# **Piezoelectric Scattering in Semiconductors**\*

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The theory of the scattering of electrons by acoustic modes in piezoelectric semiconductors is generalized so as to properly take account of the anisotropic scattering probability. The Herring-Vogt approximate solution to the Boltzmann equation is used, which is accurate if the resulting relaxation-time tensor components do not differ by more than a factor of two or so. The other main simplifying assumption consists of treating the frequencies and polarizations of the acoustic modes by a simple approximation. The theory is applied to three symmetry classes of known piezoelectric semiconductors : zincblende and wurtzite symmetry (as typified by the III-V and II-VI compounds) and  $\alpha$ -quartz symmetry (as typified by selenium and tellurium). The electron mobility anisotropy calculated for CdS (based on the measured electroelastic properties and cyclotronresonance masses) agrees quite well with the value deduced from experiment.

#### INTRODUCTION

**PIEZOELECTRIC** scattering was first discussed by Meijer and Polder<sup>1</sup> who estimated the magnitude of the relaxation time for piezoelectric scattering in crystals with zincblende symmetry. They found that the piezoelectric mobility depends only weakly on temperature  $(\mu \sim T^{-1/2})$  which implies that piezoelectric scattering should dominate deformation potential scattering  $(\mu \sim T^{-3/2})$  at low enough temperatures in crystals having the piezoelectric effect. The calculation of Meijer and Polder was approximate in that at the onset they took a weighted average of the piezoelectric constants appropriate to phonons traveling in the  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ , and  $\langle 111 \rangle$  directions. Harrison<sup>2</sup> found the relaxation times for electrons traveling in these directions and then performed the weighted average. More recently, Hutson<sup>3</sup> applied the theory to crystals having wurtzite symmetry. In his calculation he took a spherical average of the piezoelectric constants before calculating the relaxation time.

The purpose of this paper is to calculate the relaxation time tensor for piezoelectric scattering in crystals with zincblende symmetry (as typified by the III-V compounds and by the cubic II-VI compounds), wurtzite symmetry (as typified by the hexagonal II-VI compounds), and  $\alpha$ -quartz symmetry (as typified by selenium and tellurium), assuming ellipsoidal energy surfaces. The anisotropies of the scattering probability and the effective mass are treated by the method which Herring and Vogt<sup>4</sup> used for deformation potential scattering.

#### GENERAL THEORY

The present paper applies to the scattering of electrons (or holes) in a simple single-valley or simple many-valley semiconductor. We shall restrict our discussion to scattering events within a particular valley and shall choose our coordinate system so that the effective mass tensor of the valley is diagonal. Thus, the energy of an electron is given in terms of the components of its propagation vector **k**, as follows:

$$\mathcal{E} = \frac{\hbar^2}{2} \left( \frac{k_1^2}{m_1} + \frac{k_2^2}{m_2} + \frac{k_3^2}{m_3} \right), \qquad (1)$$

where  $m_1$ ,  $m_2$ , and  $m_3$  are the diagonal components of the effective mass tensor.

We are concerned with the interaction of the electrons with the long wavelength acoustic modes, i.e., the normal modes of the crystal for which the atoms in the same primitive cell move in the same direction in phase with each other (physically, this is the same motion undergone by the crystal during the measurement of the elastic and piezoelectric properties). There will, in general, be three such normal modes for a given direction of propagation, corresponding to the three degrees of freedom of the primitive cell as a whole. In general, the normal modes will be neither purely transverse nor purely longitudinal and will propagate with different velocities. The theory of elastic wave propagation in piezoelectric crystals, as discussed for example, by Kyame<sup>5</sup> and by Hutson and White,<sup>6</sup> is fundamental in setting up the problem.

Let  $x_1'$ ,  $x_2'$ , and  $x_3'$  be an arbitrary set of Cartesian coordinates which we shall call the "phonon coordinate system" rotated with respect to  $x_1$ ,  $x_2$ , and  $x_3$ , the coordinate system which diagonalizes the mass tensor, and let us consider a long wavelength acoustic normal mode (i.e., an elastic wave) propagating along the 3'axis with wave vector  $\boldsymbol{\sigma}$ , frequency  $\omega_{\alpha}(\boldsymbol{\sigma})$ , and amplitude  $U_0^{\sigma,\alpha}$ , where  $\alpha = 1, 2$ , or 3 labels the three normal modes having the same  $\sigma$ . The displacement of the lattice from its equilibrium position is then a plane wave which we may write in the form:

$$U_{j^{\sigma,\alpha}} = U_{0j^{\sigma,\alpha}} \cos(\sigma x_{3}' - \omega_{\alpha} t), \quad j = 1, 2, 3; \quad (2)$$

where  $U_{0j}^{\alpha}$  are the components of  $\mathbf{U}_{0}^{\sigma,\alpha}$  in the phonon coordinate system (the primed system). By the nature

<sup>6</sup> J. J. Kyame, J. Acoust. Soc. Am. 21, 159 (1949). <sup>6</sup> A. R. Hutson and D. L. White, J. Appl. Phys. 33, 40 (1962).

<sup>\*</sup> Some of the results of this work were described previously; see D. Zook, Bull. Am. Phys. Soc. II 9, 274 (1964). <sup>1</sup> H. J. G. Meijer and D. Polder, Physica 19, 255 (1953).

<sup>&</sup>lt;sup>2</sup> W. A. Harrison, thesis, Physica Department, University of Illinois, 1956 (unpublished); and Phys. Rev. 101, 903 (L) (1956).
<sup>3</sup> A. R. Hutson, J. Appl. Phys. (Suppl.) 32, 2287 (1961).
<sup>4</sup> C. Herring and E. Vogt, Phys. Rev. 101, 944 (1956).

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of the plane wave there are three nonzero strain components in the phonon coordinate system:

$$S_{j3}{}^{\sigma,\alpha} = \partial U_{j}{}^{\sigma,\alpha} / \partial x_{3}{}' = -\sigma U_{0j}{}^{\sigma,\alpha} \sin(\sigma x_{3}{}' - \omega_{\alpha} t), \quad (3)$$

where  $S_{i3}$  are the components of the strain tensor S.<sup>7</sup>

Since piezoelectric scattering will usually be important only in high-purity crystals, we will assume that currents can be neglected (high resistivity) and can therefore set the electric displacement **D** equal to a constant<sup>6</sup> (e.g., zero). Our theory will be valid in the low carrier concentration limit (screening effects must be included at higher concentrations<sup>3</sup>) and the electric field **E** is the fundamental dependent electrical variable. It is convenient to write the piezoelectric equations of state in the form<sup>8</sup>:

$$\mathbf{E} = -h\mathbf{S}$$
$$\mathbf{T} = \boldsymbol{c}^{D}\mathbf{S} \tag{4}$$

where  $\mathbf{T}$  is the stress,  $\boldsymbol{h}$  is the piezoelectric tensor, and  $c^{D}$  is the elastic stiffness tensor at constant displacement (we shall hereafter omit the superscript on  $c^{D}$ ). The electric field is, in terms of its components in the phonon coordinate system:

$$E_{i^{\sigma,\alpha}} = \sigma h_{ij3}' U_{0j^{\sigma,\alpha}} \sin(\sigma x_3' - \omega_{\alpha} t), \qquad (5)$$

where the summation convention is followed, and the prime means the piezoelectric tensor components are in the phonon coordinate system. It has been shown<sup>6</sup> that the longitudinal electric field  $E_3$  is much larger than the transverse fields  $E_1$  and  $E_2$ , and  $E_3$  is derivable from the potential

$$\varphi_{\sigma,\alpha} = h_{3j3}' U_{0j}^{\sigma,\alpha} \cos(\sigma x_3' - \omega_\alpha t) = h_{3j3}' U_j^{\sigma,\alpha}. \tag{6}$$

