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Citation: *Journal of Applied Physics* **45**, 1463 (1974); doi: 10.1063/1.1663435

View online: <http://dx.doi.org/10.1063/1.1663435>

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Mobility of electrons in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$

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(Received 19 March 1973; in final form 4 June 1973)

Electron mobility in semiconducting $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ at room temperature has been calculated in the range $0.2 \leq x \leq 1.0$ by an iterative solution of the Boltzmann equation incorporating the two-mode nature of the polar optical scattering and the nonparabolicity of the conduction band. The effects of the deformation potential acoustic, ionized impurity, and electron-hole scattering have also been considered. The calculated results agree with the measured values to within a factor of 2 for $x = 0.6$ and 0.4, whereas for $x = 0.2, 0.8,$ and 1.0 the agreement is within a factor of 1.4.

The continuous variation of band parameters with composition in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ has caused a great deal of interest in its electrical and optical properties. At low temperatures the observed electron mobilities for these alloys in the vicinity of $x=0.2$ can be explained by considering ionized impurity scattering alone.^{1,2} However, at room temperature, consideration of ionized impurity and electron-hole scattering only yields mobility values an order of magnitude larger than the measured ones.¹ Calculations of Segall *et al.*³ indicate that in CdTe the polar-mode scattering predominates at room temperature. The same conclusion may also be made for HgTe at room temperature by considering the results of Aliev *et al.*⁴ and Ivanov-Omskii *et al.*⁵ One may, hence, expect that polar optical scattering would be the predominant scattering mechanism also in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ at room temperature. However, the polar-scattering-limited mobility, as calculated by Scott,¹ is found to be much larger than the measured values, particularly at low values of x .

The mixed crystal $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ is characterized by two modes of optical vibrations with frequencies close to those of the end members, CdTe and HgTe. The strengths of the two modes are nearly proportional to the constituent mole fractions.⁶⁻⁸ The effect of this two-mode behavior was taken into account by Scott¹ in an approximate way. Use was made of the expression for mobility, derived by Ehrenreich,⁹ which is valid for a material having a single longitudinal optical frequency and a parabolic band structure. The mobility of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ was estimated from a weighted average of the values obtained from this expression by using the parameters of HgTe and CdTe. A rigorous approach would be to calculate the mobility by incorporating the scattering terms for the two modes of optic vibrations including the effect of the nonparabolicity of the band structure directly in the Boltzmann equation. Results obtained from such calculations are presented in this paper.

We have assumed the electron distribution to be non-degenerate in our analysis. Schmit¹⁰ has shown that at a doping level of 10^{15} cm^{-3} (which is the usual doping level for the samples under discussion) $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ remains nondegenerate at room temperature for x greater than 0.24. A meaningful comparison of our results with experiments would therefore be possible for $x \geq 0.2$, and it is this range of x over which numerical calculations have been performed.

The effect of nonparabolicity has been included by using the dispersion relation

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E) = E \left(1 + \frac{E}{E_g} \right), \quad (1)$$

where \hbar is the Dirac constant, k the magnitude of the carrier wave vector, m^* the band-edge effective mass, E the carrier energy, and E_g the band-gap energy.

Writing the electron distribution function as

$$f(\mathbf{k}) = f_0(E) + kg(E) \cos \theta, \quad (2)$$

where θ is the angle between the wave vector \mathbf{k} and the applied electric field \mathcal{E} , the Boltzmann equation for the problem becomes¹¹

$$\sum_{i=1,2} M_i \nu_i^{(0)} g(E) = \sum_{i=1,2} M_i [\nu_i^+ g(E + \hbar\omega_i) + \nu_i^- g(E - \hbar\omega_i)] - \frac{e\hbar\mathcal{E}}{m^*(d\gamma/dE)} \frac{df_0}{dE}. \quad (3)$$

The subscripts $i=1$ and 2 denote the two modes characteristic of the optic vibrations in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. The strength of the two optic vibrations corresponding to HgTe and CdTe would be, respectively, proportional to $(1-x)$ and x . The multiplying factor M_i for a given composition, therefore, has values $(1-x)$ and x , respectively, for the two modes. $\nu^{(0)}$ is the scattering-out rate for polar scattering; ν^+ and ν^- are the corresponding scattering-in rates due to the processes of phonon emission and absorption. Expressions for $\nu^{(0)}$, ν^+ , and ν^- were obtained from a paper by Conwell and Vassell.¹² It should be mentioned that these expressions ignore the admixture of p -type valence-band wave functions. Inclusion of this admixture reduces the scattering rate, and thus to some extent offsets the effect of nonparabolicity. As we are mainly interested in the degree to which nonparabolicity affects the mobility, we have not considered this admixture. Also, the parameter values of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ have not yet reached the state of precision as to warrant the incorporation of these refinements in the calculations.

