Many-Valley Dipole Scattering of Electrons in Germanium and Silicon

Allan D. Boardman

Department of Pure and Applied Physics, Royal College of Advanced Technology, Salford, Lancashire, England

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The theory of dipole scattering is developed for germanium and silicon, whose conduction-band structure can be described by a simple many-valley model. A formalism is used which employs a linear approximation to the distribution function, and is due to Herring and Vogt. It is shown that, in the approximation, an alternative approach due to Samoilovich et al. gives an identical result. The relaxation-time ratio τ_{11}/τ_1 is computed as a function of energy and it is shown analytically that, as $E \to \infty$, $\tau_{II}/\tau_1 \to 3.69$. This is approximately the square root of the corresponding result for point ions. Thus the scattering due to dipoles is less sensitive to the anistropy of the energy surfaces than in the point-ion case. This can be explained by considering the form of the cross sections presented by each type of scattering center. Finally, some numerical work on the mobility and the effective anisotropy parameter is presented.

1. INTRODUCTION

HE problem of dipole carrier scattering arises in semiconductors containing approximately equal numbers of donors and acceptors. As has already been described in I¹ the donors and acceptors may relax to form dipole centers which then constitute a new scattering mechanism. The most favorable conditions for such scattering are a low temperature (to reduce the importance of lattice scattering) and a high degree of compensation.

There has been, to the author's knowledge, only one detailed experimental study of ion pairing in semiconductors.² This work concerned the Hall mobility of holes in p-type germanium. Unfortunately, these results are difficult to discuss, for a realistic band structure, because of the complex nature of the valence band. Furthermore, the sample used was not very heavily compensated $(N_D = 2.8 \times 10^{17} \text{ cm}^{-3}, N_A = 3 \times 10^{17} \text{ cm}^{-3})$ and the effect on the mobility in this case can almost be explained by subtracting out the dipoles and neglecting them.

The theoretical calculation in I was based on the assumption of spherical energy surfaces and was in fact a generalization of calculations due to Stratton³ and Samoilovich et al.⁴ The new feature was the relaxation of the usual Brooks-Herring restriction on the screened scattering potential but, as is well known, the assumed simple model of the band structure cannot be justified for materials like Ge and Si.

In this paper we will introduce a more realistic manyvalley band structure but the generalization discussed in I is not included because the scattering matrix elements⁵ are so complex. However, it was shown in I that

the Brooks-Herring potential is satisfactory for a study of the more lightly doped materials (say 1017 or 1018 cm⁻³) so we will confine our attention to these and use an impurity potential of the form discussed in $I^{3,4}$

$$V(\mathbf{r}) = Ze^2 R \cos\phi[(1+q\mathbf{r})/\epsilon r^2] \exp(-q\mathbf{r}), \quad (1)$$

where \mathbf{r} is a position vector, Z is the degree of ionization of the impurity centers, R is the dipole length, ϕ is the angle between \mathbf{r} and the dipole vector, $\boldsymbol{\epsilon}$ is the dielectric constant, and q is the reciprocal of the screening length. The expression for q, assuming nondegenerate statistics is

$$q^2 = 4\pi n e^2 / \epsilon k_B T , \qquad (2)$$

where k_B is Boltzmann's constant, T is absolute temperature, and n is the free-carrier density.

The formalism we shall use assumes that the disturbed distribution function $f(\mathbf{k})$ of the electrons is a linear function of the momentum \mathbf{k} and that the scattering occurs in a many-valley solid such as Ge. The necessary technique in this approximation has been fully discussed by Herring and Vogt⁶ and a completely general approach has been discussed by Samoilovich et al.7

We shall calculate $K_{\tau} = \tau_{11}/\tau_{1}$, where τ_{11} and τ_{1} are the principal values of the relaxation time tensor τ_{ij} and the anisotropy parameter $K = (m_{11}/m_1)(\langle \tau_1 \rangle / \langle \tau_{11} \rangle)$ for a combination of lattice and point-ion scattering. m_{11} and m_{1} are the principal values of the energyindependent mass tensor m_{ij} .

Finally, we will calculate the electron mobility as a function of temperature.

2. GENERAL THEORY

In the first instance we will develop expressions for the relaxation times with the aid of the Herring and Vogt formalism. We will then show how these expressions can be transformed into expressions which can be derived from the linear approximation of Samoilovich et al.7

¹ A. D. Boardman, Proc. Phys. Soc. (London) 85, 141 (1965). Hereafter referred to as I. ² H. Reiss, C. S. Fuller, and F. J. Morin, Bell System Tech. J.

^{35, 535 (1956).} ³ R. Stratton, J. Phys. Chem. Solids 23, 1011 (1962).

⁴A. G. Samoilovich, M. V. Nitsovich, Fiz. Tverd. Tela 5, 2981 (1963) [English transl.: Soviet Phys.—Solid State 5, 2182 (1964)].

⁵ Throughout this work we will neglect the role of intervalley impurity scattering.