We need to find  $W_{\alpha}(\mathbf{k},\mathbf{k}^{S})$ , the probability per unit time and per unit volume of  $\mathbf{k}$  space that an electron with propagation vector  $\mathbf{k}$  will be scattered by the elastic wave to a volume  $d^{3}k^{S}$  centered on  $\mathbf{k}^{S}$ . Assuming that the perturbation energy  $e_0\varphi_{\sigma,\alpha}$  is small ( $e_0$  is the electron charge) we can use the usual formula from time-dependent perturbation theory:

$$W_{\alpha}(\mathbf{k},\mathbf{k}^{S}) = \left(\frac{2\pi}{\hbar}\right) \frac{V}{8\pi^{3}} |\langle \mathbf{k}^{S} | e_{0}\varphi_{\sigma,\alpha} | \mathbf{k} \rangle|^{2} \\ \times \delta [\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}^{S}) \pm \hbar\omega_{\alpha}] \\ \equiv W_{\alpha}^{0}(\mathbf{k},\mathbf{k}^{S}) \delta [\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}^{S}) \pm \hbar\omega_{\alpha}], \quad (7)$$

where  $V/8\pi^3$  is the number of final states per unit volume of  $\mathbf{k}^{s}$  space and V is the crystal volume.

The matrix elements  $\langle \mathbf{k}^{S} | e_{0} \varphi_{\sigma, \alpha} | \mathbf{k} \rangle$  can be calculated using plane waves for the electron wave functions. The result is

$$\langle \mathbf{k}^{S} | e_{0} \varphi_{\sigma, \alpha} | \mathbf{k} \rangle = \frac{1}{2} e_{0} h_{3j3}' U_{0j}^{\sigma, \alpha}, \qquad (8)$$

where  $\mathbf{k}^{s}$  must equal  $\mathbf{k} \pm \mathbf{\sigma}$ , the usual selection rule for phonon emission or absorption.

The amplitudes  $U_0^{\sigma,\alpha}$  at any temperature  $T_0$  can be obtained by setting the potential energy  $(\frac{1}{2}\mathbf{S}\cdot\mathbf{T}$  integrated over the crystal) associated with the elastic wave equal to one-half the average energy as given by the Bose-Einstein distribution<sup>9</sup>:

$$(V/2)\sigma^2 U_{0i}{}^{\sigma,\alpha} U_{0j}{}^{\sigma,\alpha} c_{i3j3} \cong k_0 T_0, \qquad (9)$$

where  $k_0$  is Boltzmann's constant and the approximation holds at temperatures such that  $k_0 T_0 \gg \hbar \omega_{\alpha}$  (a condition satisfied in most nondegenerate semiconductors above a few degrees Kelvin).

If the elastic anisotropy of the crystal is not too large,  $c_{i_{3}j_{3}}'$  will be approximately diagonal,<sup>10</sup> and the normal modes will lie approximately along the axes of the phonon coordinate system (if the 1' and 2' directions are chosen properly<sup>11</sup>). To first order in the elastic anisotropy we can write:

$$U_{0j}{}^{\sigma,\alpha} = U_0{}^{\sigma,\alpha}\delta_{j\alpha}, c_{i3\alpha3}{}' = c_{\alpha3\alpha3}{}'\delta_{i\alpha},$$
(10)

where  $\alpha = 3$  denotes the mainly longitudinal mode and  $\alpha = 1,2$  denote the mainly transverse modes. To this approximation we can write the squares of the matrix elements as:

$$|\langle \mathbf{k}^{S} | e_{0} \varphi_{\sigma,\alpha} | \mathbf{k} \rangle|^{2} = e_{0}^{2} k_{0} T_{0} (h_{3\alpha 3}')^{2} / \sigma^{2} c_{\alpha 3\alpha 3}', \quad (11)$$

which also includes a factor of 2 due to adding the matrix elements squared for both absorption and emission of phonons. The directional dependence of  $c_{\alpha 3\alpha 3}$  is much less pronounced than that of  $h_{3\alpha 3}$  since, for example, some or all of the components of the piezoelectric tensor will vanish for  $\sigma$  along a symmetry axis. We shall therefore use spherical averages<sup>12</sup> of the stiffness coefficients, i.e., we shall replace  $c_{3333}'$  by  $\langle c_{3333}' \rangle = c_l$ , and we shall replace both  $c_{1313}'$  and  $c_{2323}'$  by  $\frac{1}{2}\langle c_{1313}'+c_{2323}'\rangle=c_t$ , where the angular brackets denote spherical averages. These replacements are not essential but result in simpler expressions for the relaxation times. In the closely related case of deformation potential scattering, the expressions for  $\tau$  are not particularly sensitive to the elastic anisotropy, and average elastic constants can be used with little loss in accuracy.<sup>4,13</sup>

Methods for calculating the components of a tensor relaxation time have been given by Herring and Vogt<sup>4</sup>

 <sup>&</sup>lt;sup>7</sup> See, for example, Ref. 5.
 <sup>8</sup> Standards on Piezoelectric Crystals, Proc. IRE 37, 1378 (1949).

<sup>&</sup>lt;sup>9</sup> R. A. Smith, *Wave Mechanics of Crystalline Solids* (Chapman and Hall, Ltd., London, 1961), p. 421. <sup>10</sup> J. R. Neighbours and C. S. Smith, J. Appl. Phys. 21, 1338

<sup>(1950).</sup> 

<sup>&</sup>lt;sup>11</sup> Degenerate perturbation methods can be used to calculate the frequencies and polarization directions of the normal modes. In this paper the two transverse modes are averaged together (except for wurzite symmetry where this is not necessary) so that in this approximation the directions of the 1' and 2' axes are

that in this approximation the directions of the 1' and 2' axes are arbitrary. <sup>12</sup> Spherical averaging yields average elastic constants for germanium and silicon very close (less than 2% difference) to the averages calculated by A. G. Samoilovich and V. D. Iskra, Fiz. Tverd. Tela 2, 2827 (1960) [English transl.: Soviet Phys.— Solid State 2, 2517 (1961)]. <sup>13</sup> A. G. Samoilovich, I. Ya. Korenblit, I. V. Dakhovskii, and V. D. Iskra, Fiz. Tverd. Tela 3, 3285 (1961) [English transl.: Soviet Phys.—Solid State 3, 2385 (1962)].

and by Samoilovich et al.,14 whose first-order result for ellipsoids of revolution agrees with Herring and Vogt. The Herring-Vogt formula can be written in the form (see Appendix):

$$\frac{1}{\tau_{ii}} = \frac{3}{4} \frac{(2m_1m_2m_3\,\varepsilon)^{1/2}}{\hbar^3} \int \frac{q_i^2}{q} W^0(\mathbf{k},\mathbf{k}^S) d^3q \,, \quad (12)$$

where **q** is the phonon propagation vector  $\boldsymbol{\sigma}$  in a coordinate system chosen so that the energy surfaces become spheres of unit radius and the integration is over a sphere of radius two. The components of q in the ellipsoid (unprimed) coordinate system are given by:

$$q_{i} = \hbar \sigma_{i} / (2m_{i} \varepsilon)^{1/2} = \hbar (k_{i} - k_{i}^{S}) / (2m_{i} \varepsilon)^{1/2}, \quad (13)$$

where  $\sigma_i$  are the components of  $\sigma$  in the ellipsoid coordinate system. Equation (12) is valid only if the scattering is not too anisotropic, since it is based on retaining only the leading term in an expansion of the distribution function in spherical harmonics.4,14

