way CP could avoid this difficulty would have been to add many more basis states to their secular equation.

A complete treatment of spin effects should, of course, start from the Dirac equation. This can be done, as for example in KI.²⁷ For Ge there would be little advantage to this approach over what one can do by starting from

²⁷ Y. Onodera, M. Okazaki, and T. Inui, J. Phys. Soc. Japan 21, 2229 (1966); for an application of the Dirac equation in the OPW approach, see P. Soven, Phys. Rev. 137, A1706 (1965).

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Dirac equation.

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Calculation of Ionized-Impurity Scattering Mobility of Electrons in $Hg_{1-x}Cd_xTe^{\dagger}$

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A study is made of the magnitude of the ionized-impurity scattering mobility of conduction electrons in *n*-type $Hg_{1-x}Cd_xTe$ at 4.2°K, covering the alloy composition range 0 < x < 0.3. Calculations of the mobility have been made, assuming the Born approximation for scattering by singly ionized donors in degenerate material having a nonparabolic conduction band. They account well for available mobility data.

1. INTRODUCTION

HE pseudo-binary alloy system of the II-VI compounds HgTe and CdTe can be represented by the formula $Hg_{1-x}Cd_xTe$, where x denotes the mole fraction of HgTe in the alloy. This alloy system has been of great interest in recent years¹ for two reasons. First, it is a mixture of a semimetal (HgTe) with a semiconductor (CdTe), such that the electronic energy gap E_g vanishes at an intermediate alloy composition; very interesting properties occur around this composition at which $E_g = 0$. Second, narrow-gap semiconducting alloys in this system have proved useful as materials for high-performance intrinsic infrared photon detectors. Thus most studies of $Hg_{1-x}Cd_xTe$ have been on the alloys which are semimetals or narrow-gap semiconductors, occurring, as we will see, in the composition range 0 < x < 0.3.

The energy gap in $Hg_{1-x}Cd_xTe$ varies practically linearly between its values at 4.2°K for the "endpoint" compounds, HgTe and CdTe, of -0.301 and 1.606 eV, respectively. The energy gap, which is really the $\Gamma_6 - \Gamma_8$ energy difference, is "negative" in HgTe, corresponding to the semimetallic nature of that compound. Figure 1 shows the E_{g} -versus-x curve for $Hg_{1-x}Cd_{x}Te$ for very low temperatures (4.2°K). Using Fig. 1 and the momentum matrix element, $P = 9 \times 10^{-8} \text{eV cm}$, believed generally applicable for the II-VI compounds,² the curve of the conduction-band edge effective mass versus x shown in Fig. 2 for the 0 < x < 0.3 range has been calculated by the $\mathbf{k} \cdot \mathbf{p}$ method.² Figures 1 and 2 will be used in the ensuing analysis.

Eq. (2), which is derived as the limiting form of the

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Since the beginning of research on $Hg_{1-x}Cd_xTe$, many attempts have been made to analyze and explain the electrical properties, especially, of course, for alloys



FIG. 1. $\Gamma_6 \cdot \Gamma_8$ energy gap versus alloy composition x in $Hg_{1-x}Cd_xTe$ at 4.2°K. The assumed linear variation between the "endpoint" gaps of 1.606 eV in CdTe and -0.301 eV in HgTe agrees well with available data of various types; see Ref. 1.

² M. Cardona, J. Phys. Chem. Solids 24, 1543 (1963),

[†] This research supported in part by the U. S. Air Force and

This research supported in part by the U. S. Air Force and the Advanced Research Projects Agency. ¹ D. Long [*Energy Bands in Semiconductors* (John Wiley & Sons, Inc., New York, 1968), pp. 156–159] reviews the properties and band structure of $Hg_{1-x}Cd_xTe$. Very recent results give the value for the "negative" energy gap of HgTe of 0.301 eV at 4.2°K used here; see C. R. Pidgeon and S. H. Groves, in *Proceedings of the International Conference on II-VI Compounds* (W. A. Benjamin, Inc. New York 1967) p. 1080 Inc., New York, 1967), p. 1080.