⁶ C. Herring and E. Vogt., Phys. Rev. **101**, 944 (1956). ⁷ A. G. Samoilovich *et al.*, Fiz. Tverd. Tela **3**, 2939 (1961) [English transl.: Soviet Phys.—Solid State **3**, 2148 (1962).

FIG. 1. Coordinate axes defining ϕ space: $\phi_x = \phi \sin\theta \cos\alpha$; $\phi_y = \phi \sin\theta \sin\alpha$, $\phi_z = \phi \cos\theta$.

The anisotropy can be described in terms of a mass tensor m_{ij} and a relaxation time tensor $\tau_{ij}(E)$. Since the valence-band structure is more difficult to deal with for Ge and Si we will assume that the majority carriers are electrons which lie in energy minima near the zone boundaries. For simplicity the energy surfaces are taken to be ellipsoids of revolution about the (111) axes in Ge and the (100) axes in Si. We, of course, obtain an isotropic drift mobility since the crystals are cubic.

Following Herring and Vogt, let us now define a ϕ space in which the energy surfaces are again spherical, i.e.,

$$\phi_{\alpha} = \frac{\hbar}{(m_{\alpha}^{*})^{1/2}} (k_{\alpha} - k_{\alpha}^{(i)}),$$

$$\phi^{2} = 2E.$$
(3)

where α labels the principal axes of the *i*th ellipsoid, m^* are the eigenvalues of the effective mass tensor, and $k_{\alpha}^{(i)}$ is the band-edge momentum vector.

The differential cross section for elastic electron scattering from a state **k** to \mathbf{k}^1 is proportional to $|\tilde{V}(\mathbf{k}-\mathbf{k}')|^2$ $= |\tilde{V}(\mathbf{K})|^2$, where \tilde{V} is the Fourier transform¹ of (1). If we therefore consider an array of randomly orientated dipoles we obtain

$$\tilde{V}(\mathbf{K})|^{2} = \frac{16\pi^{2}Z^{2}e^{4}R^{2}h^{2}}{3\epsilon^{2}} \times \left\{ \frac{\sum_{i} m_{i}^{*}(\phi_{i} - \phi_{i}')^{2}}{\left[h^{2}q^{2} + \sum_{i} m_{i}^{*}(\phi_{i} - \phi_{i}')^{2}\right]^{2}} \right\}, \quad (4)$$

where the summations are over the principal axes of the ellipse. The ϕ space is defined in Fig. 1. At this stage, from the symmetry, we write $m_x^* = m_y^* = m_{\perp}^*$ and $m_{z}^{*}=m_{II}^{*}$. The notation is conventional. We can also note that, if $d\Omega_{\phi}$ is an element of solid angle in ϕ space.

$$\int \phi_{z}^{2} d\Omega_{\phi} = \int \phi_{x}^{2} d\Omega_{\phi} = \int \phi_{y}^{2} d\Omega_{\phi} = \frac{4}{3} \pi \phi^{2},$$

$$d\mathbf{K} = \frac{(m^{*}{}_{1}^{2} m^{*}{}_{11})^{1/2}}{\hbar^{3}} \phi d\Omega_{\phi} dE.$$
(5)

Point-ion scattering has already been discussed by Ito⁸ and Samoilovich et al.⁹ and in the notation used by Ito, namely, $x = \cos\theta$, $y = \cos\theta'$, $r = m^*_{1}/m^*_{11}$, and $Q = \hbar^2 q^2 / 2m^*_{11} E$, Eq. (4), becomes

$$|\tilde{V}(\mathbf{K})|^{2} = \frac{16\pi^{2}Z^{2}e^{4}R^{2}\hbar^{2}}{3\epsilon^{2}\phi^{2}m^{*}_{11}} \left\{ \frac{(x-y)^{2} + r\{(2-x^{2}-y^{2})-2\{(1-y^{2})(1-x^{2})\}^{1/2}\cos(\alpha-\alpha')\}}{[Q+(x-y)^{2}+r\{(2-x^{2}-y^{2})-2[(1-y^{2})(1-x^{2})]^{1/2}\cos(\alpha-\alpha')\}]^{2}} \right\}.$$
 (6)

In I we introduced a parameter $\gamma^2 = (\pi \hbar^2 e^2/2m^* \epsilon k_B^2)(n/T^2)$ which delineated the applicability of a Brooks-Herring potential. If, in this case, we replace m^* by $m^*_{||}$ we obtain $Q = 4\gamma_{||}^2/\eta$ where $\eta = E/k_BT$ and the condition $\gamma_{||}^2 \ll 1$ is again the necessary condition for a Brooks-Herring treatment to be valid.

Since the Herring and Vogt theory is so well known it is not necessary to dwell on the details leading to the relaxation-time expression.