The total transition probability  $W(\mathbf{k}, \mathbf{k}^{S})$  consists of the sum of the probabilities for the three modes with different polarizations. Since we use an average of the stiffness coefficients for the two transverse modes, we can combine the transverse modes and write:

$$\frac{1}{\mu_{ii}{}^{t}} = \frac{m_{i}}{e_{0}\tau_{ii}{}^{t}} = \frac{3}{8\pi} \frac{m_{i}}{A_{t}} \int \frac{q_{i}{}^{2}}{q} \frac{h_{313}{}^{\prime 2} + h_{323}{}^{\prime 2}}{m_{1}q_{1}{}^{2} + m_{2}q_{2}{}^{2} + m_{3}q_{3}{}^{2}} d^{3}q \quad (14a)$$

for the transverse modes, and

$$\frac{1}{\mu_{ii}{}^{l}} = \frac{m_{i}}{e_{0}\tau_{ii}{}^{l}} = \frac{3}{8\pi} \frac{m_{i}}{A_{l}} \int \frac{q_{i}{}^{2}}{q} \frac{h_{333}{}^{\prime 2}}{m_{1}q_{1}{}^{2} + m_{2}q_{2}{}^{2} + m_{3}q_{3}{}^{2}} d^{3}q \quad (14b)$$

for the longitudinal modes, where

$$\frac{1}{A_{t,l}} = \frac{e_0 k_0 T_0}{4\pi \hbar^2 c_{t,l}} \left(\frac{2m_1 m_2 m_3}{\varepsilon}\right)^{1/2}.$$
 (15)

The two mobilities are then combined by adding reciprocals to give the reciprocal of the mobility due to scattering by both types of modes.

The mobilities given above depend on energy through the factor  $A(\varepsilon)$  and must be averaged over the energy spectrum of the entire electron population. For Maxwell-Boltzmann statistics<sup>3,15</sup> we replace  $\mu(\varepsilon)$  by  $\mu((64/9\pi)k_0T_0)$  since  $\mu \sim \varepsilon^{1/2}$ . We can then write a convenient form for the average value of A (in mksa units):

$$A_{t,l}\left(\frac{64}{9\pi}k_0T_0\right) = 3.274 \times 10^7 c_{t,l}\left(\frac{m_0}{m^*}\right)^{3/2} \left(\frac{77}{T_0}\right)^{1/2}, \quad (16)$$

where  $m^* = (m_1 m_2 m_3)^{1/3}$  is the density-of-states mass for a single ellipsoid and  $T_0$  is in degrees Kelvin. In the equations that follow, the ratio  $A/\mu$  is energy inde-

pendent, so that if an energy-dependent mobility is desired, Eq. (15) is to be used, while if mobility averaged over all energies for classical statistics is desired, Eq. (16) is to be used for A.

The integration over the magnitude of q in Eq. (14) can be carried out immediately, giving a factor of 2. The integration over solid angle can be simplified in the case of energy ellipsoids of revolution  $(m_1 = m_2)$  and we can express the solid angle  $d\Omega_q$  in terms of  $d\Omega_q$ , a more convenient variable of integration. Making the substitution, we obtain:

$$\frac{A_{t}}{\mu_{ii}^{t}} = \frac{3}{4\pi} \left(\frac{m_{1}}{m_{3}}\right)^{1/2} \int \left(\frac{\sigma_{i}}{\sigma}\right)^{2} \left[1 + \frac{m_{1} - m_{3}}{m_{3}} \left(\frac{\sigma_{3}}{\sigma}\right)^{2}\right]^{-3/2} \times (h_{313}'^{2} + h_{323}'^{2}) d\Omega_{\sigma}, \quad (17a)$$

and

$$\frac{A_{l}}{\mu_{ii}^{l}} = \frac{3}{4\pi} \left(\frac{m_{1}}{m_{3}}\right)^{1/2} \int \left(\frac{\sigma_{i}}{\sigma}\right)^{2} \left[1 + \frac{m_{1} - m_{3}}{m_{3}} \left(\frac{\sigma_{3}}{\sigma}\right)^{2}\right]^{-3/2} \times h_{333}{}^{\prime 2} d\Omega_{\sigma}. \quad (17b)$$

Note that if  $m_3 = m_1$  and if  $h^2$  does not depend on direction (or if an average value of  $h^2$  is used), then the mobility is equal to A divided by  $h^2$ .

The remaining problem is that of expressing the piezoelectric constants  $h_{3\alpha3}'$  in terms of the direction cosines of  $\sigma$ , i.e.,  $\sigma_i/\sigma$ . In general, the piezoelectric constants in the phonon coordinate system will be given by:

$$h_{3\alpha3}' = a_{3i}a_{\alpha j}a_{3k}h_{ijk}, \qquad (18)$$

where the  $a_{ij}$  are the components of the rotation matrix which take vectors in the unprimed system into vectors in the primed system, and  $h_{ijk}$  are the piezoelectric constants in the ellipsoid (unprimed) coordinate system. The 3' axis is defined to be along  $\sigma$  with the 1' and 2' axes arbitrary<sup>11</sup>; we now choose the 2' axis to be in the (1,2) plane<sup>16</sup> so that we can write the transformation matrix in the following ways:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \cos\vartheta \cos\varphi & \cos\vartheta \sin\varphi & -\sin\vartheta \\ -\sin\varphi & \cos\varphi & 0 \\ \sin\vartheta \cos\varphi & \sin\vartheta \sin\varphi & \cos\vartheta \end{bmatrix}$$
$$= \begin{bmatrix} \frac{\sigma_1\sigma_3}{\sigma\sigma_1} & \frac{\sigma_2\sigma_3}{\sigma\sigma_1} & \frac{\sigma_1}{\sigma} \\ -\frac{\sigma_2}{\sigma_1} & \frac{\sigma_1}{\sigma_1} & 0 \\ \frac{\sigma_1}{\sigma} & \frac{\sigma_2}{\sigma} & \frac{\sigma_3}{\sigma} \end{bmatrix}, \quad (19)$$

 <sup>&</sup>lt;sup>14</sup> A. G. Samoilovich, I. Va. Korenblit, I. V. Dakhovskii and V. D. Iskra, Fiz. Tverd. Tela 3, 2939 (1961) [English transl.: Soviet Phys.—Solid State 3, 2148 (1962)].
 <sup>15</sup> See, for example, Ref. 9, p. 324.

<sup>&</sup>lt;sup>16</sup> For wurtzite symmetry this choice of coordinates is such that normal lattice modes lie nearly along the 1' and 2' axes and only one of the transverse modes has a piezoelectric effect associated is the transverse modes. with it [see Eq. (30)].

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where  $\sigma_1 = (\sigma_1^2 + \sigma_2^2)^{1/2}$  and  $(\vartheta, \varphi, \sigma)$  are the polar coordinates of  $\sigma$ . The integration of (17) is therefore over  $\vartheta$  and  $\varphi$  and is quite simple. The integration over  $\varphi$  is of the form

$$\int_0^{2\pi} \sin^n \varphi \, \cos^m \varphi d\, \varphi$$

with n and m integers, and it is not hard to show that the integrations over  $\vartheta$  can always be written in terms of the quantities:

$$I_{n} = \frac{1}{2} \left( \frac{m_{1}}{m_{3}} \right)^{1/2} \int_{0}^{\pi} \frac{\cos^{n}\vartheta \sin\vartheta d\vartheta}{\{1 + \left[ (m_{1} - m_{3})/m_{3} \right] \cos^{2}\vartheta \}^{3/2}}$$
(20a)

$$=\frac{(\alpha^2+1)^{1/2}}{\alpha^3}\int_0^1\frac{z^ndz}{(\alpha^{-2}+z^2)^{3/2}}$$
(20b)

$$=\frac{\beta^{2}+1}{\beta^{3}}\int_{0}^{1}\frac{z^{n}dz}{\{[(\beta^{2}+1)/\beta^{2}]-z^{2}\}^{3/2}}$$
(20c)

where n=0, 2, 4, 6, or 8;  $\alpha^2 = (m_1 - m_3)/m_3$ ; and  $\beta^2 = (m_3 - m_1)/m_1$ . Equation (20b) is the convenient form for oblate ellipsoids, while (20c) is convenient for prolate ellipsoids. In either case the integrals can be found in a standard table of integrals,<sup>17</sup> and in the case of isotropic mass they reduce simply to  $I_n = 1/(n+1)$ .

