

Low-Temperature Transverse Resistivity of Saturation-Stressed Degenerately Doped n -Type Germanium

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Upper and lower bounds to the transverse resistivity due to ionized impurity scattering in saturation-stressed degenerately doped n -type germanium (single conduction-band valley occupied at $T=0$ °K) have been calculated for Brooks-Herring scattering. The bounds are obtained by solving exactly the Boltzmann equation including the mass anisotropy for two different scattering rates which either overestimate or underestimate the Brooks-Herring scattering rate. The use of Kohler's variational principle also yields an upper bound to the resistivity, which is found to be approximately 20% higher than the lower bound previously obtained, but is smaller than the experimental results of Katz. The calculation is approximately corrected for the inaccuracies of the Born approximation together with contributions from multiple scattering and dressing effects. The final results are in excellent agreement with experiment.

I. INTRODUCTION AND CONCLUSIONS

When a semiconductor is heavily doped with donor atoms, the energy levels of the donor electrons are raised relative to the conduction-band minima because of the electron-electron interaction between them.¹ For sufficiently high donor densities, there are no bound states for these electrons, and consequently the donor electrons occupy states in the conduction band of the material at all temperatures.^{2,3} Such materials are called degenerately doped semiconductors, and the electron distribution is statistically degenerate for temperatures well below the Fermi or degeneracy temperature, the latter being of the order of a few tens to thousands of degrees Kelvin.

The theory of the electrical conductivity of such materials has been given by Brooks and Herring,⁴ who treated the conduction electrons as free electrons with isotropic effective masses, which undergo scattering via a Thomas-Fermi potential which takes into consideration the fact that the semiconductor is a polarizable medium. The Born approximation is used to obtain the differential scattering cross section. The calculation above has often been used to explain the resistivity of degenerately doped semiconductors with an anisotropic band structure by an appropriate choice of the conductivity mass for the effective mass. However, the choice of the effective mass which gives agreement with experiment will, in general, be a function of the electron concentration, and cannot be precisely anticipated until the experimental results are known. Furthermore, experimental results on unstressed germanium indicate that, for a reasonable choice of effective mass, the Brooks-Herring result underestimates the observed resistivity by a factor of 4.⁵ Similar observations have also been made for

degenerately doped silicon.⁶

One of the earliest attempts to take the anisotropic band structure of Ge and Si into account in transport calculations was made by Ham.⁷ He assumed that only small-angle scattering appreciably contributed to the resistivity, and as a result obtained the anisotropy in the ratio of the relaxation time for transverse and longitudinal conductivity. Ito⁸ has observed that because of the electron screening of the scattering ion, small-angle scattering is not as significant as in the case of the unscreened, or Rutherford, scattering and a more careful analysis is necessary. He, instead, used the Herring-Vogt⁹ formalism to calculate a relaxation-time tensor as a function of the energy by truncating a spherical-harmonic expansion of the electron distribution after the $l=1$ term. Since the usual criterion for the justification of this technique is that the anisotropy in the relaxation times be small, his results must be considered questionable since he finds just the opposite results for Ge at low temperatures. Truncated expansions have also been used by Samoilovich *et al.* with similar results.¹⁰

The above-mentioned calculations were all performed for the unstressed, and hence many-valley, Ge and Si semiconductors. Since these materials have cubic symmetry, the total conductivity tensor is a constant times the unit tensor even though the conductivity tensor for each separate valley is not. The anisotropy in the relaxation times is deduced from magnetoconductivity experiments, usually analyzed by assuming the existence of relaxation times which are at most a function of the energy only.¹¹ Since this assumption may be questionable for energy bands as anisotropic as those in Ge, where there exists a 19:1 mass ratio, it is preferable to compare the theoretical calculation directly with the conductivity anisotropy if at all possible.