Thus:

$$\frac{1}{\tau_{11}} = \frac{3B(\eta)}{8_{\tau}} \int_{-1}^{1} \int_{-1}^{1} (x-y)^2 \langle M \rangle dx dy, \qquad (7)$$

where

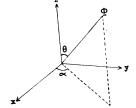
$$B(\eta) = \frac{42^{-e^{2}K^{-1}\sqrt{dM^{-1}}}}{3\sqrt{2}\epsilon^{2}h^{2}(m^{*}_{11}k_{B}T)^{1/2}}\frac{1}{\eta^{1/2}}$$
(8)

and $\langle M \rangle$ means the integration over α and α' of (6). After the integration in $\langle M \rangle$ has been performed, we obtain

72-4 D2 M ...

$$\frac{1}{\tau_{11}} = \frac{3}{2}\pi B(\eta) \int_{-1}^{1} \int_{-1}^{1} \frac{(x-y)^2 [(x-y)^2 (Q+(x-y)^2) + r(2-x^2-y^2) (Q+(x-y)^2) + r^2 (x^2-y^2)^2] dx dy}{[(Q+(x-y)^2)^2 + 2r(2-x^2-y^2) (Q+(x-y)^2) + r^2 (x^2-y^2)^2]^{3/2}}.$$
(9)

This integral can only be solved analytically in the limit $r \rightarrow 0$. We must therefore resort to numerical quadrature. Equation (9) is similar to the expression for pointion scattering obtained by Ito,8 indeed the denominator is identical. However, as discussed in the Appendix, the Herring and Vogt treatment is a linear approximation and is therefore *identical* to the Samoilovich treatment in this approximation. This point has not previously been explicitly made.



⁸ R. Ito, J. Phys. Soc. Japan 18, 1604 (1963). ⁹ A. G. Samoilovich, Fiz. Tverd. Tela 3, 3285 (1961) [English transl.: Soviet Phys.—Solid State 3, 2385 (1962)].

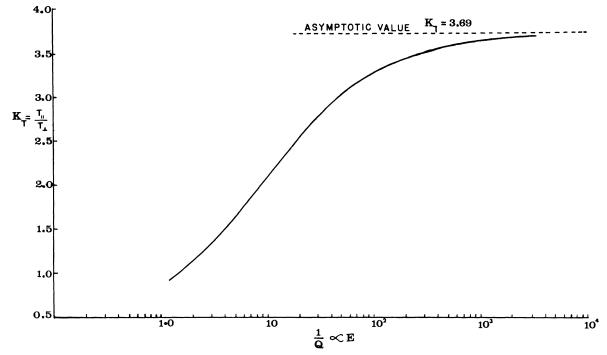


FIG. 2. The ratio of the longitudinal relaxation time to the traverse relaxation time for one valley in Ge plotted against energy. The asymptotic form was obtained from Eq. (14).

Thus, in the Samoilovich formalism Eq. (9) becomes

$$\frac{1}{\tau_{11}} = \frac{6\pi B(\eta)}{(1-r)} \int_{-1}^{1} \frac{x^2 dx}{\left[x^2 + r/(1-r)\right]} \times \left\{\frac{1+2A^2}{2(1+A^2)} - A^2 \ln\left(1 + \frac{1}{A^2}\right)\right\}, \quad (10)$$

where

$$4^{2} = \frac{\gamma_{11}^{2}}{\eta [(1-r)x^{2} + r^{2}]},$$
 (11)

and in a similar fashion we obtain

$$\frac{1}{\tau_{1}} = \frac{3\pi B(\eta)}{(1-r)} \int_{-1}^{1} \frac{dx}{\left[x^{2} + r/(1-r)\right]} \times \left\{\frac{1+2A^{2}}{2(1+A^{2})} - A^{2} \ln\left(1+\frac{1}{A^{2}}\right)\right\} - \frac{1}{2\tau_{11}}.$$
 (12)

These one-dimensional integrals can be handled more conveniently, e.g., the asymptotic forms are especially easy to find. It has always of course been implicit that the two approaches must be entirely equivalent in the linear approximation. The work of Ito8 and Samoilovich9 on point-ion scattering should therefore be in exact agreement.

If the limit $r \rightarrow 1$ is taken in Eqs. (10) and (12) we obtain the usual isotropic case.^{1,3,4}

The theory described here can only be used to calculate quantities which depend only on the first power of τ , e.g., the drift mobility. If we desire to calculate the Hall mobility which depends on τ^2 then the inherent error in the results is multiplied by 2.10 However, to go beyond the Herring and Vogt approximation we need to employ the sophisticated techniques of Samoilovich so we will concentrate only on the quantities μ and K.

Even if the linear approximation is transcended, the formal Herring and Vogt expressions for the galvanomagnetic coefficients are sufficient provided one uses the more accurate expressions for τ_{11} and τ_{1} obtainable from the work of Samoilovich.¹⁰⁻¹³

3. SCATTERING PARAMETER

It has been noted in previous calculations of point-ion scattering^{8,9} that the ratio τ_{11}/τ_1 tends asymptotically to a finite limit as $E \rightarrow \infty$. This limit is often called the maximum anisotropy and of course exists in this case also (cf. Fig. 2). We can discuss this limit by considering small-A expansion of the integrands of (10) and (12).