#### APPLICATION TO CRYSTALS WITH ZINCBLENDE SYMMETRY AND [000] OR [100]-TYPE VALLEYS

In the case of zincblende symmetry (point group  $\bar{4}3m$ ) there is only one independent piezoelectric constant in the cubic crystal coordinate system<sup>18</sup> with axes along the fourfold axes. For energy minima at points along the cube axes of reciprocal space ( $\Delta$  points), the effective mass tensor is diagonal in the crystal coordinate system and two of the diagonal components are equal. At the center of the Brillouin zone (a  $\Gamma$  point) all three effective mass tensor components are equal. In either case the ellipsoid coordinate system is the same as the crystal coordinate system and the piezoelectric tensor is of the form<sup>18</sup>:

$$\boldsymbol{h} = \begin{bmatrix} 0 & 0 & 0 & h_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{14} \end{bmatrix}, \quad (21)$$

where we use the two subscript notation for piezoelectric tensor components in the crystal coordinate system.

Although we could express the piezoelectric tensor components in the primed coordinate system using Eq. (18) directly, in practice it is more convenient to use

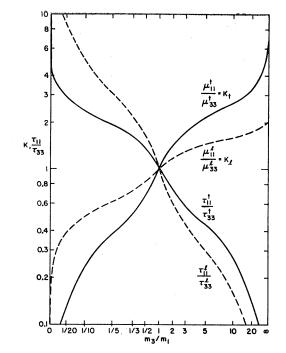


FIG. 1. The mobility and relaxation-time tensor anisotropy as functions of the mass anisotropy for piezoelectric scattering in crystals with zincblende symmetry and [100]-type valleys. The subscripts refer to the directions of the principal axes of an energy ellipsoid (the "3" direction is along the axis of revolution), while *t* and *l* refer to scattering by the mainly longitudinal and mainly transverse modes.

the tables of Hearmon.<sup>19</sup> From Hearmon's tables 3 and 4 and our rotation matrix, Eq. (19), we obtain

$$h_{333}' = 6h_{14}(\sigma_1 \sigma_2 \sigma_3 / \sigma^3), h_{323}' = 2h_{14}[\sigma_3(\sigma_1^2 - \sigma_2^2) / \sigma_1^2], h_{313}' = 2h_{14}[\sigma_1 \sigma_2(2\sigma_3^2 - \sigma_1^2) / \sigma_1^3].$$

$$(22)$$

When the transverse modes are combined, the squares of the piezoelectric constants are given by

$$h_{333}'^{2} = 36h_{14}^{2}(\sigma_{1}^{2}\sigma_{2}^{2}\sigma_{3}^{2}/\sigma^{6}),$$

$$h_{313}'^{2} + h_{323}'^{2} = 4h_{14}^{2}[(\sigma_{2}^{2}\sigma_{3}^{2} + \sigma_{1}^{2}\sigma_{3}^{2} + \sigma_{1}^{2}\sigma_{2}^{2})/\sigma^{4}] - h_{333}'^{2},$$
(23)

which exhibit the cubic symmetry.

The integration of Eq. (17) can be written in terms of the differences of the  $I_n$  integrals:

$$A_{t}/\mu_{33}^{t} = \frac{3}{2}h_{14}^{2}\{(I_{2}-I_{4})-2(I_{4}-I_{6})+9(I_{6}-I_{8})\},$$
  
$$A_{t}/\mu_{11}^{t} = \frac{3}{4}h_{14}^{2}\{(I_{0}-I_{2})-3(I_{2}-I_{4})+11(I_{4}-I_{6})$$

$$A_{l}/\mu_{33}^{l} = \frac{27}{2} h_{14}^{2} \{ (I_{4} - I_{6}) - (I_{6} - I_{8}) \}, \qquad (24)$$

$$A_{1}/\mu_{33}^{l} = \frac{27}{4}h_{14}^{2}\{(I_{2}-I_{4})-2(I_{4}-I_{6})+(I_{6}-I_{8})\}.$$

<sup>19</sup> R. F. S. Hearmon, Acta Cryst. 10, 121 (1957).

<sup>&</sup>lt;sup>17</sup> For example, H. B. Dwight, Tables of Integrals and Other Mathematical Data (The Macmillan Company, New York, 1947). <sup>18</sup> W. P. Mason, Piezoelectric Crystals and Their Application to Ultrasonics (D. Van Nostrand Company, Inc., New York, 1950), p. 40.

The reduction formulas for integrals of binomial differentials<sup>17</sup> (integration by parts) can be used to show that the  $I_n$  integrals obey the recurrence relation:

$$I_{n} - I_{n+2} = \frac{\beta^{2} + 1}{n\beta^{2}} \left[ 1 + \frac{\beta^{2} + n + 1}{\beta^{2} + 1} I_{n} \right]$$
(25a)

$$= (n\alpha^2)^{-1} [-1 + (n\alpha^2 + n + 1)I_n], \quad (25b)$$

which are the convenient forms for prolate and oblate ellipsoids, respectively.

The mobility anisotropy  $K = \mu_{11}/\mu_{33}$  and the  $\tau$ -tensor anisotropy  $\tau_{11}/\tau_{33}$  are plotted in Fig. 1 for the longitudinal and transverse modes as functions of the mass anisotropy. In both the oblate and prolate cases the scattering becomes anisotropic quite rapidly as the mass anisotropy is increased. As mentioned above. when the scattering is too anisotropic Eq. (12) can no longer be used with confidence, and the curves are extended to this region only to show the qualitative features of the scattering. The error incurred by the use of Eq. (12) has not been investigated but could be determined by calculating higher-order terms using the equation of Samoilovich et al.<sup>13,14</sup> At any rate, the error should not be appreciable if  $\tau_{11}$  and  $\tau_{33}$  differ by less than a factor of two.<sup>4</sup>

The magnitude of the scattering is also dependent on the mass anisotropy as shown in Fig. 2. The important point is that the average mobility

$$\bar{\mu} = \frac{1}{3}(2\mu_{11} + \mu_{33})$$

. . .

is only weakly dependent on the mass ratio, so that the isotropic formulas can be used to estimate the magnitude of the piezoelectric mobility in a crystal if the density-of-states mass of a single valley is known, even if the mass anisotropy is not known. In the isotropic case the mobilities are simply given by

$$A_t/\mu_{ii}^t = (16/35)h_{14}^2,$$
  

$$A_t/\mu_{ii}^l = (12/35)h_{14}^2.$$
(26)

These values are also obtained if one takes a spherical average of the piezoelectric constants at the onset [using Eq. (23)], and they are quite close to the values estimated by Harrison,<sup>2</sup> who calculated a relaxation time for an electron along the (100), (110), and (111)directions using the method of Herring<sup>20</sup> and Brooks<sup>21</sup> and to the values estimated by Meijer and Polder<sup>1</sup> who took averages of the piezoelectric constants along the (100), (110), and (111) directions (see discussion section below).

