As might be expected, the temperature dependence of the mobility of the carriers in the grain-boundary space-charge sheath is such as to indicate that the principle scattering mechanism is impurity or defect scattering However, the marked difference between the mobilities (Fig. 9) of samples with different orientation of the grain boundary is not understood.

PHYSICAL REVIEW

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Hot Electron Problem in Semiconductors with Spheroidal Energy Surfaces

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Shockley has derived the expression $E_c = (1.51)C_l/\mu$ for the critical electric field strength E_c at which the current-voltage relation in a semiconductor departs from Ohm's law. Here C_l is the velocity of longitudinal phonons and μ the conductivity mobility of the carrier. Experimental values of E_{σ} for Ge and Si are from two to four times larger than those predicted by this formula. We therefore have extended the theory to take account ellipsoidal energy surfaces in the Brillouin Zone and scattering by shear modes of vibration. The effect of the more general effective mass tensor is to raise the theoretical value of E_c by a factor of about 2 for *n*-type Ge and 1.3 for *n*-type Si, whereas shear mode scattering lowers E_c by a factor that is between 1 and the value of the ratio of the velocity of transverse modes to that of longitudinal modes. Moreover, Ec should vary with the direction of the current. The present study still fails to close the gap between theory and experiment : the remaining discrepancy is possibly the result of neglecting intervalley scattering.

INTRODUCTION AND SUMMARY

HE deviation from Ohm's law in semiconductors such as Ge and Si in strong electric fields has been studied both theoretically¹⁻⁷ and experimentally^{8,9} by many investigators. This problem has been called the "hot-electron" problem by Shockley because the average kinetic energy of the electrons in strong fields becomes larger than the usual thermal energy, so that the "electron temperature" becomes larger than the lattice temperature. There are, however, quantitative discrepancies between theory and experiment in some respects, such as in the value of the critical field E_c where the deviation from Ohm's law occurs. The experimental values in Ge and Si are about twice to four times larger than those obtained from the formula

$$E_c^s = 1.51 C_l / \mu. \tag{1}$$

The superscript s on E_c indicates that this value is obtained from the scalar effective mass theories, C_{l} is the longitudinal velocity of the phonons, and μ is the weakfield conductivity mobility of electrons.

Previous calculations have assumed spherical energy

surfaces in the Brillouin zone. It is now believed that for *n*-type Ge and Si one must use spheroidal surfaces in discussing the electrical properties. Further, as has been pointed out by Adams¹⁰ and by Herring,¹¹ shear waves are as important as pure compressional waves in the lattice scattering of electrons in these crystals. Therefore we have attempted to solve the hot-electron problem with the spheroidal model, including the effect of shear waves. A number of drastic approximations are made in solving the Bloch equation, and we finally get the expression for the critical field in the following form:

$$E_c = ASE_c^s, \tag{2}$$

where the factor A is an anisotropy factor and the other factor S results from the effect of the shear waves. When we neglect the effect of the latter, S equals 1, and when the mass component ratio $r=m_2/m_1$ is equal to 1, A becomes independent of the direction of the current vector and is also 1. The larger the departure of r from 1, the larger is the value of A. The factor S is a complicated function of the mass ratio r, the ratios of the characteristic coefficients of the deformation potentials of shear waves and of pure compressional waves, and the ratio $C = C_t / C_l$ of the transverse and longitudinal velocities of the acoustical modes of lattice vibration. However, the value of S is almost always between C and 1. This fact may be qualitatively understood, because both

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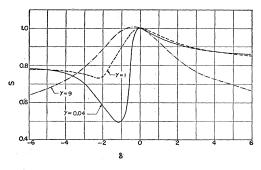


FIG. 1. S versus δ for r = 0.04, 1 and 9.

transverse and longitudinal modes of vibration contribute to shear-wave scattering, so that the effective average velocity for lattice scattering is between C_t and C_{l} . We already found scalar conductivity for cubic crystals in weak electric fields without magnetic fields even in the spheroidal approximation,¹² because of the cubically symmetric distribution of spheroids. In the hot-electron problem, on the contrary, anisotropic effects do not vanish with the same spheroidal model. Thus the factor A depends not only upon the model but also upon the direction of the current vector. In addition, when the current is not parallel to the symmetry axes of the cubic crystal such as the (100), (110), and (111) axes, there appears a small induced transverse field. Although the angle ϵ between the current and field vectors is very small, about a few degrees, its maximum value is about one hundred times larger than the mosaic angle in the case of Ge. There have been no experimental observations of the transverse voltage and the directional dependence of the critical field arising from the anisotropy of the spheroids. However, we believe that this effect should be detectable.