The expression for K_{τ} then becomes

$$K_{r} \approx \frac{1}{2} \left\{ \int_{-1}^{1} \frac{dx}{[x^{2} + r/(1 - r)]} / \int_{-1}^{1} \frac{x^{2} dx}{[x^{2} + r/(1 - r)]} - 1 \right\}$$
(13)

¹⁰ I. Ya. Korenblit, Fiz. Tverd. Tela 4, 168 (1962) [English transl.: Soviet Phys.—Solid State 4, 120 (1962)]. ¹¹ P. M. Eagles and D. M. Edwards, Phys. Rev. 138, A1706

^{(1965).}

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 ¹² I. V. Dakhovskii, Fiz. Tverd. Tela 5, 2332 (1963) [English transl.; Soviet Phys.—Solid State 5, 1695 (1964)].
 ¹³ D. G. Andrianov *et al.*, Fiz. Tverd. Tela 6, 2825 (1964) [English transl.: Soviet Phys.—Solid State 5, 1695 (1964)].

which becomes

$$K_{\tau} \approx \frac{1}{2} \left\{ \frac{\left[(1-r)^{1/2}/r^{1/2} \right] \tan^{-1} \left[(1-r)^{1/2}/r^{1/2} \right]}{1 - \left[r^{1/2}/(1-r)^{1/2} \right] \tan^{-1} \left[(1-r)^{1/2}/r^{1/2} \right]} - 1 \right\}.$$
(14)

The parameters for Ge are $m^*_{11} = 1.588$, $m^*_{12} = 0.08152$, r=0.0513 and for Si are $m^*_{11}=0.80$, $m^*_{12}=0.192$. Thus the analytical form (14) predicts

$$K_{\tau} \approx 3.694 \quad (Ge),$$

$$K_{\tau} \approx 1.924 \quad (Si).$$
(15)

If we now define the part of the integrand of (10) which depends on A as

$$f(A) = \frac{1+2A^2}{2(1+A^2)} - A^2 \ln\left(1+\frac{1}{A^2}\right), \quad (16)$$

we see that when $A \rightarrow \infty$

$$f(A) \to (6A^4)^{-1}$$
. (17)

This means that in the low-energy region

$$\frac{1}{\tau_{11}} \approx \frac{32(1-r)\pi B(\eta)}{Q^2} \left(\frac{1}{5} + \frac{r}{3(1-r)}\right), \qquad (18)$$

$$\frac{1}{\tau_{1}} \approx \frac{32(1-r)\pi B(\eta)}{Q^{2}} \left(\frac{1}{15} + \frac{r}{3(1-r)}\right), \qquad (19)$$

so that the value of K_{τ} becomes

$$K_r \approx (1+4r)/(3+2r)$$
. (20)

Thus, numerically

$$K_{\tau} \approx 0.3884 \quad (Ge),$$

$$K_{\tau} \approx 0.5405 \quad (Si).$$
(21)

The quantity K_{τ} which refers to one valley is a measure of the scattering anisotropy. It has been discovered that, as $E \to \infty$, for point-ion scattering $K_{\tau} \approx 12.^{8,9,14}$ However, Eq. (15) shows that the anisotropy in the scattering due to dipoles is much less, so it is of interest to consider a rather nonrigorous argument which leads us to expect this result.

A single valley is represented by a prolate energy

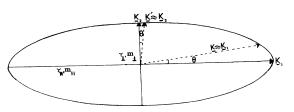


FIG. 3. The prolate energy surface of revolution as a model of one valley. The effective masses and relaxation times associated with the longitudinal and transverse axes are shown.

surface of revolution¹⁵ whose longitudinal axis lies along a symmetry axis. (See Fig. 3).

As a rough measure of τ_{11}/τ_1 we will take $\tau(\mathbf{K}_1)/\tau(\mathbf{K}_2)$ where we consider, in turn, an electron traveling along the minor or major axis of the ellipsoid. Essentially the relaxation time is proportional to the probability of a transition from a state **K** to state \mathbf{K}^1 , and the scattering matrix element is a function of $|\mathbf{K} - \mathbf{K}'|$. The distinction between the action of dipoles and point ions can be

TABLE I. A comparison of scattering matrix elements as a function of carrier energy.

Scattering mechanism	Matrix element	Energy of carrier
Point Ions	$ \mathbf{K} - \mathbf{K}' ^{-4}$ Constant	High Low
Dipoles	K-K' ⁻² K-K' ²	High Low

made by referring to Table I. Thus we can predict the trend of the K_{τ} values by setting (for $E \rightarrow \infty$)

$$\frac{\tau_{11}}{\tau_1} \sim \frac{\tau(\mathbf{K}_1)}{\tau(\mathbf{K}_2)} \propto \frac{K_1^4/K_2^4 \quad \text{(point ions)}}{K_1^2/K_2^2 \quad \text{(dipoles)}}.$$
(22)

Therefore, since $K_{\tau} \sim 12$ for point-ions, we expect in the dipole case that $K_{\tau} \sim (12)^{1/2}$, which is roughly what we obtain. A previous attempt to predict the trend of K_{τ} for point-ion scattering in this way, due to Herring,^{15,16} led to the opposite conclusion.