Price¹² has shown that if stress is appropriately applied to a many-valley semiconductor, it is possible to lower the energy of one of the valleys relative to the others, and thus, for sufficient stress, have all the electrons in a single valley. More recently, these experiments have been performed and a large amount of data exists on the anisotropy in the conductivity contributed by a single-ellipsoidal conduction-band valley.¹³ Furthermore, since the experiments were performed at liquid-helium temperature, the data presumably are related only to the screened ionized scattering and not to any appreciable electron-phonon scattering. Finally, we note that since the analysis of the transport properties of a degenerate electron gas is simpler than that for the nondegenerate case because it is not necessary to take a thermal average over a Boltzmann distribution, it is possible to gain some insight into the transport properties of charge carriers in anisotropic bands. This is significant for an understanding of the conductivity of not only these semiconductors but also for semimetals.

In Sec. II, we show that it is possible to obtain rigorous upper and lower bounds for the resistivity predicted by the Boltzmann equation by finding the exact solution for two different scattering rates which either are always greater than (or equal to) the true scattering rate or always less than (or equal to) the true scattering rate. The technique is applied to the calculation of the transverse resistivity of saturation-stressed degenerately doped germanium, assuming the validity of the Born approximation for electron scattering using the Thomas-Fermi potential of the screened ionized impurities, i. e., Brooks-Herring scattering. In Sec. III, another upper bound to the resistivity is obtained from a direct application of Kohler's variational principle.¹⁴ This result is found to be only approximately 20% higher than a lower bound obtained in Sec. II, but is lower than the experimental results.

The calculations are approximately corrected for the known inaccuracies of the Born approximation, together with the contributions from multiple-scattering and dressing effects.^{15,16} The final results are found to be in excellent agreement with experiment, although the quantum corrections to the resistivity are larger than the Brooks-Herring result alone.

II. UPPER AND LOWER BOUNDS TO TRANSVERSE RESISTIVITY

In the Thomas-Fermi approximation, the screened Coulomb potential for an electron interacting with a singly ionized donor is

$$V(\vec{r}) = -(e^2/\kappa r) e^{-qr}, \quad (1)$$

where κ is the static dielectric constant of the semi-

conductor and q is the Thomas-Fermi inverse-screening length which, for a degenerate electron gas at $T = 0^\circ\text{K}$, is given by

$$q^2 = (4\pi e^2/\kappa) g(\epsilon_F), \quad (2)$$

where $g(\epsilon_F)$ is the electron density of states at the Fermi energy.

In the first Born approximation, the transition probability that an electron with wave vector \vec{k} is scattered into a state with wave vector \vec{k}' is

$$S_{\sigma\sigma'}(\vec{k}, \vec{k}') = n_i \frac{2\pi}{\hbar} \left(\frac{4\pi e^2}{\kappa} \right)^2 \frac{1}{[(\vec{k} - \vec{k}')^2 + q^2]^2} \delta(\epsilon - \epsilon') \delta_{\sigma\sigma'}, \quad (3)$$

where n_i is the number of ionized donors in the unit normalization volume and σ and σ' are the initial and final spin projections. The current density, and hence the conductivity, may be determined from

$$\vec{J} = e \int \vec{v}(\vec{k}) f(\vec{k}) \frac{d\vec{k}}{4\pi^3}, \quad (4)$$

where $\vec{v}(\vec{k})$ is the velocity of a Bloch electron with wave vector \vec{k} and $f(\vec{k})$ is the distribution function obtained by solving the linearized Boltzmann equation, i. e.,

$$e\vec{E} \cdot \vec{v} \left(-\frac{\partial f_0}{\partial \epsilon} \right) = \sum_{\vec{k}', \sigma'} S_{\sigma\sigma'}(\vec{k}, \vec{k}') [f(\vec{k}) - f(\vec{k}')], \quad (5)$$

where f_0 is the Fermi-Dirac distribution and \vec{E} is the electric field. It is well known that for S given by Eq. (3), Eq. (5) may be solved exactly in terms of an energy-dependent relaxation time, provided the energy is an isotropic function of \vec{k} .¹⁴ However, for a single-conduction-band valley of germanium the dispersion relation for the energy relative to the band minima is given by¹³

$$\epsilon(\vec{k}) = (\hbar^2/2m_n)k_x^2 + (\hbar^2/2m_l)(k_y^2 + k_z^2), \quad (6)$$