FIG. 2. Conduction-band edge effective-mass ratio versus alloy composition x in Hg_{1-x}Cd_xTe for $0 \le x \le 0.3$ at 4.2°K. This is a theoretical curve derived by the $\mathbf{k} \cdot \mathbf{p}$ method, using Fig. 1 and a momentum matrix element $P = 9 \times 10^{-8}$ eV cm.

with x in the above range.³⁻¹³ The electrical properties are understood in a general, qualitative way, but a full quantitative understanding remains to be reached. Earlier analyses of electrical properties were generally inhibited by uncertainties about crystal perfection, composition, and impurity content and also by an incomplete understanding of the energy band structure. Even now, for example, peculiar Hall curves observed in studies of annealing effects are difficult to explain.¹³ By "explaining" electrical properties we mean being able to account for such properties as shapes of Hallcoefficient-versus-temperature and mobility-versustemperature curves, and for the magnitudes of observed mobilities, in terms of the band structure (effective masses and energy gap) and reasonable theories of carrier scattering mechanisms. Crystal-growth technology and band-structure knowledge have now advanced far enough that it makes sense to attack anew the problem of analyzing the electrical properties of $Hg_{1-x}Cd_{x}Te.$

In the present treatment we will not attempt to explain all features of the electrical properties, but will

⁵ M. V. Kot, V. G. Tyrziu, A. V. Simashkevich, Y. Y. Maron-

- chuk, and V. A. Mshenskii, Fiz. Tverd. Tela 4, 1535 (1962) [English transl.: Soviet Phys.—Solid State 4, 1128 (1962)]. ⁶ A. D. Shneider and I. V. Gavrischak, Fiz. Tverd. Tela 5, 1208 (1963) [English transl.: Soviet Phys.—Solid State 5, 881 (1963)].
- ⁷ R. R. Galazka, Acta Phys. Polon. 24, 791 (1963). ⁸ M. Rodot, H. Rodot, and C. Verié, in *Proceedings of the Seventh International Conference on the Physics of Semiconductors*, edited by M. Hulin (Academic Press Inc., New York, 1964),
- ¹⁰ C. Verié, Phys. Status Solidi 13, 215 (1966).
 ¹⁰ C. Verié, Phys. Status Solidi 17, 889 (1966).
 ¹¹ R. R. Galazka and L. Sosnowski, Phys. Status Solidi 20, 113 (1967).
- 12 R. R. Galazka and T. Zakrzewski, Phys. Status Solidi 23, K39 (1967)
 - ¹³ P. W. Kruse and J. L. Schmit (unpublished).

restrict ourselves simply to trying to account for the magnitude of the conduction-band electron mobility at very low temperatures (4.2°K) as a function of alloy composition x in the range 0 < x < 0.3; limited variations of carrier concentration will also be permitted. Many samples of $Hg_{1-x}Cd_xTe$ taken from crystals grown from a melt by Bridgman methods exhibit Hall and resistivity-versus-temperature curves like those of a conventional n-type semiconductor in which the donor activation energy is vanishingly small, so that no freeze-out of extrinsic carriers occurs at low temperatures. In these samples, the extrinsic carrier concentration is thus a constant, independent of temperature. The Hall mobility increases with decreasing temperature from room temperature downward, and becomes nearly independent of temperature as the liquid-helium range is approached¹³; see Fig. 3. The temperatureindependent behavior is observed where statistical degeneracy exists. One can hope to understand the mobility in this region in terms of the scattering of a statistically degenerate carrier population by ionized impurities. That is, the sample is n-type because it contains donor impurities, each of which gives one electron to the conduction band and thereby becomes a singly ionized scattering center. The mobility is then limited at 4.2°K by ionized-impurity scattering. Let us assume that this model is correct, and that the Born approximation can legitimately be employed in the analysis, and then see how well such a model accounts for existing data. We focus mainly on alloys in the x=0.2 vicinity, which are narrow-gap semiconductors with small electron effective masses and nonparabolic conduction bands, qualitatively analogous to InSb.