The mobilities for the longitudinal and transverse modes must be combined by adding reciprocals to give

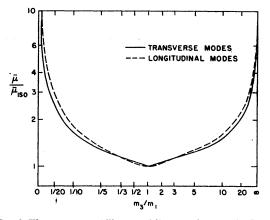


FIG. 2. The average mobility  $\overline{\mu}_a = \frac{1}{3}(2\mu_{11} + \mu_{33})$  normalized to the isotropic  $(m_1 = m_3)$  mobility for piezoelectric scattering in crystals with zincblende symmetry and (100)-type valleys.

the total mobility. Because the longitudinal modes are stiffer than the transverse modes (larger sound velocity), the transverse modes usually dominate the scattering. The stiffness coefficients in the phonon coordinate system are given by<sup>10,19</sup>

$$c_{3333}' = c_{11} + 2c^* \Gamma(\mathbf{\sigma}),$$
  
$$\frac{1}{2} (c_{1313}' + c_{2323}') = c_{44} - c^* \Gamma(\mathbf{\sigma}), \qquad (27)$$

where and

$$\Gamma(\boldsymbol{\sigma}) = (\sigma_2^2 \sigma_3^2 + \sigma_3^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2) / \sigma^4$$

 $c^* = 2c_{44} + c_{12} - c_{11},$ 

The spherical average of  $\Gamma$  is  $\frac{1}{5}$ , so that

$$c_{l} = c_{11} + \frac{2}{5}c^{*}$$

$$c_{t} = c_{44} - \frac{1}{5}c^{*}.$$
(28)

Except for an effective mass factor, the numerical value of the piezoelectric mobility can be calculated for GaAs, ZnŠ, ZnTe, ZnSe, and CdTe, whose piezo-electric constants  $^{6,22-25}$  and elastic constants  $^{25,26}$  have been recently measured. We assume an isotropic effective mass  $m^*$ , and combine Eqs. (16), (26), and (28). The relevant parameters derived from the measurements are summarized in Table I, along with the calculated piezoelectric mobility at 77°K. The mobility at other temperatures can be obtained from the  $T^{-1/2}$ dependence. Cyclotron resonance of electrons in GaAs<sup>27</sup> and CdTe<sup>28</sup> indicates that the energy surfaces are spherical<sup>29</sup> with the effective masses given in Table I.

<sup>&</sup>lt;sup>20</sup> C. Herring, Bell system Tech. J. 34, 237 (1955), Appendix A. (The formula for  $\tau(\mathbf{k})$  is not written out explicitly but is described is the basis for calculations of deformation potential scattering. These calculations disagree with the later ones of Ref. 4.

<sup>&</sup>lt;sup>21</sup> H. Brooks, Advan. Electron. Electron Phys. 7, 85 (1957), Eq. 6.21.

 <sup>&</sup>lt;sup>22</sup> H. Kaplan and J. L. Sullivan, Phys. Rev. 130, 120 (1963).
 <sup>23</sup> E. J. Charlson and G. Mott, Proc. IEEE 51, 1239 (1963).
 <sup>24</sup> M. Zerbst and H. Boroffka, Z. Naturforsch. 18a, 642 (1963).
 <sup>25</sup> D. Berlincourt, H. Jaffe, and L. R. Shiozawa, Phys. Rev.

 <sup>129, 1009 (1963).
 &</sup>lt;sup>26</sup> T. B. Bateman, H. J. McSkimin, and J. M. Whelan, J. Appl.

Phys. 30, 544 (1959).
 <sup>27</sup> E. D. Palik, S. Teitler, and R. F. Wallis, J. Appl. Phys. (Suppl.) 32, 2132 (1961).
 <sup>28</sup> K. K. Kanazawa, Bull. Am. Phys. Soc. 8, 620 (1963).

<sup>&</sup>lt;sup>29</sup> For a review of other band structure data, see, for example, D. Long, J. Appl. Phys. 33, 1682 (1962).

Units	h <sub>14</sub> (Ref.) 10 <sup>9</sup> V/M	$c_l$ (Ref.) $10^{10} N/M^2$	$c_t$ (Ref.) $10^{10} N/M^2$	$\frac{m^*}{m_0}$ (Ref.)	μ at 77°K M²/VS
GaAs (~300°K)	$ \begin{array}{c} \approx 1.2 & (6,22) \\ 1.57 & (23) \\ 1.57^{a} & (24) \end{array} $	14.03 (26)	4.86 (26)	0.071 (27)	77 <sup>b</sup>
ZnS (77°K)	2.26 (25)	12.89 (25)	3.60 (25)		$0.42\left(\frac{m_0}{m^*}\right)^{3/2}$
ZnTe (298°K)	0.314 (25)	8.41 (25)	2.48 (25)		$14.8 \left(\frac{m_0}{m^*}\right)^{3/2}$
ZnSe (298°K)	0.61 (25)	10.34 (25)	<b>3.29</b> (25)	•••	$5.1\left(\frac{m_0}{m_0}\right)^{3/2}$
CdTe (77°K)	0.394 (25)	6.97 (25)	1.55 (25)	0.096 (28)	\ <i>m</i> */ 206

TABLE I. Calculated piezoelectric mobility of certain zincblende-type semiconductors based on the piezoelectric and elastic quantities shown.

<sup>a</sup> We have assumed that kp means kilogram weight in Ref. 24. <sup>b</sup> Using  $h_{14} = 1.57 \times 10^9 V/M$ .

#### APPLICATION TO CRYSTALS WITH WURTZITE SYMMETRY AND [0001]-TYPE VALLEYS

The symmetries of second-, third-, and fourth-rank tensors for wurtzite symmetry (point group 6mm) are the same as the corresponding symmetries for a material having axial symmetry.<sup>18</sup> The piezoelectric tensor is of

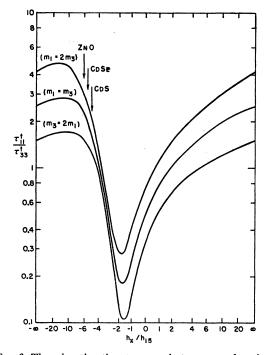


FIG. 3. The relaxation-time tensor anisotropy as a function of the ratio of piezoelectric constants for piezoelectric scattering by the mainly transverse modes in wurtzite-type crystals. The experimentally observed ratios of the piezoelectric constants are shown for those crystals in which they have been measured. The relationship between the effective masses assumed for each curve is shown in parentheses.

the form<sup>18</sup>

$$\boldsymbol{h} = \begin{bmatrix} 0 & 0 & 0 & 0 & h_{15} & 0 \\ 0 & 0 & 0 & h_{15} & 0 & 0 \\ h_{31} & h_{31} & h_{33} & 0 & 0 & 0 \end{bmatrix}, \quad (29)$$

where the 3-axis is the symmetry axis. Points on the 3-axis ( $\Delta$  points) of reciprocal space also have the axial symmetry, so that for valleys centered at these points the effective mass tensor is diagonal,  $m_2 = m_1$ , and the ellipsoid axes are the same as the crystal coordinate axes. We shall consider here only such [0001]-type energy minima.

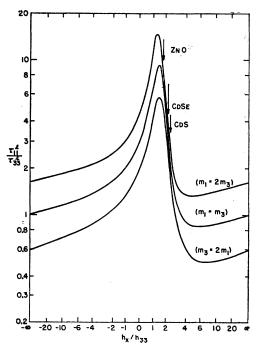


FIG. 4. Same as Fig. 3 for the mainly longitudinal modes.