where $m_n/m_l \approx 19$. Thus, the usual assumption of an isotropic effective mass is not even approximately satisfied, and a different analysis is required. The techniques previously employed by others to solve this problem are all approximate without any estimate of the error introduced by the use of the various methods. Consequently, when discrepancies between experiment and calculations have occurred, it has not been clear whether the conventional transport theory has failed or merely that the approximations in obtaining the solutions are not applicable.⁵ We show below how to obtain rigorous upper and lower bounds to the resistivity. When the technique is applied to the transverse resistivity of degenerately doped germanium, these bounds differ by only a few percent over the entire range of doping for which the semiconductor is degenerate.

It is an immediate consequence of Kohler's prin-

ciple¹⁴ that if the scattering function is written as a sum, i.e.,

$$S(\vec{k}, \vec{k}') = S_1(\vec{k}, \vec{k}') + S_1'(\vec{k}, \vec{k}'),$$

with

$$S_1(\vec{k}, \vec{k}') = S_1(\vec{k}', \vec{k}), \quad S_1'(\vec{k}, \vec{k}') = S_1'(\vec{k}', \vec{k}),$$

$$S_1, S_1' \geq 0,$$

then

$$\rho \geq \rho_1 + \rho_1',$$

where ρ_1 (ρ_1') is the resistivity if only S_1 (S_1') were present, and ρ is the resistivity if the total S is present. Since $\rho_1, \rho_1' \geq 0$, it immediately follows that $\rho \geq \rho_1$, provided $S \geq S_1$, which is merely equivalent to the statement that if the scattering is increased then the resistivity is also.

Similarly, if

$$S(\vec{k}, \vec{k}') = S_2(\vec{k}, \vec{k}') - S_2'(\vec{k}, \vec{k}'),$$

with

$$S_2(\vec{k}, \vec{k}') = S_2(\vec{k}', \vec{k}) \geq 0,$$

$$S_2'(\vec{k}, \vec{k}') = S_2'(\vec{k}', \vec{k}) \geq 0,$$

then

$$S_2 = S + S_2', \quad \rho_2 \geq \rho.$$

Thus, if we can find two symmetric positive definite functions S_1 and S_2 which underestimate and overestimate S , respectively, and for which the exact resistivities ρ_1 and ρ_2 can be obtained, then

$$\rho_2 \geq \rho \geq \rho_1. \quad (7)$$

There are, of course, many functions S_i satisfying the above conditions. However, it is clear that if we are to obtain ρ_1 and ρ_2 , which are nearly equal, we must choose the S_i in such a way that they closely approximate the given S .

For an electric field in the y direction and a scattering function $S_i(\vec{k}, \vec{k}')$, which allows transitions only into states with the same spin projection, Eq. (5) may be written

$$eE v_y(\vec{k}) = \int S_i(\vec{k}, \vec{k}') [\phi(\vec{k}) - \phi(\vec{k}')] \frac{d\vec{k}'}{(2\pi)^3}, \quad (8)$$

where

$$f(\vec{k}) = f_0(\epsilon) + \phi(\vec{k}) \left(-\frac{\partial f_0}{\partial \epsilon} \right), \quad (9)$$

but

$$v_y(\vec{k}) = \hbar k_y / m_1,$$

and hence, if $S_i(\vec{k}, \vec{k}')$ is unchanged when $\vec{k}_t' \rightarrow -\vec{k}_t'$, where t denotes the plane normal to the k_x axis, and $\phi(\vec{k})$ is odd in k_y , then the second term on the right-hand side of Eq. (8) is odd in k_y , and the exact solution of Eq. (8) is

$$\phi(\vec{k}) = eE v_y(\vec{k}) / \int S_i(\vec{k}, \vec{k}') \frac{d\vec{k}'}{(2\pi)^3}, \quad (10)$$

which is odd as required.

Thus, we can obtain the exact solution to the transport equation for the transverse resistivity provided the scattering function is unchanged when $\vec{k}_t' \rightarrow -\vec{k}_t'$.

