 | 0.93 | 0.93 |
| $1-\cos^2\beta+\frac{1}{4}\cos^4\beta$ | 4.00 | 1.62 | 0.89 | 0.93 |
| $1+4\cos^2\beta$ | 0.20 | 0.53 | 0.88 | 0.84 |
| $1+\infty\cos^2\beta$ | 0 | 0.33 | 0.56 | 0 |
| $1-\cos^2\beta$ | $\infty$ | 2.00 | 0 | 0.83 |

Since equivalence to a relaxation time is a rather special property for a scattering function, it is of interest to compare $d\mathbf{j}$ and $d\mathbf{j}^*$ for scattering functions not possessing this property. To do this, we need to construct such more general functions which will still permit easy solution of the transport equation. One way of doing this is suggested by the fact that the transport equation can be transformed into an integral equation of the Fredholm type,[27] and the fact that the solution of such an equation can be reduced to the solution of linear simultaneous equations if the kernel is expressible as a finite sum of terms of the form $f_1(\boldsymbol{\varphi})f_2(\boldsymbol{\varphi}')$. It turns out that for the Fredholm kernel to be of this form it is necessary and sufficient that $\Lambda(\boldsymbol{\varphi},\boldsymbol{\varphi}')$ be of this form. Since in our problem $\Lambda$ is symmetrical, we shall investigate a few cases for which

$$\Lambda(\boldsymbol{\varphi},\boldsymbol{\varphi}') = \Lambda_0[1 + \lambda_1 L_1(\beta)L_1(\beta') + \lambda_2 L_2(\beta)L_2(\beta')]. \tag{A7}$$

If we wish $\Lambda$ not to be describable by a relaxation time, the functions $L_1$, $L_2$ must not both be even in $\beta \rightleftarrows \pi-\beta$.

The cases of this form for which we have made calculations are summarized in Table X; the results seem at least as encouraging as those of Table IX. For the scattering function given in the first line the approximation is exact, since this $\Lambda$ takes any first-order harmonic into a first-order harmonic. It is noteworthy that for the case $\Lambda \propto 1+\cos(\beta'-\beta)$ our approximation works very well, better than for the cases of Table IX which had a comparable $\tau_{\parallel}/\tau_{\perp}$. This is a $\Lambda$ which tends to limit the scattering to final states with a polar angle not far from that of the initial state, wherever the latter may lie. This is just the type of anisotropy which is most prominent for semiconductors with prolate energy surfaces when $\tau_{\parallel}/\tau_{\perp} > 1$; a similar effect may occur in impurity scattering also. There is thus a suggestion that our approximations are not hopelessly poor even near the maxima of the $\tau_{\parallel}/\tau_{\perp}$ curves computed in Secs. 5 and 6 (Figs. 5 and 6).

In accordance with the remark already made in Sec. 2, the last two columns of Tables IX and X are all $\leq 1$. The fact that the entries in these two columns are usually even closer to each other than they are to unity

TABLE X. Comparison of approximate current $d\mathbf{j}^*$ with exact current $d\mathbf{j}$, for some cases not describable by a simple relaxation time.

| $\Lambda(\beta,\beta')/\Lambda_0$ | $\tau_{\parallel}/\tau_{\perp}$ | $dj_{\parallel}^*/dj_{\parallel}$ | $dj_{\perp}^*/dj_{\perp}$ |
|---|---|---|---|
| $1+\lambda\cos\beta\cos\beta'$ | 1.33 to 0.67 | 1.00 | 1.00 |
| $1\pm\cos^3\beta\cos^3\beta'$ | 1.14, 0.89 | 0.997, 0.997 | 1.00 |
| $1\pm\cos(\beta'-\beta)$ | 1.53, 0.35 | 0.98, 0.94 | 0.99, 0.91 |

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[27] M. Kohler, Ann. Physik **27**, 201 (1936).

implies that properties of a semiconductor which involve only $\tau_{\parallel}/\tau_{\perp}$ can probably be calculated even more reliably using our approximations than can those which involve absolute values of the $\tau$'s. In fact, if one is not interested in calculating $\tau$'s from first principles, as we did in Secs. 4 to 6, one may be tempted to define $\tau_{\parallel}$ and $\tau_{\perp}$ from the anisotropy of conductivity of a valley, and then to hope that the $\tau$'s so defined will give very good results when applied to magnetoresistance theory, etc. While this may sometimes be the case, it is easy to show that for sufficiently anisotropic scattering functions there is no limit to the amount by which, for example, the magnetoresistance can depart from the value estimated by putting such empirical $\tau$'s into the theory of Sec. 3. Thus although we believe the approximations of Sec. 2 provide a good basis for transport theory when the anisotropy of the scattering function is slight to moderate, we doubt that any major improvement in the accuracy of the method can be made by very simple means.