In the phonon coordinate system the relevant piezoelectric constants are:

$$\begin{array}{l} h_{333}' = \cos\vartheta \left( h_{33} - h_x \sin^2 \vartheta \right) \\ h_{323}' = 0 \\ h_{313}' = -\sin\vartheta \left( h_{15} + h_x \cos^2 \vartheta \right), \end{array}$$
(30)

where we have defined the anisotropic piezoelectric constant  $h_x = h_{33} - h_{31} - 2h_{15}$ . Because of the axial symmetry, the integrations over  $\varphi$  in Eq. (17) give a factor of  $2\pi$ , while the integrations over  $\vartheta$  can be written in terms of the  $I_n$ . The mobilities are then given by:

$$\frac{A_{t}}{\mu_{33}^{t}} = 3h_{15}^{2} \left\{ (I_{2} - I_{4}) + 2(I_{4} - I_{6}) \left(\frac{h_{x}}{h_{15}}\right) + (I_{6} - I_{8}) \left(\frac{h_{x}}{h_{15}}\right)^{2} \right\},$$

$$\frac{A_{t}}{\mu_{11}^{t}} = \frac{3}{2}h_{15}^{2} \left\{ (I_{0} - 2I_{2} + I_{4}) + 2(I_{2} - 2I_{4} + I_{6}) \left(\frac{h_{x}}{h_{15}}\right) + (I_{4} - 2I_{6} + I_{8}) \left(\frac{h_{x}}{h_{15}}\right)^{2} \right\},$$

$$\frac{A_{t}}{\mu_{11}^{t}} = 3h_{t}^{2} \left\{ I_{t} - 2(I_{t} - I_{t}) \left(\frac{h_{x}}{h_{t}}\right) \right\},$$
(31)

$$\frac{1}{\mu_{33}^{l}} = 3h_{33}^{2} \left\{ I_{4} - 2(I_{4} - I_{6}) \left( \frac{1}{h_{33}} \right) + (I_{4} - 2I_{6} + I_{8}) \left( \frac{h_{x}}{h_{33}} \right)^{2} \right\},$$

$$\frac{A_{l}}{\mu_{11}^{l}} = \frac{3}{2}h_{33}^{2} \left\{ (I_{2} - I_{4}) - 2(I_{2} - 2I_{4} + I_{6}) \left( \frac{h_{x}}{h_{33}} \right) + (I_{2} - 3I_{4} + 3I_{6} - I_{8}) \left( \frac{h_{x}}{h_{33}} \right)^{2} \right\}.$$

In this case there are two parameters which determine the mobility anisotropy for either the transverse or longitudinal modes, namely, the mass anisotropy and the ratios of the piezoelectric constants. Figures 3 and 4 show the ratios  $\tau_{11}/\tau_{33}$  as functions of the ratios  $h_x/h_{15}$ and  $h_x/h_{33}$  for several cases of mass anisotropy. It is clear that the scattering anisotropy can be quite sensitive to the ratios of the piezoelectric constants. Measurements<sup>25</sup> of the piezoelectric properties of CdS and CdSe show that the ratios  $h_x/h_{15}$  and  $h_x/h_{33}$  are quite close to the values obtained theoretically by comparing the ideal wurtzite structure to the zincblende structure,<sup>25,30</sup> namely, -5 and 2.5, respectively. The mobility anistropy K is plotted in Fig. 5 for these values and also for  $h_x/h_{15} = -6$  and  $h_x/h_{33} = 2$  as a function of the mass anisotropy. Again, we must caution that the calculated values of K can be considered accurate only if  $\tau_{11}/\tau_{33}$  is not too far from unity.

To combine the scattering by the transverse and

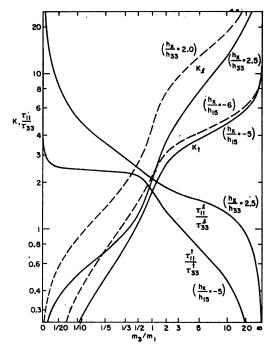


FIG. 5. The mobility tensor anisotropy K and relaxation-time tensor anisotropy  $\tau_{11}/\tau_{33}$  for both longitudinal and transverse modes as functions of the effective mass anisotropy. The ratio of the piezoelectric constants assumed for each curve is shown in parentheses.

longitudinal modes we must know the average stiffness coefficients. In the phonon coordinate system the relevant stiffness coefficients are given by

$$c_{3333}' = \frac{\sigma_{1}^{4}}{\sigma^{4}} c_{11} + \frac{\sigma_{3}^{4}}{\sigma^{4}} c_{33} + 2 \frac{\sigma_{1}^{2} \sigma_{3}^{2}}{\sigma^{4}} (c_{13} + 2c_{44}),$$
  

$$c_{1313}' = c_{44} + (\sigma_{1}^{2} \sigma_{3}^{2} / \sigma^{4}) c_{x},$$
(32)

where  $c_x = c_{11} + c_{33} - 2c_{13} - 4c_{44}$  and  $c_{2323}'$  is not relevant since  $h_{323}' = 0$  by symmetry and thus only one transverse mode contributes to the scattering. A spherical average of (32) gives

$$c_{l} = \frac{1}{3}(2c_{11} + c_{33}) - (2/15)c_{x},$$
  

$$c_{t} = c_{44} + (2/15)c_{x}.$$
(33)

As in the case of cubic symmetry, the magnitude of the scattering is not sensitive to the mass anisotropy, and thus the combined mobilities for transverse and longitudinal modes can be estimated by choosing  $m_1 = m_3$ . Table II lists the calculated mobilities and the relevant elastic and piezoelectric quantities which have been measured for CdS<sup>25</sup>, CdSe<sup>25</sup>, and ZnO.<sup>3,31,32</sup> Cyclotron resonance of electrons in CdS<sup>33,34</sup> indicates that

<sup>&</sup>lt;sup>30</sup> See L. J. Touchard, J. Appl. Phys. **34**, 2694 (1963), for a similar comparison of the elastic constants for these two structures.

<sup>&</sup>lt;sup>31</sup> A. R. Hutson, Phys. Rev. Letters 4, 505 (1960). <sup>32</sup> T. B. Bateman, J. Appl. Phys. 32, 3309 (1962). The author thanks an attentive referee for calling this reference to his attention.

W. S. Baer and R. N. Dexter, Bull. Am. Phys. Soc. 8, 516 (1963).

<sup>&</sup>lt;sup>34</sup> K. Sawamoto, J. Phys. Soc. Japan 18, 1224 (1963).

Units	h <sub>33</sub> 10 <sup>9</sup> V/M	(Ref.) ſ	h <sub>15</sub> 10 <sup>9</sup> V/M	(Ref.) 1	h <sub>x</sub> 10 <sup>9</sup> V/A	(Ref.)	cı 10 <sup>10</sup> N/M	(Ref.) [ <sup>2</sup>	c <sub>t</sub> 10 <sup>10</sup> N/M	(Ref.) 1²	$m_1/m_0$ $m_3/m_0$ 		μ33 at 77°K M²/VS	$K = \frac{\mu_{11}}{\mu_{33}}$
CdS	5.21	(25)	-2.63	(25)	13.4	(25)	8.95	(25)	1.902	(25)	0.171 0.153' 0.20 <sup>a</sup> 0.20 '	(33) (40)	1.03 0.77	1.69 1.82ª
CdSe	3.84	(25)	-1.77	(25)	8.95	(25)	7.40	(25)	1.716	(25)			$0.135 \left(\frac{m_0}{m^*}\right)^{3/2}$	1.89
ZnO	15	(3)	-4.3	(3)	26	(3)	21.0	(32)	5.01,	(32)			$0.036 \left(\frac{m_0}{m^*}\right)^{3/2}$	2.8 <sup>b</sup>

TABLE II. Calculated piezoelectric mobility tensor components for certain wurtzite-type semiconductors, based on the piezoelectric and elastic quantities shown.

<sup>a</sup> We assume here that the effective mass without the piezoelectric polaron correction is isotropic in order to illustrate the effect of mass anisotropy on K. <sup>b</sup> The value of K for ZnO is subject to a large uncertainty since it is quite sensitive to the ratios  $h_x/h_{33}$  and  $h_x/h_{16}$  which are not known with accuracy for ZnO.

the energy surfaces are oblate ellipsoids of revolution in terms of the  $I_n$  integrals: with the effective masses indicated in Table II.