It is convenient to transform the ellipsoidal constant-energy surfaces into spheres. Letting

$$\begin{aligned} k_x &= (2m_{\parallel}\epsilon/\hbar^2)^{1/2} x, \\ k_y &= (2m_{\perp}\epsilon/\hbar^2)^{1/2} y, \\ k_z &= (2m_{\perp}\epsilon/\hbar^2)^{1/2} z, \end{aligned} \quad (11)$$

we have $x^2 + y^2 + z^2 = 1$, i.e., the constant-energy surface has been transformed to the surface of a sphere of radius 1. Since we are considering only elastic scattering, only one energy shell at a time need be considered. Defining

$$S(\vec{k}, \vec{k}') = n_i \frac{2\pi}{\hbar} \left(\frac{4\pi e^2}{\kappa} \right)^2 \left(\frac{2m_{\parallel}\epsilon}{\hbar^2} \right)^{-2} R(\vec{r}, \vec{r}') \delta(\epsilon - \epsilon'), \quad (12)$$

we have

$$R(\vec{r}, \vec{r}') = \frac{1}{\{(x-x')^2 + K_m^{-1}[(y-y')^2 + (z-z')^2] + \beta\}^2}, \quad (13)$$

where

$$\beta = q^2/k_{\parallel}^2, \quad \hbar^2 k_{\parallel}^2 / 2m_{\parallel} = \epsilon,$$

$$K_m^{-1} = m_{\perp}/m_{\parallel} \approx 0.052$$

for Ge.

Using the fact that \vec{r} and \vec{r}' have unit length, we obtain, after employing the law of cosines,

$$R(\vec{r}, \vec{r}') = \frac{1}{\{(x-x')^2 + K_m^{-1}[(1-x^2) + (1-x'^2) - 2(1-x^2)^{1/2}(1-x'^2)^{1/2}\cos\theta] + \beta\}^2}, \quad (14)$$

where θ is the angle between \vec{r} and \vec{r}' projected in the yz plane. We define

$$R_1 = \frac{1}{\{(x-x')^2 + K_m^{-1}[(1-x^2) + (1-x'^2) + 2(1-x^2)^{1/2}(1-x'^2)^{1/2}|\cos\theta|] + \beta\}^2} \leq R,$$

$$R_2 = \frac{1}{\{(x-x')^2 + K_m^{-1}[(1-x^2) + (1-x'^2) - 2(1-x^2)^{1/2}(1-x'^2)^{1/2}|\cos\theta|] + \beta\}^2} \geq R. \quad (15)$$

Then both R_1 and R_2 remain unchanged when $\vec{k}'_t \rightarrow -\vec{k}'_t$ since the latter transformation changes θ to its supplement and, hence, leaves $|\cos\theta|$ invariant. Consequently, the exact solutions for $\phi_1(\vec{k})$ and $\phi_2(\vec{k})$ can be obtained from Eq. (10), where S_1 and S_2 are obtained by replacing R in Eq. (12) by Eq. (15).

Transforming the volume element in \vec{k} space, we have

$$d\vec{k}' = \frac{dS' d\epsilon'}{|\vec{\nabla}_{\vec{k}'} \epsilon'|} = \frac{m_{\perp}}{\hbar^2} \left(\frac{2m_{\parallel} \epsilon'}{\hbar^2} \right)^{1/2} d\theta dx' d\epsilon',$$

which together with Eqs. (10) and (15) leads to ϕ_1 and ϕ_2 proportional to B_1 and B_2 , respectively, where

$$\begin{aligned} \frac{1}{B_1(x)} &= \int_{-1}^{+1} \int_0^{2\pi} R_1(x, x', \theta) \frac{d\theta}{2\pi} dx' \\ &= -\frac{\partial}{\partial \beta} \int_{-1}^{+1} \frac{4}{\pi} \frac{1}{(a^2 - b^2)^{1/2}} \\ &\quad \times \tan^{-1} \left(\frac{a-b}{a+b} \right)^{1/2} dx', \\ \frac{1}{B_2(x)} &= \int_{-1}^{+1} \int_0^{2\pi} R_2(x, x', \theta) \frac{d\theta}{2\pi} dx' \\ &= -\frac{\partial}{\partial \beta} \int_{-1}^{+1} \frac{4}{\pi} \frac{1}{(a^2 - b^2)^{1/2}} \\ &\quad \times \tan^{-1} \left(\frac{a+b}{a-b} \right)^{1/2} dx', \end{aligned} \quad (16)$$