2. FORMULATION OF THEORY

The general expression for the carrier mobility which can be applied to a nonparabolic band with spherical energy surfaces is14

$$\mu = \frac{\sigma}{ne_0} = -\frac{4e_0}{3h^2n} \int_0^\infty \tau k^2 \left(\frac{dE}{dk}\right) \left(\frac{\partial f_0}{\partial E}\right) dE.$$
(1)

See the list of symbol definitions in Table I. For a narrow-gap semiconductor obeying the $\mathbf{k} \cdot \mathbf{p}$ model,^{2,15,16} with its valence-band spin-orbit splitting energy much larger than the energy gap (as it is in the alloys of interest), one has the following relationships¹⁴:

$$k^{2} = (2m_{0}^{*}/\hbar^{2})(E/E_{g})(E+E_{g}), \qquad (2)$$

$$dE - \sqrt{2}\hbar E_g^{1/2} E^{1/2} (E + E_g)^{1/2}$$
⁽³⁾

$$dk = m_0^{*1/2}(2E+E_g)$$
 , (5)

$$m^*(E) = m_0^* [(2E + E_g)/E_g].$$
(4)

¹⁴ T. C. Harman and J. M. Honig, J. Phys. Chem. Solids 23, 913 (1962); T. C. Harman, J. M. Honig, and B. M. Tarmy, *ibid*. 24, 835 (1963). ¹⁵ Reference 1, Chap. 3.

- ¹⁶ E. O. Kane, J. Phys. Chem. Solids 1, 249 (1957).

⁸ W. D. Lawson, S. Nielsen, E. H. Putley, and A. S. Young, J. Phys. Chem. Solids 9, 325 (1959). ⁴ T. C. Harman, A. J. Strauss, D. H. Dickey, M. S. Dresselhaus,

G. B. Wright, and J. G. Mavroides, Phys. Rev. Letters 7, 403 (1961).



FIG. 3. Typical Hall-mobility-versus-temperature curve for a melt-grown sample of *n*-type $Hg_{1-x}Cd_xTe$ with $x \approx 0.2$.

Substitution of (2) and (3) into (1) gives

$$\mu = \frac{2\sqrt{2}e_0m_0^{*1/2}}{3\pi^2 n\hbar^3} \int_0^\infty \tau \frac{E^{3/2}(E+E_g)^{3/2}}{E^{1/2}(2E+E_g)} \left(\frac{\partial f_0}{\partial E}\right) dE.$$
 (5)

The relaxation time for scattering by ionized impurities in the Born approximation is given by

$$\tau_I = \frac{\hbar \kappa^2}{2\pi e_0^4 N_{Ig}(b)} k^2 \frac{dE}{dk} \tag{6}$$

for the general case of a nonparabolic band with spherical surfaces of constant energy.¹⁷ The screening factor g(b) in (6) is given by

$$g(b) = \ln(1+b) - \frac{b}{(1+b)},$$
 (7)

where

$$b \equiv 4k^2 R^2 = \frac{\kappa}{\pi e_c^2} k^2 \left(\frac{dn}{dE_n}\right)^{-1}, \qquad (8)$$

since,18 in general,

$$R^2 = \frac{\kappa}{4\pi e_0^2} \left(\frac{dn}{dE_F}\right)^{-1} \tag{9}$$

for the case under consideration.