4. ELECTRON MOBILITY

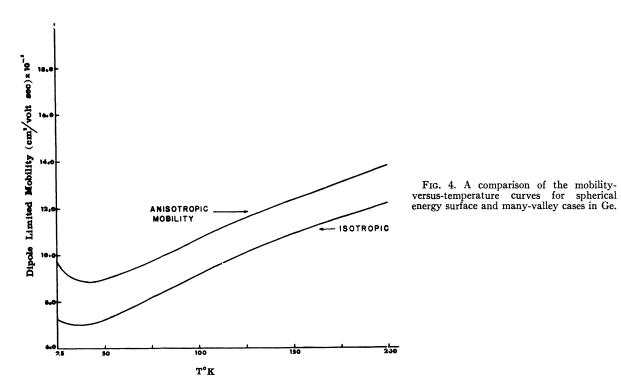
Since a Brooks-Herring potential has been used throughout, the electron mobility is evaluated at $\eta = E_F/k_BT = 2$ (cf. I) when the averaging is performed. The isotropic result is^{1,3}

$$\mu_{I} = \frac{2^{1/2} \epsilon^{2} \hbar^{2} (k_{B}T)^{1/2}}{\pi^{3/2} Z^{2} R^{2} m^{*3/2} \epsilon^{3} V_{\alpha} [(2+2/\gamma^{2})/(1+2/\gamma^{2}) - \gamma^{2} \ln(1+2/\gamma^{2})]}.$$
(23)

We must now compare this result with the anisotropic mobility obtained from

$$\mu_{A} = \frac{4e}{9\pi^{1/2}} \left\{ \frac{2}{m^{*}_{1}} \langle \tau_{1} \rangle + \frac{1}{m^{*}_{11}} \langle \tau_{11} \rangle \right\}, \qquad (24)$$

 ¹⁴ F. S. Ham, Phys. Rev. 100, 1251 (1955).
 ¹⁵ C. Herring, Bell System Tech. J. 34, 237 (1955).
 ¹⁶ J. D. Zook, Phys. Rev. 136, A869 (1964).



where $\langle \tau \rangle = \int_0^\infty d\eta \ \tau(\eta) e^{-\eta} \eta^{3/2}$. The mobility averaged in the way described above becomes

$$\mu_{A} = \frac{2^{5/2} \epsilon^{2} h^{2} (m^{*}_{11} k_{B} T)^{1/2}}{9 \pi^{3/2} Z^{2} e^{3} R^{2} N_{d} m^{*}_{1}} \left\{ \frac{2}{m^{*}_{1} J(2)} \frac{1}{m^{*}_{11} I(2)} \right\}$$
$$= \frac{2^{1/2} \epsilon^{2} h^{2} (m^{*}_{11} k_{B} T)^{1/2} (1-r)}{9 \pi^{3/2} Z^{2} e^{3} R^{2} N_{d} m^{*}_{1}} \left\{ \frac{2}{m^{*}_{1} L(2)} + \frac{1}{m^{*}_{11} M(2)} \right\}, \qquad (25)$$

where $I(\eta)$, $J(\eta)$ are the double integrals such as (9) and $L(\eta)$, $M(\eta)$ are the integrals involved in (10) and (12). As an illustration we consider Ge containing 3×10^{17} cm⁻³ donors and 2.8×10^{17} cm⁻³ acceptors; this is the *n*-type counterpart of the case described in the Introduction. The compensation is 0.0345. This is really representative of a minimum required degree of compensation; the dipole density² is $\sim N_A$ while the carrier density is $\sim (N_D - N_A)$. For the sake of simplicity we will neglect freeze-out of electrons at low temperatures. We can now express μ_A as

$$\mu_{A} = \frac{2^{7/2} \epsilon^{2} h^{2} (m^{*}_{11} k_{B} T)^{1/2}}{9 \pi^{3/2} Z^{2} \epsilon^{3} R^{2} N_{d} m^{*}_{1}^{2} J(2)} \left\{ 1 + \frac{r K_{r}}{2} \right\} , \qquad (26)$$

where K_{τ} is to be evaluated at $E = 2k_BT$. If we now compare this result with (23) we obtain

$$\frac{\mu_A}{\mu_I} = \frac{8m_{11}^{1/2}m^{*3/2}}{9m_1^2 J(2)} \left(1 + \frac{rK_\tau}{2}\right) f(\gamma^2)$$
(27)

which can easily be seen to reduce to unity for r=1. For Ge $\epsilon \sim 16$, $m^* \sim 0.25$, so that numerically Eqs. (23) and (25) become

$$\mu_{A} = \frac{\frac{1.934 \times 10^{6} T^{1/2}}{F(T)J(2)} [1 + 0.0257 K_{\tau}] \text{ cm}^{2}/\text{V sec},$$

$$\mu_{I} = \frac{9.173 \times 10^{4} T^{1/2}}{F(T)[(2 + 2/\gamma^{2})/(1 + 2/\gamma^{2}) - \gamma^{2} \ln(1 + 2/\gamma^{2})]} \text{ cm}^{2}/\text{V sec},$$
(28)