where

$$\begin{aligned} a &= (x-x')^2 + K_m^{-1}(2-x^2-x'^2) + \beta, \\ b &= 2K_m^{-1}(1-x^2)^{1/2}(1-x'^2)^{1/2}. \end{aligned} \quad (17)$$

Furthermore, using the fact that $v_y \sim y$ and that the transverse current is the same if the electric field is in the z direction, we find that the conductivity at $T = 0^\circ\text{K}$ corresponding to $R_1(R_2)$ is proportional to $I_1(I_2)$ where

$$I_i = \int_0^1 (1-x^2) B_i(x) dx. \quad (18)$$

Here we have made use of the fact that B_1 and B_2 are even in x , and ϵ is evaluated at the Fermi energy. Using Eq. (2) and

$$g(\epsilon_F) = \frac{3}{2}(n/\epsilon_F),$$

we have

$$\beta = \frac{q^2}{k_{\parallel}^2} = \frac{4}{\pi a_{\perp} (3\pi^2 n)^{1/3}} \left(\frac{m_{\perp}}{m_{\parallel}} \right)^{1/3}, \quad (19)$$

where

$$a_{\perp} = \hbar^2 \kappa / m_{\perp} e^2.$$

Finally, using Eqs. (4), (10), (12), (15), and (18), the transverse resistivity is given by

$$\rho_t = 16m_{\perp}^3 e^2 / 9\pi m_{\parallel} \kappa^2 \hbar^3 n I_i. \quad (20)$$

Figure 1 shows the calculated upper and lower bounds for the transverse resistivity as a function of donor concentration. The boxes correspond to the experimental results of Katz¹³ at 4°K . We see that the upper bound is approximately twice the lower bound at $n = 10^{18}/\text{cm}^3$ with the ratio increasing to approximately 3.7 at $n = 5 \times 10^{19}/\text{cm}^3$. But in all

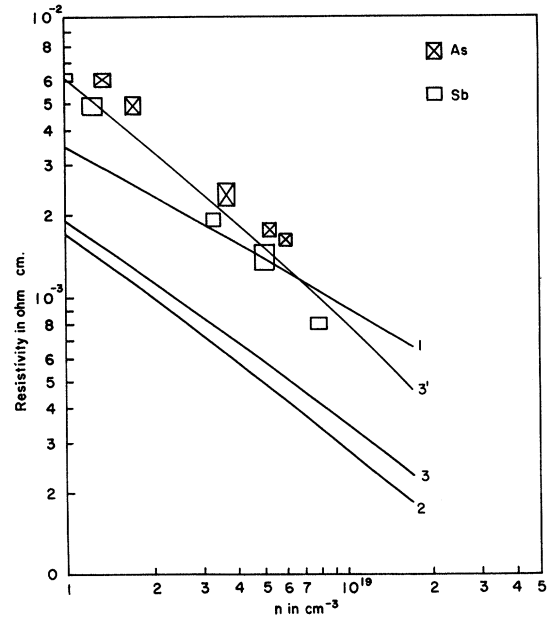


FIG. 1. Transverse resistivity of degenerately doped Ge vs n , the impurity concentration. The experimental results are those of Katz given in Ref. 13. The curves labeled 1 and 2 correspond to the theoretical upper and lower bounds ρ_1 and ρ_2 to the resistivity due to Brooks-Herring scattering discussed in Sec. II. The curve labeled 3 is the theoretical upper bound ρ_3 to the resistivity due to Brooks-Herring scattering discussed in Sec. III. The curve labeled 3' is obtained by multiplying the results given by curve 3 by the Moore-Ehrenreich correction factor discussed in Sec. IV. In the above calculations we have taken $m_{\perp} = 0.082 m_0$, $m_{\parallel} = 1.59 m_0$, and $\kappa = 16$.

cases, the experimental points fall between the upper and lower bounds with the average value of these two estimates giving a good approximation to the experimental results, especially as n increases. However, this apparent consistency is actually meaningless, i.e., we show in Sec. III that a rigorous upper bound for ρ obtained by the variational principle is given by the curve numbered 3, and hence the resistivity corresponding to the scattering rate given by Eq. (3) is actually bounded by the curves 2 and 3.