Substituting the results of the preceding paragraph into (5), we obtain

$$\mu_{I} = \frac{32\kappa^{2}m_{0}^{*}}{3e_{0}^{3}h^{3}N_{I}n} \int_{0}^{\infty} \frac{E^{3}(E+E_{g})^{3}}{E_{g}(2E+E_{g})^{2}g(b)} \left(\frac{\partial f_{0}}{\partial E}\right) dE. \quad (10)$$

For complete statistical degeneracy, Eq. (10) reduces to

$$\mu_{I} = \frac{32\kappa^{2}m_{0}^{*}}{3e_{0}^{3}h^{3}N_{I}n} \frac{E_{F}^{3}(E_{F} + E_{g})^{3}}{E_{g}(2E_{F} + E_{g})^{2}g(b)}.$$
 (11)

The expression for the carrier concentration in the

degenerate limit,¹⁴

$$n = \frac{32\pi m_0^{*3/2}}{3h^3\sqrt{2}} \frac{E_F^{3/2} (E_F + E_g)^{3/2}}{E_g^{3/2}}, \qquad (12)$$

can be substituted into (11) to give

$$\mu_{I} = \frac{\sqrt{2}\kappa^{2}}{\pi e_{0}^{3}m_{0}^{*1/2}N_{I}} \frac{E_{F}^{3/2}(E_{F} + E_{g})^{3/2}E_{g}^{1/2}}{(2E_{F} + E_{g})^{2}g(b)}$$
$$= \frac{3\hbar^{3}\pi\kappa^{2}n}{2e_{0}^{3}m_{0}^{*2}N_{I}} \frac{E_{g}^{2}}{(2E_{F} + E_{g})^{2}g(b)}.$$
(13)

When $n = N_I$, Eq. (13) can be simplified further to

$$\mu_I = \frac{3\hbar^3 \pi \kappa^2}{2e_0{}^3 m_0{}^{*2}g(b)} \frac{E_g{}^2}{(2E_F + E_g)^2} \,. \tag{14}$$

This last equation is valid for a nonparabolic band, complete statistical degeneracy, and a sample in which the carrier concentration equals the concentration of singly ionized impurities. Equation (14) in practical units is

$$\mu_I = \frac{0.20\kappa^2}{(m_0^*/m)^2 g(b)} \frac{E_g^2}{(2E_F + E_g)^2}, \ \mathrm{cm}^2/\mathrm{V} \ \mathrm{sec.}$$
(15)

The expression for the screening factor in Eq. (14) in terms of the dependence of b on material parameters, for complete statistical degeneracy, is

$$b = \frac{h\kappa}{\sqrt{2}e_0^2 m_0^{*1/2}} \frac{E_F^{1/2} E_g^{1/2} (E_F + E_g)^{1/2}}{(2E_F + E_g)}, \qquad (16)$$

TABLE I. Definitions of symbols.

| Symbol | Meaning | | | | | | |
|----------------|--|--|--|--|--|--|--|
| a_0 | first Bohr radius | | | | | | |
| e_0 | electronic charge | | | | | | |
| J0 | equilibrium statistical distribution function | | | | | | |
| n L | hanck's constant | | | | | | |
| n k | $n/2\pi$ | | | | | | |
| n h- | magnitude of carrier wave vector at Fermi level in | | | | | | |
| ĸŗ | degenerate material | | | | | | |
| m | mass of free electron | | | | | | |
| m_0^{\star} | effective mass at band edge $(\mathbf{k}=0)$ | | | | | | |
| $m^{\star}(E)$ | effective mass at energy E above band edge | | | | | | |
| m_F | effective mass at Fermi level in degenerate material | | | | | | |
| k _B | Boltzmann's constant | | | | | | |
| IV I | ionized-impurity concentration | | | | | | |
| n | conduction-electron concentration | | | | | | |
| x | mole fraction of CdTe in $Hg_{1-x}Cd_x$ Te alloy | | | | | | |
| | carrier energy | | | | | | |
| E_g | energy gap | | | | | | |
| E_F | Fermi energy level | | | | | | |
| P | momentum matrix element | | | | | | |
| ĸ | screening radius | | | | | | |
| 1 | absolute temperature | | | | | | |
| η_F | reduced Fermi level, E_F/k_BT | | | | | | |
| к | static dielectric constant | | | | | | |
| μ | carrier mobility | | | | | | |
| μ_I | ionized-impurity scattering carrier mobility | | | | | | |
| σ | electrical conductivity | | | | | | |
| au | scattering relaxation time | | | | | | |

 ¹⁷ R. Barrie, Proc. Phys. Soc. (London) **69B**, 553 (1956).
 ¹⁸ F. Stern, Phys. Rev. **148**, 186 (1966).

or, in numerical terms,

$$b = \frac{0.85\kappa}{(m_0^*/m)^{1/2}} \frac{E_F^{1/2} E_g^{1/2} (E_F + E_g)^{1/2}}{(2E_F + E_g)}, \qquad (17)$$

where E_F and E_g are in eV.