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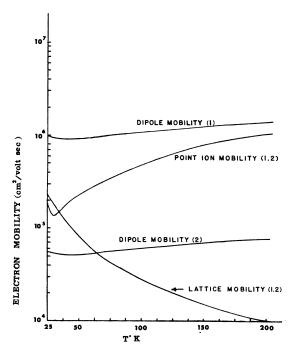


FIG. 5. The various contributions to the electron mobility of Ge for $N_D=3\times10^{17}$ cm⁻³; $N_A=2.8\times10^{17}$ cm⁻³ (curves 1) and for $N_D=5\times10^{18}$ cm⁻³; $N_A=4.98\times10^{18}$ cm⁻³ (curves 2).

where $F(T) = 1 + (3.253 \times 10^{-4})T + (3.702 \times 10^{-7})T^2$ represents the temperature dependence of R, the dipole separation.

It should be emphasized at this point that we are considering a random array of dipoles. This means that we have replaced a collection of anisotropic scatterers, oriented at random, by an equivalent set of isotropic scatterers, since this is the most probable experimental situation.

The dipole "length" R can be obtained from the work of Reiss *et al.* which employs the ionic theory of liquids. The appropriate expression has been developed by Stratton, i.e., $R^2 \approx R_0^2 f(T)$, where R_0 is the minimum dipole length. In the above calculations we take $R_0=1.8$ Å this being the value calculated by Reiss *et al.* It can be seen in Fig. 4 that the anisotropic mobility is higher than in the isotropic case. This of course is expected¹⁷ because a simple argument shows that the value of the effective masses are such that an increase must occur. The order of magnitude of the increase is 24% at 50°K so that in a situation where dipoles are the dominant scattering mechanism this is significant.

In Figs. 5 and 6, we can see the various contributions made to the total mobility. The lattice mobility, given by Dakhovskii,12 is

$$\mu_L = 2.82 \times 10^7 T^{-3/2} \,\mathrm{cm}^2 / \mathrm{V} \,\mathrm{sec} \tag{29}$$

and the ion-mobility, obtained from the Samoilovich formalism,¹² is

$$u_{i} = \frac{2.144 \times 10^{3} T^{3/2}}{(\ln Q/4 + 1.7)} \times \left[1 + 0.373 \left(\frac{\ln Q/4 + 2.76}{\ln Q/4 + 1.7} \right) \right] \text{ cm}^{2}/\text{V sec}.$$
(30)

It can be seen in Fig. 6 that a large rise in the observed mobility is to be observed when compensation occurs. However, if we assume simply that the ion population is decreased to $N_D - N_A$ and neglect the role of the resultant dipoles we could almost reproduce these results. A significant error of $\sim 10\%$ can be made by such a procedure in the lower temperature range.

If the compensation were an order of magnitude better, as it is in curves 2 of Fig. 5, then the mobility will be limited mainly by dipoles and the lattice. It is not possible to comment on any experimental work on Ge but it is possible that dipole scattering may be dominant in solid solutions of Cd Te in InAs.¹⁸

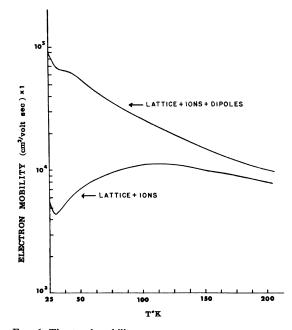


FIG. 6. The total mobility versus temperature for Ge $(N_D = 3 \times 10^{17} \text{ cm}^{-3}, N_A = 2.8 \times 10^{17} \text{ cm}^{-3})$. The lower curve assumes that there is no ion-pairing to produce dipoles or otherwise. The mobilities have been added reciprocally.

¹⁸ A. D. Stuckes and R. P. Chasmar, J. Phys. Chem. Solids 25, 469 (1964). This problem is currently being examined by the author.

¹⁷ I. J. Boiko, Fiz. Tverd. Tela 1, 574 (1959) [English transl.: Soviet Phys.—Solid State 1, 518 (1959)]. In this work Boiko deduced from an extension, using the Herring and Vogt formalism, of the Conwell-Weisskopf formula that the predicted mobilities are a factor of 2 greater than the corresponding isotropic case. We expect that with a reduced sensitivity to the anisotropy the difference will be less.

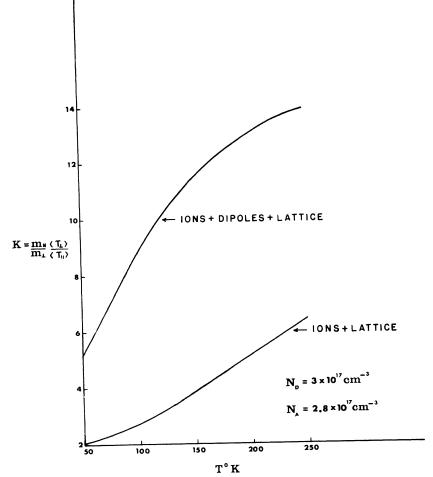


FIG. 7. Effective anisotropy parameter versus temperature for Ge. $(N_A = 2.8 \times 10^{17} \text{ cm}^{-3}; N_D = 3.0 \times 10^{17} \text{ cm}^{-3})$. The lower curve assumes that all the ions behave as separate scattering centers.