### APPLICATIONS TO CRYSTALS WITH TELLURIUM SYMMETRY AND [001]-TYPE VALLEYS

Tellurium and selenium have the same symmetry (point group 32) as that of  $\alpha$ -quartz and can therefore, in principle, be piezoelectric, although the physical basis of piezoelectricity in elemental crystals has never been discussed, to the author's knowledge. A large piezoelectric effect has been measured in the case of selenium,<sup>35</sup> the piezoelectric constant  $d_{11}$  being thirtytwo times as large as that of  $\alpha$ -quartz. In the crystal coordinate system (3-axis along the trigonal axis, and 1-axis along the binary axis) the piezoelectric tensor is of the form:

$$\boldsymbol{h} = \begin{bmatrix} h_{11} & -h_{11} & 0 & h_{14} & 0 & 0\\ 0 & 0 & 0 & 0 & -h_{14} & h_{14}\\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} .$$
(34)

Again, for simplicity we discuss the type of valley for which the effective mass tensor is diagonal in the crystal coordinate system and the ellipsoid coordinate system is the same as the crystal coordinate system. In the phonon coordinate system the piezoelectric constants of interest are:

$$h_{333}' = h_{11} \sin^3 \vartheta \cos 3\varphi,$$
  

$$h_{323}' = -h_{11} \sin^2 \vartheta \sin 3\varphi + h_{14} \sin \vartheta \cos \vartheta, \qquad (35)$$
  

$$h_{313}' = h_{11} \sin^2 \vartheta \cos \vartheta \cos 3\varphi.$$

As before, for  $\Gamma$  and  $\Delta$  points the two transverse effective masses must be equal and the mobilities can be written

$$\frac{A_{t}}{\mu_{33}^{t}} = h_{11}^{2} \{ (I_{2} - 2I_{4} + I_{6}) - \frac{1}{2} (I_{2} - 3I_{4} + 3I_{6} - I_{8}) \} + h_{14}^{2} (I_{4} - I_{6}), \\
\frac{A_{t}}{\mu_{11}^{t}} = \frac{h_{11}^{2}}{2} \{ (I_{0} - 3I_{2} + 3I_{4} - I_{6}) - \frac{1}{2} (I_{0} - 4I_{2} + 6I_{4} - 4I_{6} + I_{8}) \} + \frac{h_{14}^{2}}{2} (I_{2} - 2I_{4} + I_{6}), \\
\frac{A_{t}}{\mu_{33}^{t}} = \frac{1}{2} h_{11}^{2} \{ I_{2} - 3I_{4} + 3I_{6} - I_{8} \}, \\
A_{t}$$

$$\frac{2I_{l}}{\mu_{11}^{l}} = \frac{1}{4}h_{11}^{2}\{I_{0} - 4I_{2} + 6I_{4} - 4I_{6} + I_{8}\}.$$
(36)

For isotropic effective mass these reduce simply to:

$$\frac{A_{t}}{\mu_{33}^{t}} = \frac{16}{315} h_{11}^{2} + \frac{2}{35} h_{14}^{2},$$

$$\frac{A_{t}}{\mu_{11}^{t}} = \frac{8}{63} h_{11}^{2} + \frac{4}{105} h_{14}^{2},$$

$$\frac{A_{t}}{\mu_{33}^{t}} = \frac{8}{315} h_{11}^{2},$$

$$\frac{A_{t}}{\mu_{33}^{t}} = \frac{32}{315} h_{11}^{2},$$
(37)

which shows that the scattering is quite anisotropic with  $K = \mu_{11}/\mu_{33} < 1$  if  $h_{14}^2 < h_{11}^2$  (in  $\alpha$ -quartz,  $h_{11}^2 \approx 32h_{14}^2$ ).

Note added in proof. A piezoelectric effect in tellurium has been measured recently by G. Quentin and J. M.

<sup>&</sup>lt;sup>35</sup> H. Gobrecht, H. Hamisch, and A. Tausend, Z. Physik 148, 209 (1957).

Thuillier [Solid State Commun. 2, 115 (1964)] who found that  $d_{11}^2/s_{11}\epsilon_1=0.12$ . Recent cyclotron-resonance results at 68 Gc/sec [J. H. Mendum and R. N. Dexter (private communication)] have shown that the valence band of tellurium is characterized by a single energy extremum with effective masses  $m_1/m_0=0.126$ ,  $m_3/m_0$ =0.243. Using the approximate relationships:  $n_{11}^2/c_1$  $\approx d_{11}^2/s_{11}\epsilon_1^2$ ,  $\epsilon_1 \approx n_1^2\epsilon_0$  and the index of refraction  $n_1=4.8$  measured by R. S. Caldwell and H. Y. Fan [Phys. Rev. 114, 664 (1959)], and assuming that  $h_{14}^2=0$ and that  $c_i/c_i=1.5$  [the elastic constants have been measured by J. L. Malgrange, G. Quentin, and J. M. Thuillier, Phys. Stat. Solidi 4, 139 (1964)] we obtain for the piezoelectric mobility:

$$\mu_{11} = 3.8(77/T)^{1/2} \times 10^4 \text{ cm}^2/\text{V sec}, \quad \mu_{33} = 2.4 \ \mu_{11}.$$

The theory as developed above may not be adequate, however, since tellurium is quite anisotropic elastically. For example, along the l axis the stiffness coefficients for the two transverse modes differ by a factor of seven, and averaging them together is not justified. Also, the cyclotron mass should be corrected for piezoelectric polaron effects, as in the case of CdS.

## DISCUSSION

The piezoelectric mobility of electrons (or of holes) has been calculated for the three classes of known piezoelectric semiconductors, assuming energy surfaces which are ellipsoids of revolution with principal axes along the crystal axes. For other types of valleys the piezoelectric tensor must first be expressed in the ellipsoid coordinate system. Two main simplifying approximations are used: an approximate solution to the Boltzmann equation valid if the scattering is not too anisotropic, and approximate formulas for the frequencies and polarizations of the long wavelength acoustic modes. Improvements in either of these approximations are difficult in general, but in specific cases numerical calculations could be used to give improved accuracy for comparison with accurate experiments. The piezoelectric mobilities in semiconductors for which all the elastoelectric properties have been measured are listed in Tables I and II. The effective mass has been included in the tables only for those crystals in which cyclotron resonance has been measured.

In the case of zincblende symmetry and [000]-type valleys the present results [Eq. (26)] agree quite well with the previous calculations<sup>1,2</sup> which invoked various averaging techniques. It is easy to show, by examination of Eq. (17), that in the case of an isotropic effective mass tensor a spherical average of the piezoelectric constants gives the average mobility  $\mu_a$ , where

$$\frac{1}{\mu_a} = \frac{1}{3} \left( \frac{1}{\mu_{11}} + \frac{1}{\mu_{22}} + \frac{1}{\mu_{33}} \right). \tag{38}$$

For cubic symmetry the  $\mu_{ii}$  are equal to each other and to  $\mu_a$ , thus it is not surprising that the present calculations are in good agreement with the results of Meijer and Polder<sup>1</sup> who took a weighted average of the piezoelectric constants in the  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ , and  $\langle 111 \rangle$  directions. Harrison<sup>2</sup> used the formula for  $\tau(\mathbf{k})$  postulated by Herring<sup>20</sup> and Brooks<sup>21</sup> and took a weighted average of  $\tau(\mathbf{k})$  for  $\mathbf{k}$  along the (100), (110), and (111) directions. This formula, however, is basically incorrect for calculating relaxation-time anisotropy since it is not based on a solution of the Boltzmann equation for anisotropic scattering, but rather on a generalization of the exact solution which exists for isotropic scattering. The incorrectness of this formula for calculating the anisotropy can be judged from the fact that it predicts the wrong *direction* of the relaxation time tensor anisotropy for ionized impurity scattering.<sup>36</sup> It is not hard to show, however, that for isotropic effective mass a spherical average of  $1/\tau(\mathbf{k})$  gives the same result as Eq. (38). It is therefore not surprising that Harrison's results also agree well with Eq. (26).