III. APPLICATION OF KOHLER'S PRINCIPLE

In Sec. II, we obtained rigorous upper and lower bounds to the resistivity corresponding to the scattering rate given by Eq. (3). In the limit of infinite-mass anisotropy, i.e., $K_m \rightarrow \infty$, the coefficient of $|\cos\theta|$ in Eq. (14) would be zero, and hence both R_1 and R_2 would be equal to R and we would have the exact solution. However, because $K_m \approx 19$, the term proportional to $|\cos\theta|$ is appreciable compared to β in the degenerate doping range and the derived upper and lower bounds are significantly different. Consequently, it is desirable to obtain yet another estimate of the resistivity.

According to Ziman,¹⁴ if the Boltzmann equation is written

$$e\vec{E} \cdot \vec{v}(\vec{k}) \left(-\frac{\partial f_0}{\partial \epsilon} \right) = \int [\phi(\vec{k}) - \phi(\vec{k}')] \left(-\frac{\partial f_0}{\partial \epsilon} \right)$$

$$I_3^{-1} = \frac{9}{16\pi} \int_{-1}^{+1} \int_{-1}^{+1} \int_0^\pi \frac{[(1-x^2) + (1-x'^2) - 2(1-x^2)^{1/2}(1-x'^2)^{1/2} \cos\theta] dx' dx d\theta}{\{(x-x')^2 + K_m^{-1} [(1-x^2) + (1-x'^2) - 2(1-x^2)^{1/2}(1-x'^2)^{1/2} \cos\theta] + \beta\}^2} \quad (25)$$

The results for ρ_3 are plotted in Fig. 1, where it is seen that ρ_3 closely approximates the lower bound given by ρ_1 . More significantly, however, ρ_3 lies below the experimental results for all densities, indicating that the scattering rate given by Eq. (3) cannot entirely account for the resistivity. It is also interesting to note that a calculation of the resistivity for Brooks-Herring scattering using a relaxation-time approximation gives results which are only a few percent smaller than the lower bound reported here.¹³ However, when the same technique is applied to the longitudinal case, the results are significantly larger than found experimentally,¹³ and are an order of magnitude larger than a rigorous upper bound obtained by employing the variational principle.¹⁷

IV. CORRECTIONS TO BROOKS-HERRING SCATTERING

The techniques employed in Secs. II and III have enabled us to calculate upper and lower bounds to the resistivity which differ by only approximately

$$\times S(\vec{k}, \vec{k}') \frac{d\vec{k}'}{(2\pi)^3}, \quad (21)$$

then the exact resistivity is given by

$$\rho = \langle \phi, P\phi \rangle / [\langle \phi, X(E=1) \rangle]^2, \quad (22)$$

where X and $P\phi$ are the left- and right-hand sides of Eq. (21), respectively, and

$$\langle f, g \rangle \equiv \int f(\vec{k}) g(\vec{k}) \frac{d\vec{k}}{4\pi^3}.$$

Furthermore, if any function ϕ' is substituted into Eq. (22), the resulting expression is either greater than or equal to the exact result. Thus

$$\rho_3 = \langle \phi', P\phi' \rangle / [\langle \phi', X(E=1) \rangle]^2 \quad (23)$$

is an upper bound to the resistivity for arbitrary choice of ϕ' . Now in the relaxation-time approximation, $\phi' = e\vec{E} \cdot \vec{v} \tau = cv_y$, for \vec{E} in the y direction. Taking this as an approximate solution we have from Eq. (23)

$$\rho_3 = \frac{\langle v_y, P v_y \rangle}{[\langle v_y, X(E=1) \rangle]^2} \geq \rho. \quad (24)$$