5. EFFECTIVE ANISOTROPY PARAMETER

The anisotropy of one valley can be studied directly from magnetoresistance and piezoresistance experiments.¹⁹ The results here will apply only to the linear range of piezoresistance¹⁹ since the valleys shift relative to each other at large stresses²⁰ and the varying number of carriers in each valley alter the effective screening radius we would have to use.

We consider the quantity $K = (m_{11}^*/m_{11}^*)(\langle \tau_1 \rangle / \langle \tau_{11} \rangle)$ as a function of temperature. The brackets $\langle \rangle$ represent the usual Maxwellian average. In Fig. 7 we see K computed for a combination of ions, lattice, and dipoles. As we commented in the last section, the upper curve can be roughly explained by assuming the ion population to be N_D-N_A . However at 100°K an error ~15% would be made by such an assumption.

If highly compensated materials become available, then it should be possible to specifically examine the dipole scattering anisotropy K_{τ} directly, i.e., the validity of $K_{\tau} \rightarrow 3.69$ as $Q \rightarrow 0$ can be checked. This was done experimentally for point-ions by Laff and Fan.¹⁹

6. DISCUSSION

We have calculated the anisotropy in the scattering of electrons from a set of randomly orientated dipoles. Naturally the experimental situation will be such that partial alignment of the dipoles will occur.^{21,4} We would then have to consider the anisotropy of the cross section and the energy surfaces. This problem has yet to be solved.

The degree of anisotropy cannot be compared to an experimental result because there are no relevant available data on Ge or Si.

However, some work done on the InAs-CdTe alloy system¹⁸ may provide a means of comparing part of the theory with experiment. In this case the band would be spherical but the nonparabolicity would have to be included.

The calculations presented here are based on the first Born approximation. This leads to results of limited applicability below 50°K²² because the cross section is

 ¹⁹ R. A. Laff and H. Y. Fan., Phys. Rev. **112**, 317 (1958).
 ²⁰ M. J. Katz, Phys. Rev. **140**, A1323 (1965).

²¹ J. Appel and W. B. Teutsch, J. Phys. Chem. Solids 23, 1521 (1962). ²² F. Blatt, J. Phys. Chem. Solids 1, 262 (1957).

overestimated. It is clear that partial-wave calculation²³ must be performed to account for the temperature range $T \le 50^{\circ}$ K more accurately. The difficulty here is that for spherical energy surfaces the radial Schrödinger equations, which must be solved numerically, are coupled. Also there is a basic defect in such a partialwave analysis, namely, the lack of a self-consistency condition. Such a condition exists for metals in the form of the Friedel sum rule. In semiconductor work we can only assume the scattering potential and then devise qualitative arguments which lead to a choice of the screening length, or the cutoff parameter, which yields results which are insensitive to the detailed form of the potential.24

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APPENDIX

We will now demonstrate that the procedures of Herring and Vogt⁶ and Samoilovich *et al.*⁷⁻⁹ are entirely equivalent in the linear approximation. In the Herring-Vogt formalism the departure of the distribution function from equilibrium is written as

$$n_{\mathbf{k}} = \sum_{m=-\rho}^{m=+\rho} \sum_{\rho} F_{\rho m}(\boldsymbol{\phi}) Y_{\rho m}(\boldsymbol{\phi}) , \qquad (A1)$$

where $Y_{\rho m}(\hat{\phi})$ is the usual spherical harmonic. The relaxation times are then assumed and are generated from the collision equation^{7,9}

$$Rn_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}(n_{\mathbf{k}} - n_{\mathbf{k}'}), \qquad (A2)$$

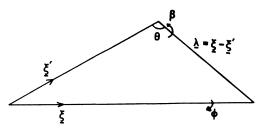


FIG. 8. Vector diagram showing the scattering from ξ to ξ' together with the polar angles.

where R is a collision operator and $V_{kk'}$ is the scattering matrix element. In the Herring-Vogt notation we obtain [neglecting all harmonics above $\rho = 1$ in (A1)]

$$\frac{1}{\tau_{ii}} = -A \int \int d\Omega_{\phi} d\Omega_{\phi'} \phi_i(\phi_i' - \phi_i) \\ \times W(\phi \to \phi') \bigg/ \int \phi_i^2 d\Omega_{\phi}, \quad (A3)$$

where for dipole scattering

$$A = \frac{4e^4 N_d (m^* {}_{1}^2 m^* {}_{11})^{1/2} R^2}{3\epsilon^2 \hbar^4}$$

and the transition probability is

$$W(\phi \to \phi') = \phi \frac{\sum_{i} m^{*}_{i}/\hbar^{2}(\phi_{i} - \phi_{i}')^{2}}{\left[q^{2} + \sum_{i} m^{*}_{i}/\hbar^{2}(\phi_{i} - \phi_{i}')^{2}\right]^{2}}$$