## APPENDIX B. INTERPOLATION FORMULAS FOR THE MATRIX ELEMENT

We wish to approximate $|M(\mathbf{q},l)|^2$ and $|M(\mathbf{q},t_1)|^2+|M(\mathbf{q},t_2)|^2$ by combinations of spherical harmonic functions of the direction of $\mathbf{q}$.

According to Table IV, there are, for either type of valley, five independent directions of $\mathbf{q}$ along symmetry axes of the crystal. For a (111) valley, the five simplest even spherical harmonic functions with the symmetry of the valley are

$$1,\ P_2(\cos\theta),\ P_4(\cos\theta),\ P_6(\cos\theta),\ \text{and}\ \sin^3\theta\cos\theta\cos3\alpha, \quad \text{(B1)}$$

where $\theta$ is the angle of $\mathbf{q}$ with the (111) direction, and $\alpha$ the azimuthal angle relative to a $(1\bar{1}0)$ plane. The entries of Table IV for the two transverse modes were added, and the sums fitted to these five spherical harmonics. Averaging the resulting expression on $\alpha$ gave the last line of Table V.

For a (100) valley, the five simplest spherical harmonics with the proper symmetry are similar to (B1), but with the last expression replaced by $\sin^4\theta\cos4\alpha$. When these are fitted to the transverse contributions of Table IV the coefficients of the first and last terms obviously vanish, since there are two types of symmetry directions with $\cos\theta=0$, for which the matrix element vanishes. The second line of Table V was obtained from the fit to the remaining three harmonics. An alternative interpolation using $\sin^2\theta\cos^2\theta\cos4\alpha$ instead of the spherical harmonic $\sin^4\theta\cos4\alpha$ gave azimuthal averages which differed from these by only a negligible amount.

For the longitudinal modes a similar fit can be made; however, there is an alternative procedure which is probably more accurate. This is based on the assumption that for arbitrary direction of $\mathbf{q}$ the displacements in the longitudinal mode are exactly longitudinal, so that $f_{xx}=q_x^2$, $f_{xy}=2q_xq_y$, etc. This assumption is valid for symmetry directions of $\mathbf{q}$, and though not exactly valid for other directions, is probably not far off. If we adopt it, we find after a little algebra

$$|M(\mathbf{q},l)|^2=\frac{kT}{V}\frac{(\Xi_d+\cos^2\theta\,\Xi_u)^2}{c_{12}+2c_{44}+(q_{1x}^4+q_{1y}^4+q_{1z}^4)c^*}, \quad \text{(B2)}$$

where $\mathbf{q}_1$ is the unit vector in the direction of $\mathbf{q}$, $x$, $y$, $z$ refer to the crystal axes, $\theta$ is the angle of $\mathbf{q}$ with the valley axis $\mathbf{K}^{(i)}$, and $c^*=c_{11}-c_{12}-2c_{44}$. Since the term in $c^*$ in the denominator is fairly small, it suffices to represent (B2) by the first two terms of its Taylor expansion in powers of $c^*$. The first and third lines of Table V were obtained from these by carrying out the averaging operation over all azimuths of $\mathbf{q}$ about the valley axis.

It is interesting to compare the results of the interpolation procedure just described with those obtained from a spherical harmonic fitting of the $|M(\mathbf{q},l)|^2$ in symmetry directions, as described for the transverse case above. The two procedures must of course agree exactly as far as the term independent of $c^*$ is concerned and also in the terms first-order in $c^*$ which are proportional to $\Xi_d^2$ and $\Xi_d\Xi_u$. For the term in $\Xi_u^2c^*$, the spherical harmonic treatment gives, for a (111) valley, an expression containing

$$(-0.186\cos^2\theta+0.023\cos^4\theta+0.563\cos^6\theta) \quad \text{(B3)}$$

instead of the

$$(0.15-1.50\cos^2\theta+1.75\cos^4\theta)\cos^4\theta \quad \text{(B4)}$$

occurring in the third line of Table V. These agree, as they must, at $\cos^2\theta=0$ and 1, but differ somewhat in between. With the values of $I_n$, $J_n$ appropriate to germanium, the contribution of (B3) to $1/\tau_{\parallel}$ is about 10% too high compared with that of (B4), while for $1/\tau_{\perp}$, (B3) is about 50% too high. These figures give a clue to the size of the error involved in using the spherical harmonic interpolation for the transverse modes: the procedure is crude, but is probably in error by only a fraction of the small anisotropy term in Table V.