For a scattering rate given by Eq. (3) we find ρ_3 is given by Eq. (20) with

20% with no adjustable parameters. Furthermore, it is possible to conclude that ρ_3 overestimates the results of an exact calculation with the assumed scattering rate by only a couple percent, by comparing the results of using the variational principle with an exact calculation in the case of infinite mass anisotropy.¹⁷

The fact that the experimental results are larger than the calculated resistivity is not unusual for Brooks-Herring scattering even for spherical energy bands and has been discussed by Moore and Ehrenreich^{15,16} for degenerately doped GaAs. More specifically, they show that for an isotropic effective mass

$$\rho/\rho_B = 1 + \delta_B + \delta_M + \delta_N,$$

where ρ_B is the resistivity derived from using the first-order Born approximation (Brooks-Herring scattering) and δ_B , δ_M , and δ_N are correction terms arising from the failure of the Born approximation, the effects of multiple-scattering and dressing

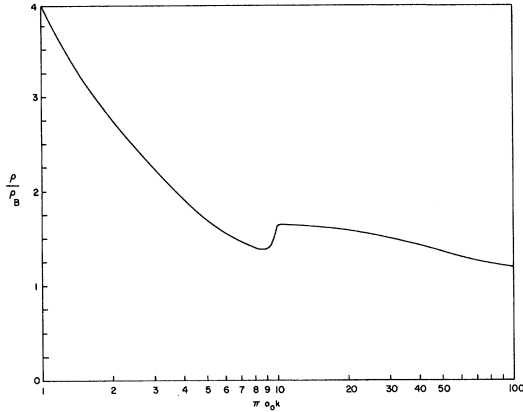


FIG. 2. Resistivity ρ as calculated by Moore and Ehrenreich divided by ρ_B , the resistivity given by the Brooks-Herring result vs $\pi a_0 k$. Here, a_0 is the radius of the first Bohr orbit in the material for an isotropic effective mass and k is the Fermi wave number.

corrections, respectively. For completely degenerate statistics, these corrections are given by

$$\delta_B = \frac{4zm^{3/2}e^3}{\pi^{3/2}\kappa^{3/2}\hbar^3(3n_e)^{1/2}} Q_B(y),$$

$$\delta_M = C_M Q_M(y),$$

$$\delta_N = \left(1 - \frac{C_M}{4} \frac{y}{(1+y)}\right)^{-2} - 1,$$

where

$$C_M = \frac{z^2 \pi^{1/6} m^{1/2} e n_i}{\hbar \kappa^{1/2} (3n_e)^{7/6}},$$

$$y = \frac{\pi^{5/3} \kappa \hbar^2 (3n_e)^{1/3}}{m e^2}.$$

Here, z is the number of electrons lost by the impurity, m is the electron effective mass, n_e is the number of electrons/cm³, n_i is the number of impurities/cm³, and Q_B and Q_M are functions which are given graphically.

For the case of singly ionized impurity scattering ($z=1$) in uncompensated material ($n_i = n_e \equiv n$) these expressions can be written

$$\delta_B = (4\pi/y^{3/2}) Q_B(y),$$

$$\delta_M = (\pi/3y^{1/2}) Q_M(y),$$

$$C_M = \pi/3y^{1/2},$$

$$y = \pi a_0 k,$$

where $a_0 = \hbar^2 \kappa / m e^2$ is the radius of the first Bohr orbit in the material, and $k = (3\pi^2 n)^{1/3}$ is the Fermi wave number. Hence, in the completely degenerate limit the correction factor for singly ionized impurity scattering in uncompensated material is the same function of $a_0 k$ for all semiconductors. Using the values of $Q_B(y)$ and $Q_M(y)$ given graphically by Moore¹⁶ and Ehrenreich, we have calculated the correction factors. A graph of the results is given in Fig. 2.