The Samoilovich formalism generates relaxation times by setting

$$Rn_{\mathbf{k}} = -\sum_{mn} F_{1m}(\phi) B_{11}(mn) Y_{1n}(\hat{\phi});$$

the relaxation times τ_{11} and τ_{1} are then $B_{11}^{-1}(0)$ and $B_{11}^{-1}(1)$, respectively. The functions $B_{jk}(m)$ are obtained from⁴

$$B_{jk}(m) = \frac{(2m^{*}{}_{1}^{2}m^{*}{}_{1!}E)^{1/2}}{\pi^{2}h^{3}} \sum_{(s, \text{ even})} \frac{(2j+1)(2k+1)(j-s)!(k-s)!}{(j+s)!(k+s)!} \int_{0}^{\pi} d\alpha \sin\alpha \int_{0}^{\pi/2} d\theta \sin\theta \times \cos\theta W(\theta, \alpha) P_{j}^{s}(\cos\theta) P_{k}^{s}(\cos\theta) P_{sm}^{j}(\cos\alpha) P_{sm}^{*}(\cos\alpha), \quad (A4)$$

where $W(\theta, \alpha)$ is the transition probability once more and P_{sm}^{k} are Wigner functions.²⁵ Having defined the two formalisms we will now show how Eq. (9) of the text can be expressed as a single integral (10). We begin with (A3) which was derived using the transformation (3).

Let us now make the transformation^{7,9,16} $\xi_i = \hbar k_i / (2m^* E)^{1/2}$ so that Eq. (A3) now becomes

$$\frac{1}{\tau_{ii}} = +\frac{3}{8\pi} \int \int (\xi_i - \xi_i')^2 \Lambda(\xi \to \xi') d\Omega_{\xi} d\Omega_{\xi'}, \qquad (A5)$$

²³ This problem is currently being investigated by the author in collaboration with Dr. S. Sampanthar of the Mathematics Department.

²⁴ N. Sclar, Phys. Rev. **104**, 1548 (1956). ²⁵ These functions are clearly defined in an article by R. J. Roe, J. Appl. Phys. **36**, 2024 (1965). The author would like to thank Dr. R. A. Sack of the Mathematics Department for pointing this out to him.

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where

$$\Lambda(\xi \to \xi') = \frac{4e^4 N_d (m^*{}_1^2 m_{11}^*)^{1/2} R^2}{3\epsilon^2 \hbar^4 (2E)^{1/2}} \frac{\sum_i m^*{}_i / \hbar^2 (\xi_i - \xi_i')^2}{\left[q^2 / 2E + \sum_i m_{i\hbar}{}^* (\xi_i - \xi_i')^2\right]^2}.$$
 (A6)

Let us now consider scattering from ξ to ξ' such that $\xi - \xi' = \lambda$ (see Fig. 8). It is then a straightforward matter to write, as shown by Zook,¹⁶

$$d\Omega_{\xi} d\Omega_{\xi'} = \lambda d\Omega_{\lambda} d\lambda d\beta.$$
(A7)

Thus,16

$$\frac{1}{\tau_{ii}} = \frac{3}{4} \int d\lambda \,\lambda^2_{i/\lambda} \Lambda(|\lambda|) \,. \tag{A8}$$

However, we can proceed beyond this stage. Thus, since ξ and ξ' are unit vectors it is obvious that $0 \le \lambda \le 2$ and we can also write⁷

$$\lambda = 2\cos\theta; \quad 0 \le \theta \le \pi/2, \tag{A9}$$

where θ is the angle between λ and ξ . In λ space we have $\lambda_z = \lambda \sin \psi \cos \phi'$, $\lambda_y = \lambda \sin \psi \cos \phi'$, and $\lambda_z = \lambda \cos \psi$, and the scattering function is

$$\Lambda = \frac{4e^4 N_{\alpha} m^* R^2}{3\epsilon^2 \hbar^2 (2E)^{1/2} m^* R^2} \cos^2 \theta \left\{ \frac{\cos^2 \psi + r \sin^2 \psi}{\left[Q/4 + (\cos^2 \psi + r \sin^2 \psi) \cos^2 \theta \right]^2} \right\}.$$
 (A10)

Therefore,

$$\frac{1}{\tau_{11}} = \frac{e^4 N_d m^* R^2}{\epsilon^2 \hbar^2 (2Em^*_{11})^{1/2}} \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi/2} \frac{(8\cos^2\psi \sin\psi)(2\cos^5\theta \sin\theta)(\cos^2\psi + r\sin^2\psi)d\theta d\phi' d\psi}{[Q/4 + \cos^2\theta(\cos^2\psi + r\sin^2\psi)]^2}$$
(A11)

which can be expressed as

$$\frac{1}{\tau_{11}} = \frac{8\pi e^4 N_d m_{\perp}^* R^2}{\epsilon^2 \hbar^2 (2m_{11}^* E)^{1/2} (1-r)} \int_{-1}^1 \frac{x^2 dx}{\left[x^2 + r/(1+r)\right]} \int_0^1 \frac{y^5 dy}{(y^2 + A^2)^2}.$$
(A12)

The integral over y can easily be performed and Eq. (10) of the text is recovered.