Equation (12) for the carrier concentration can be put into the following convenient numerical form:

$$n = 4.54 \times 10^{21} \left(\frac{m_0^*}{m}\right)^{3/2} \frac{E_F^{3/2} (E_F + E_g)^{3/2}}{E_g^{3/2}}, \text{ cm}^{-3}, (18)$$

with the energies in eV.

Especially interesting is the mobility value (at 4.2°K) for the composition at which $E_g=0$. The preceding equations specialize to the following for this case:

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$$n = (\sqrt{3}/2\sqrt{2}\pi^2)(E_F^3/P^3), \qquad (19)$$

$$\mu_I = \frac{\kappa^2 P^2}{3^{3/2} \pi^{1/3} \hbar e_0^3 g(b) n^{2/3}},$$
(20)

$$b = \frac{\pi^{1/3} \kappa E_F}{3^{1/3} e_0^2 n^{1/3}} = \frac{\sqrt{2\pi\kappa P}}{\sqrt{3} e_0^2}, \qquad (21)$$

since

$$E_g/m_0^* = 4P^2/3\hbar^2,$$
 (22)

in general, according to the $\mathbf{k} \cdot \mathbf{p}$ method, and P is the momentum matrix element. At the composition at which $E_g=0$, the electron effective mass is zero, because the conduction band has no curvature. Nevertheless, the mobility is not infinite. The indeterminate ratio on the left side of Eq. (22) is simply replaced by the right side of Eq. (22) to evaluate the mobility, as



FIG. 4. Ionized-impurity scattering mobility versus alloy composition x in Hg_{1-x}Cd_xTe at 4.2°K. The curves are theoretical, and the points represent experimental data. The data points are from samples all having carrier concentrations n within a factor of 2 of 10¹⁵ cm⁻³, except for the point indicated as corresponding to a 3×10^{16} cm⁻³ sample.

in Eqs. (19)-(21), and this leads to the finite mobility given in Eq. (20).

3. APPLICATION TO EXPERIMENTAL RESULTS

Using Figs. 1 and 2 and the results of Sec. 2, we have derived the curves in Fig. 4; also involved was the assumption of a linear variation of the static dielectric constant κ with x between its value¹⁹ of 20 in HgTe and 10.6 in CdTe. The curves in Fig. 4 represent the dependence of the ionized-impurity scattering mobility on composition, with conduction-electron concentration as a parameter, calculated from the above model. These curves take full account of statistical degeneracy and conduction-band nonparabolicity.

The points plotted in Fig. 4 are data considered to be reasonably reliable. The six Honeywell data points are results typical for samples cut from melt-grown crystals, like that of Fig. 3. The theoretical model gives a very good description of the magnitudes of the measured mobilities in the $x\approx0.2$ samples. It would be interesting to have mobility data for *n*-type Hg_{1-x}Cd_xTe samples ranging over the entire 0 < x < 0.3 composition range.

Krieger and Strauss²⁰ have published recently an analysis of singly ionized-impurity scattering in degenerate material which is relevant here. Their theory determines the degree of validity of the Born approximation by comparing the results of phase-shift calculations with the mobility or resistivity calculated using the well-known Brooks-Herring formulation, which is based on the Born approximation. Krieger and Strauss take proper account of the Friedel sum rule in their analysis. Their results are expressed in terms of the ratio of the resistivity calculated by their approach to the Born-approximation resistivity, plotted versus the quantity a_0k , where a_0 is the first Bohr radius and k is the magnitude of the carrier wave vector $(k \equiv k_F \text{ in our }$ notation). In both theories the results are universal functions of a_0k .