The generalization of these results to the anisotropic mass case would involve a detailed and involved calculation which we have not performed. It is possible, however, to approximately apply their correction factor by choosing an appropriate value of $a_0 k$. Since the Brooks-Herring matrix element depends mainly on momentum changes in the longitudinal direction, we have used the value of $a_0 k$ in the longitudinal direction (here, $\hbar^2 k_{||}^2 / 2m_{||} = \epsilon_F$) to obtain the correction factor from Fig. 2. In this case, for $10^{18}/\text{cm}^3 \leq n \leq 1.6 \times 10^{19}/\text{cm}^3$, we find $1.4 \leq \pi a_{||} k_{||} \leq 3.5$. The curve labeled ρ_3 in Fig. 1 is the result of multiplying ρ_3 by the correction factor obtained in this way and is in excellent agreement with the experimental results.

In concluding, we note that according to Moore and Ehrenreich their calculation is valid provided $y = \pi a_0 k \gg 1$ and δ_B , δ_M , and δ_N are all small compared to 1. We find, using their calculations, that for $y=2$, $\delta_B \approx 1.3$, which is much larger than the correction to the Born approximation found by performing a phase-shift calculation on the Thomas-Fermi potential.¹⁸ Furthermore, when the potential is corrected so that the phase shifts satisfy the Friedel sum rule,¹⁹ the correction factor is further reduced.¹⁸ Nevertheless, they find excellent agreement between theory and experiment down to the lowest impurity concentration studied for GaAs, i.e., $n = 10^{16}/\text{cm}^3$, which corresponds to $y \approx 2$, even though $\rho/\rho_B \approx 3$ in this case. These results suggest that if their calculation for all three correction terms were correctly extended to the $y \approx 1$ domain, the results would be similar to those given by Fig. 2, i.e., their results for ρ/ρ_B apparently have a greater range of validity than their derivation would suggest, and thus justify their application in the present calculation.

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Lattice Dynamics of Grey Tin and Indium Antimonide[†]

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We have measured the phonon-dispersion relations in symmetry directions for α -Sn at 90 °K and InSb at 300 °K. A limited number of measurements were made at 240 °K in α -Sn to look for effects associated with the phase transition, but none were found. The two dispersion relations are qualitatively similar, the main differences arising from the lower symmetry and a slight general drop in frequency in going from α -Sn to InSb. Systematic trends in the comparison with other group-IV and III-V semiconductors can be seen. We have found second-neighbor shell models which give a reasonable description of the dispersion relations but in which the parameters are poorly defined and apparently devoid of physical meaning. The microscopic implications of this fact are discussed.

I. INTRODUCTION

The horizontal sequence of covalent compounds centered on tin, together with tin itself in the semiconducting phase, provides a unique system for testing theories of covalently bonded crystals. InSb and CdTe form stable compounds in the zinc-blende structure with a lattice parameter nearly identical to that of α -Sn; γ -AgI also has a similar lattice parameter but is a metastable phase.¹ Grey tin itself has a zero direct band gap,² which has led to speculations³ about a singularity in the dielectric function as $\vec{q} \rightarrow 0$ and a possible excitonic transition at low temperatures in highly pure material (Sherington and Kohn, Ref. 4). Going outwards in the horizontal sequence, the band gap increases and the compounds become more ionic (Herman, Cardona, and Greenaway, Ref. 4). Phillips⁵ has developed a microscopic theory of covalent bonding

which leads to an ionicity scale⁶ in which the ionic characters f_i of InSb, CdTe, and AgI are 0.32, 0.67, and 0.77, respectively; since $f_i = 0.785$ is taken to represent the boundary between octahedral and tetrahedral bonding, the observed polymorphism in AgI is consistent with this scale. A study of the lattice dynamics of the members of this sequence should reveal the effects of this increasing ionicity since the lattice structures and masses do not vary much. We present here measurements of phonon-dispersion curves in the first two members, α -Sn⁷ and InSb.

Grey tin is also interesting because it undergoes at normal pressures the transition to a metallic state which InSb, CdTe, Ge, and Si exhibit only under pressure.⁸ This aspect will not be discussed here, partly because it does not appear to be connected with the zero band gap⁹ and also because no evidence for it was found in the temperature depen-