The average mobilities  $\mu_a$  for wurtzite symmetry and isotropic mass agree exactly with Hutson's results,<sup>4</sup> since he used a spherical average of the piezoelectric constants. (However, the present formulas include the effect of dielectric anisotropy exactly, through the use of h rather than e for the piezoelectric tensor.) The effects of piezoelectric scattering will be larger in the wurtzite-type crystals than in the cubic crystals, because the piezoelectric effect itself is larger in these crystals.<sup>25</sup>

In the case of CdS, crystals of sufficient purity are available such that piezoelectric scattering is important in determining the mobility.<sup>37,38</sup> Zook and Dexter<sup>37</sup> invoked a combination of polar optical mode scattering, piezoelectric scattering, and impurity scattering to explain their measurements of electron mobility in CdS between 77 and 300°K. A significant result of their experiments was the observation of a temperature dependence of the mobility anisotropy which was consistent with the hypothesis that the piezoelectric mobility was anisotropic while the mobility due to other mechanisms was essentially isotropic. From these data and assumptions, a piezoelectric mobility anisotropy of  $K = \mu_{11}/\mu_{33} = 1.55 \pm 0.12$  was deduced. In that paper an

<sup>&</sup>lt;sup>36</sup> The author is indebted to D. Long for pointing out that in Ref. 20 Herring deduced a direction of the relaxation time anisotropy for ionized impurity scattering opposite to that deduced in Ref. 13. The latter theory agrees with experiments [see L. J. Neuringer and W. Little, *Proceedings of the International Conference on Semiconductors, Exeter, 1962* (The Institute of Physics and the Physical Society, London, 1962), p. 614; J. D. Maines and E. G. S. Paige, Proc. Phys. Soc. (London) 81, 767 (1963); also, L. J. Neuringer and D. Long, Phys. Rev. 135, A788 (1964)]. <sup>47</sup> D. Zook and R. N. Dexter. Phys. Rev. 129, 1980 (1963).

 <sup>&</sup>lt;sup>37</sup> D. Zook and R. N. Dexter, Phys. Rev. 129, 1980 (1963).
 <sup>38</sup> W. S. Baer, thesis, The University of Wisconsin, 1964 (unpublished).

incorrect<sup>39</sup> theoretical estimate was given of the piezoelectric mobility anisotropy for isotropic mass, based on the formula for  $\tau(\mathbf{k})$  discussed above. The calculated mobility anisotropy for CdS is given in Table II, using the recent cyclotron-resonance results<sup>33</sup> which indicate slightly oblate  $(m_1/m_3=1.12)$  ellipsoids. The measured cyclotron-resonance masses include a piezoelectric polaron correction which would not be observed in experiments done at temperatures well above a few degrees Kelvin.<sup>40</sup> Assuming the electron effective mass without the piezoelectric polaron correction is 0.20  $m_0^{40}$ and isotropic, we obtain the second set of mobilities for CdS indicated in Table II. Both calculated values of K have associated with them probable errors of about 8% due to the stated accuracy of the measurement of the piezoelectric and dielectric constants. The agreement between either of the theoretical values and the experimental value of K is quite good in view of the simplifying assumptions used in deducing both the theoretical and experimental values. A more accurate comparison of the magnitude and anisotropy of piezoelectric scattering can be made only if the experiments are repeated under conditions such that virtually all the scattering is due to the piezoelectric mechanism.

# ACKNOWLEDGMENTS

The author gratefully acknowledges helpful discussions with D. Long and O. N. Tufte, and the assistance of P. W. Chapman with the numerical calculations.

# APPENDIX. REWRITING THE HERRING-VOGT FORMULA FOR $\tau_{ii}(\epsilon)$

It is always convenient in discussing ellipsoidal energy surfaces to change to a coordinate system in which the energy surfaces are spherical. We use the notation of Ref. 14 to write such a transformation:

$$\xi_{i} = \hbar k_{i} / (2m_{i} \varepsilon)^{1/2}, \quad \xi_{i}^{S} = \hbar k_{i}^{S} / (2m_{i} \varepsilon)^{1/2}, q_{i} = \xi_{i} - \xi_{i}^{S}.$$
(A1)

The Herring-Vogt formula (Eq. (11), Ref. 4] can then be written

$$\frac{1}{\tau_{ii}(\epsilon)} = \int \int \xi_i (\xi_i - \xi_i^S) \Lambda^0(\xi - \xi^S) d\Omega_{\xi} d\Omega_{\xi^S} / \int \xi_i^2 d\Omega_{\xi}, \quad (A2)$$

where  $\Lambda^0$  is related to  $W^0$ , as follows:

$$[(2m_1m_2m_3\,\varepsilon)^{1/2}/\hbar^3]W^0(\mathbf{k},\mathbf{k}^S) = \Lambda^0(\boldsymbol{\xi} - \boldsymbol{\xi}^S). \quad (A3)$$

We have assumed that the scattering probability  $W(\mathbf{k}, \mathbf{k}^{S})$  depends only on the difference  $\mathbf{k} - \mathbf{k}^{S}$ .

The first step in rewriting (A2) is to symmetrize it by interchanging  $\xi$  and  $\xi^s$ , adding the result to the original equation and dividing by 2 to obtain

$$\frac{1}{\tau_{ii}(\varepsilon)} = \frac{3}{4\pi} \int \int \frac{1}{2} (\xi_i - \xi_i^S)^2 \Lambda^0(\xi - \xi^S) d\Omega_{\xi} d\Omega_{\xi}^s, \quad (A4)$$

since  $\Lambda$  is symmetrical with respect to interchange of  $\xi$ and  $\xi^s$ , and the denominator of (A2) is just  $4\pi/3$ . The next step is to change the integration over  $d\Omega_{\xi^s}$  to an integration over  $d\Omega_q$ , holding  $\xi$  constant. Taking the pole of a spherical coordinate system to be along  $\xi$ , we can obtain the relationship

$$d\Omega_{\xi^s} = 2qd\Omega_q, \quad 0 \le q \le 2. \tag{A5}$$

Then, interchanging the order of integration, we hold the direction of  $\mathbf{q}$  fixed and can write

$$d\Omega_{\xi} = \frac{1}{2} dq d\beta \,, \tag{A6}$$

where  $\beta$  is the azimuthal angle about the vector **q**. The integrand of (A4) depends only on **q** so that the integration over  $\beta$  yields a factor of  $2\pi$ , and we then obtain Eq. (12).

<sup>&</sup>lt;sup>39</sup> There are two other errata in Ref. 37. In the statement on page 1986 to the effect that Casella calculated appreciable longitudinal magnetoresistance for toroidal energy surfaces, the word "longitudinal" should be deleted. Casella did calculate transverse magnetoresistance for current along the c axis and pointed out the longitudinal magnetoresistance in this case is zero by symmetry. On page 1987, the value of  $\alpha$  for CdS should be 0.7 instead of 0.3. The author is indebted to R. C. Casella and W. S. Baer, respectively, for pointing out these errors, neither of which affect the rest of the discussion in Ref. 37.

<sup>&</sup>lt;sup>40</sup> G. D. Mahan and J. J. Hopfield, Phys. Rev. Letters 12, 214 (1964).