Thus we can use the results of Krieger and Strauss to determine the degree of validity of our Bornapproximation model for $Hg_{1-x}Cd_xTe$. For this purpose we have calculated a_0k_F for several representative points from the formula

$$a_0 k_F \cong \frac{0.27 \kappa E_F^{1/2}}{(m_0^*/m)^{1/2}},$$
(23)

which is easily derived from the usual expression for the Bohr radius and from the relationship

$$k_F = (2m_0^* E_F)^{1/2} / \hbar \tag{24}$$

between k_F and the Fermi level in degenerate material.

¹⁹ J. G. Mavroides and D. F. Kolesar, Solid State Commun. 2, 213 (1964); O. G. Lorimor and W. G. Spitzer, J. Appl. Phys. 36, 1841 (1965).

²⁰ J. B. Krieger and S. Strauss, Phys. Rev. 169, 674 (1968).

| | n (cm ⁻³) | | | | | | | | Basis of result |
|------------------|--------------------------------------|----------------|----------------|----------------|-------|--------------|-------------|-------------|-----------------|
| $ E_a ^{x}$ (eV) | ••• | 0.008 0.286 | 0.053 0.200 | 0.105 0.100 | 0.158 | 0.210 | 0.263 | 0.315 | Fig. 1 |
| $a_0 k_F$ | 10 ¹⁵ 10 ¹⁶ | 1.31 2.79 | 1.85 3.91 | 3.51 7.14 | ••• | 3.54 7.18 | 1.84 | 1.24 | Eq. (23) |
| m_F^*/m_0^* | 10 ¹⁵ 10 ¹⁶ | 1.01 | 1.02 | 1.08 | • • • | 1.08 | 1.02 | 1.01 | Eq. (4) |
| η_F | 10 ¹⁵ 10 ¹⁶ | 4.0 18.3 | 5.8 26.0 | 11.1 46.1 | | 11.2 48.6 | 6.4 28.7 | 4.5 20.2 | Eq. (18) |

TABLE II. Calculated parameters of $Hg_{1-x}Cd_xTe$ related to Fig. 4. See Table I for definitions of symbols. The last row, giving values of the reduced Fermi level η_F , shows the degree of validity of the assumption of complete statistical degeneracy in our model.

We are assuming a parabolic conduction band for simplicity here, since Krieger and Strauss made that assumption. The resulting values of a_0k_F are listed in Table II. Referring to Fig. 1 of Krieger and Strauss, we see that the discrepancy between the Born-approximation mobility and their more nearly exact calculation is less than 30% for most of our region of interest. Our data probably have this much uncertainty and scatter, so that the inaccuracy of the Born approximation is not significant in the present study. It would be of great interest, however, to obtain still more accurate data which could be used to investigate the Krieger-Strauss predictions; $Hg_{1-x}Cd_xTe$ is a nearly ideal material for this because of the "adjustability" of its parameters due to its alloy nature.

Krieger and Strauss also point out that when $a_0k_F > 4$ in degenerate semiconductors, the screened potentials of neighboring impurity ions overlap significantly, so that their calculation based on scattering from separate ions is no longer applicable; only for 0.05 < x < 0.25 and $n = 10^{16}$ cm⁻³ is this true in our region of interest according to Table II. The row in Table II giving values of m_F^*/m_0^* shows that our assumption of a parabolic conduction band in calculating a_0k_F is reasonable, except perhaps for the range specified in the preceding sentence.

The samples for which data are plotted in Fig. 4 must be relatively uncompensated, because our model, assuming that the only ionized impurities are the singly ionized donors, accounts well for the data. That is, there must be only a negligible concentration of compensating acceptor ions in these samples.

Finally, the energy-band parameters of $Hg_{1-x}Cd_xTe$, such as in Figs. 1 and 2, are not yet "finalized," so that further small changes in the theoretical curves of Fig. 4 may yet be necessary. However, these changes are not likely to be important.

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