We have neglected intervalley scattering and scattering due to impurities and to optical modes of vibration and made many approximations and simplifications in this calculation. Therefore it is not surprising that our formulas do not give quantitative agreement with the experimental results. However, we do not expect that the qualitative features of our results could be changed in a more rigorous theory. The factor A makes the gap between theory and experiment narrower than before, but the factor S makes it broader. If we could include the effect of intervalley scattering, we would get another modulation factor I in the Eq. (2). This factor is probably greater than unity because the higher-energy electrons should lose energy through the intervalley scattering.

OUTLINE OF CALCULATION AND RESULT

Now we briefly outline the calculation and the results upon which the above discussion is based.

Including the effect of the shear waves, the deformation potential U for a spheroid becomes, as pointed out

by Herring,¹¹

$$U = E_d\{(1+\delta)\epsilon_{11} + \epsilon_{22} + \epsilon_{33}\}$$
(3)

where ϵ_{11} , ϵ_{22} , and ϵ_{33} are the diagonal components of the strain tensor along the principal axes of the spheroid. The subscript 1 is for the rotational axis, and 2 and 3 are for the other principal axes. $E_d \delta \epsilon_{11}$ is the shear wave component of the deformation potential. Owing to this component, we must modify the scattering matrix element for the longitudinal wave by a factor

$$1+\delta\cos^2\theta,$$
 (4)

and also introduce a new matrix element for the transverse wave which can be obtained by multiplying

$$\delta \cos\theta \sin\theta$$
 (5)

into the usual longitudinal matrix element of pure dilation interaction. Of course we must not forget to replace the longitudinal velocity C_l by the transverse velocity C_t in the expression of the latter matrix element. Here θ is the angle between the wave vector of the phonon and the rotational axis of the spheroid.

Using these matrix elements, we solve the Bloch equation by the same procedure as that used by Yamashita and Watanabe⁷ or Davidow.⁴ Three following assumptions (a), (b), and (c) are used:

(a)
$$f(\mathbf{K},\mathbf{F},\mathfrak{M}) = f_0(W,\mathbf{F},\mathfrak{M}) + G(W,\mathbf{F},\mathfrak{M}) \cdot \boldsymbol{\nabla}_k W,$$
 (6)

(b)
$$\begin{cases} f_0(W \pm h\nu) = f_0(W) \pm h\nu df_0/dW \\ +\frac{1}{2}(h\nu)^2 d^2 f_0/dW^2, \quad (7) \\ \mathbf{G}(W \pm h\nu) = \mathbf{G}(W), \end{cases}$$

c)
$$h\nu \ll kT$$
, (8)

where $h\nu$ is the phonon energy. In Eq. (6) we assume that f_0 and **G** are functions of the wave vector **K** only through energy. Unfortunately this assumption leads to different expressions for the collision term along the three principal axes of the spheroid. Instead of doing a more elaborate calculation taking into account this anisotropy in the scattering, we shall simply use the average of these three collision terms. Also in the calculation of the drift term we use the approximation

$$m_1 v_1^2 = \frac{1}{2} m_2 v_2^2 = \frac{1}{2} m_2 v_3^2 = \frac{1}{3} W.$$
 (9)

Finally we get an expression for the current density in a strong field of electrons whose energy surfaces is a spheroid characterized by the mass tensor \mathfrak{M} .

1

$$\mathbf{J} = \frac{Ne\mu\pi}{2^{5/4}\Gamma(3/4)} \left(\frac{3}{\mathrm{Trace}\mathfrak{M}^{-1}}\right) p^{-\frac{1}{4}}\mathfrak{M}^{-1} \cdot \mathbf{F}.$$
 (10)

TABLE I.
$$\sqrt{A_1}$$
.

	The direction of the current vector		
Case	(100)	(110)	(111)
(A)	$\frac{1}{3}(2+r^{3/4})$	$\frac{1}{3}$ {1 +2 [$\frac{1}{2}$ (r +1)] ^{3/4} }	$[\frac{1}{3}(r+2)]^{3/4}$
(<i>B</i>)	$\frac{1}{3}\left\{1+2\left[\frac{1}{2}(r+1)\right]^{3/4}\right\}$	$\frac{1}{6} \{1 + r^{3/4} + 4 [\frac{1}{4}(r+3)]^{3/4} \}$	$\frac{1}{2}$ {1+[$\frac{1}{3}$ (2r+1)] ^{3/4} }
(C)	$[\frac{1}{3}(r+2)]^{3/4}$	$\frac{1}{2}$ {1 + [$\frac{1}{3}$ (2r + 1)] ^{3/4} }	$\frac{1}{4}$ { $r^{3/4}$ +3[(r +8)/9] ^{3/4} }

¹² M. Shibuya, Phys. Rev. 95, 1385 (1954).

Here μ is the weak field conductivity mobility defined by

$$\mu = \frac{2(2\pi)^{\frac{3}{2}} e\hbar^4 M C_l^2}{3E_d^2 (kT)^{\frac{3}{2}} \sqrt{\Delta}} \left(\frac{\mathrm{Trace}\mathfrak{M}^{-1}}{3}\right) \frac{1}{(1+2b\delta+c\delta^2)}, \quad (11)$$

and p is defined by

$$p = \frac{3\pi}{16} \left(\frac{\mu}{C_{l}}\right)^{2} \left(\frac{1+2b\delta+c\delta^{2}}{1+2a\delta+a\delta^{2}}\right) \left(\frac{3}{\operatorname{Trace}\mathfrak{M}^{-1}}\right)^{2} \times \left(\frac{3}{\operatorname{Trace}\mathfrak{M}}\right) F \cdot \mathfrak{M}^{-1} \cdot F. \quad (12)$$

Here Δ is the determinant of the mass tensor and the three constants *a*, *b*, and *c* are functions of *r* and *C* given by

$$a = 1/(2r+1),$$
 (13)

$$b = \frac{1}{3} \left\{ \frac{2(\sqrt{r+3})}{3(\sqrt{r+1})^3} + \frac{2r^2 \ln r}{(r-1)^3} - \frac{(3r-1)}{(r-1)^2} \right\},\tag{14}$$

$$c = Cb + \frac{(1-C)}{3} \left[\frac{2}{(\sqrt{r+1})^4} + \frac{(2r^2 + 5r - 1)}{(r-1)^3} - \frac{6r^2 \ln r}{(r-1)^4} \right].$$
 (15)

In order to discuss the hot-electron problem in actual crystals such as Ge and Si, we must consider the several spheroids in the Brillouin zone and sum up each current density (10) of these spheroids. Three special cases are considered: Case (A): 6 (or 3) spheroids along the cubic axes, Case (B): 12 spheroids along the face-diagonal axes, Case (C): 8 (or 4) spheroids along the body-diagonal axes.

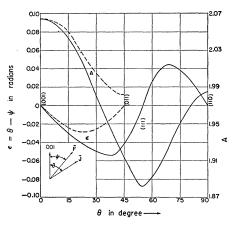


FIG. 2. A and ϵ versus θ in Case (C) with r=0.06. Here $\epsilon=\theta-\psi$; θ and ψ are the polar angles with respect to the Z-axis of current and field vectors respectively. For full curves these vectors are lying in the X=V plane and for broken curves they are lying in the X=0 plane.

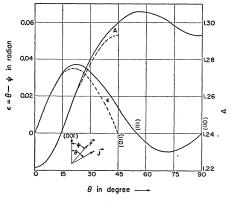


FIG. 3. A and ϵ versus θ in Case (A) with r=0.2.

The total current density J_T is given in each case by

$$\mathbf{J}_{T} = \frac{Ne\mu\pi}{2^{5/4}\Gamma(3/4)} \left(\frac{3}{\mathrm{Trace}\mathfrak{M}^{-1}}\right) \frac{1}{n} \sum_{i=1}^{n} p_{i}^{-\frac{1}{4}}\mathfrak{M}_{i}^{-1} \cdot \mathbf{F}, \quad (16)$$

where N is the total carrier density and n is the number of spheroids. Here p_i is a function of the electric field vector and of the direction of the rotational axis of the *i*th spheroid. Two factors A and S already introduced in Eq. (2) are derived from Eq. (16):

$$S = \left\{ \frac{1 + 2a\delta + a\delta^2}{1 + 2b\delta + c\delta^2} \right\}^{\frac{1}{2}},\tag{17}$$

$$A = A_1 \frac{3}{(r+2)} \left(\frac{2r+1}{3r}\right)^{\frac{1}{2}}.$$
 (18)

Here A_1 is dependent not only upon r but also upon both the spheroid arrangement and the direction of the current vector. In Table I, expressions for $\sqrt{A_1}$ are listed for the cases in which the current vector is directed along three symmetry axes of the cubic crystal. In Fig. 1, three S curves are plotted as a function of δ for r=0.04, 1 and 9, where we use 0.431 as the value of C. The anisotropy factor A and the deviation angle ϵ between the current and field vectors are the measures of the anisotropy in the hot-electron problem. They are plotted as functions of the direction of the current vector in Figs. 2 and 3, for n-type Ge and Si, respectively. In Fig. 2 we use the arrangement (C) with r = 0.2. Two special cases are considered in these figures: For broken curves we let the current vector lie in the X=0plane; the field vector then makes an angle ϵ with the current vector and lies in the same plane. For full curves both current and field vectors lie in the X = Yplane.

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