Equation (3) has been solved for $g(E)$ by numerical iteration, using the method described by Rode.¹¹ In this method, the summation terms on the right-hand side of (3) are first ignored and an approximate value of $g(E)$ is obtained by solving the resultant equation. This value of $g(E)$ is then substituted in the right-hand side to yield a more accurate value of $g(E)$, which is again used in the right-hand side. The process, when repeated a few times, gives a convergent value for mobility that is determined by the relation

TABLE I. Comparison of the results of the present analysis and those of Scott's analysis.

x	Mobilities for a parabolic band on the basis of the present analysis ($\text{cm}^2 \text{V}^{-1} \text{sec}^{-1}$)	Mobilities obtained using Scott's method and the parameter values the same as those in the previous column ($\text{cm}^2 \text{V}^{-1} \text{sec}^{-1}$)	Mobility values given by Scott ($\text{cm}^2 \text{V}^{-1} \text{sec}^{-1}$)
0.2	4.19×10^4	4.02×10^4	9.87×10^4
0.4	7.93×10^3	7.6×10^3	7.03×10^3
0.6	3.42×10^3	3.34×10^3	2.41×10^3
0.8	1.90×10^3	1.90×10^3	1.37×10^3
1.0	1.18×10^3	1.18×10^3	1×10^3

$$\mu = \frac{8\sqrt{2}\pi(m^*)^{3/2}}{3\hbar^4 n \mathcal{E}} \int_0^\infty \gamma^{3/2}(E)g(E)dE, \quad (4)$$

where n is the carrier concentration.

We have taken the values of the optic frequencies of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ from Ref. 6. Recent results given by Baars and Sorger⁸ for the composition dependence of the high-frequency dielectric constant (K_∞) of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ shows that it varies almost linearly with x from the HgTe to the CdTe value. But the variation of the static dielectric constant (K_0) is, to the knowledge of the authors, not available in the literature. For the sake of simplicity, both K_0 and K_∞ have been assumed to vary linearly with x from the HgTe to the CdTe end. Values of K_0 and K_∞ for HgTe and CdTe were taken from Refs. 13 and 14, respectively. The band-gap values (for different values of x) for room temperature as given in Ref. 15 were used.

In order to estimate the values of the band-edge effective mass, we note that it is related to the band gap by the expression^{2,10}

$$m^* = \frac{3\hbar^2 E_g}{4P^2}, \quad (5)$$

where P is the momentum matrix element. Since E_g varies almost linearly with x , it is evident from Eq. (5) that the variation of m^* will also be linear. The effective masses for different values of x have, therefore, been obtained by assuming it to vary linearly with x from zero at $x=0.093$ (where the semimetal-semiconductor transition takes place at room temperature¹⁵) to $0.111m_0$ (the value for CdTe¹⁴) at $x=1$.

For a comparison of the results of the present analysis with those obtained on the basis of the method described by Scott,¹ we have first calculated the mobility for a parabolic band. The calculated results are presented in column II of Table I. In column III we give the results obtained by Scott's method using identical values of parameters. In these calculations the factor $\exp(-\xi)G^{(1)}$ in Eq. (3) of Ref. 1 was taken to be 0.677 so as to yield the same CdTe mobility as in column II. It is found that the present analysis gives mobility values that are higher by about 4% than those obtained by Scott's method for lower values of x . For higher values of x , however, the difference between the two results becomes insignificant.

In column IV of Table I we show the theoretical values

of mobility obtained by Scott.¹ It is found that the CdTe mobility ($x=1$) given by Scott is lower than the value in column III by a factor of 1.18. The parameter values actually used by Scott are not given. The difference in the values of column III and IV, thus, indicates that Scott used slightly different values in his calculations. In order to compare the two results we have therefore multiplied the values in column IV by 1.18, so as to yield the same CdTe mobility as in column III. We then find that the mobility given in column IV is more than two times larger than that given in column III at $x=0.2$. At higher x values, however, the mobilities agree within 20%. We find that the mobility given by Scott at $x=0.2$ is obtained if the effective mass is taken as about $0.007m_0$. This mass occurs at temperatures close to absolute zero,¹⁵ where the semimetal-semiconductor transition takes place at $x \approx 0.15$. At room temperature,¹⁵ on the other hand, the transition occurs at $x=0.093$ and the effective mass at $x=0.2$ is about $0.013m_0$. This large difference in m^* gives rise to the discrepancy in the mobility values at $x=0.2$ in columns III and IV of Table I. For $x \geq 0.4$, however, the effective-mass values corresponding to the above two transitions differ within 15%. This together with small possible differences in other parameter values makes the mobilities for such values of x agree within reasonable limits. We therefore suspect that in Scott's calculation the semimetal-semiconductor transition was taken at $x \approx 0.15$, while it should be actually taken at $x \approx 0.09$.

The mobility values obtained in the present analysis incorporating the nonparabolicity of the band structure have been given in column II of Table II. On comparing these values with those in column II of Table I we find that nonparabolicity reduces the mobility particularly in the low- x samples. The decrease is 12% at $x=1.0$ and about 60% at $x=0.2$. Column IV in Table II gives the experimental results on mobility. It is found that the theoretical values given in column II are higher than the measured ones. The discrepancy is largest at $x=0.4$, where the ratio of the theoretical and the experimental mobilities is about 2. It should be mentioned that this disagreement is enhanced when the admixture of p functions is included in the calculations. This admixture reduces the scattering probability and would hence increase the calculated mobilities further.

In order to examine how far the agreement between theory and experiment is improved by the incorporation

TABLE II. Comparison of the theoretical and the experimental values of mobility.

x	Mobilities including the band nonparabolicity and polar-mode scattering only ($\text{cm}^2 \text{V}^{-1} \text{sec}^{-1}$)	Mobilities including the band nonparabolicity and the effects of polar-mode, acoustic, impurity, and electron-hole scattering ($\text{cm}^2 \text{V}^{-1} \text{sec}^{-1}$)	Experimental values (Ref. 1) ($\text{cm}^2 \text{V}^{-1} \text{sec}^{-1}$)
0.2	1.65×10^4	1.44×10^4	1.03×10^4
0.4	5.6×10^3	5.2×10^3	2.74×10^3
0.6	2.73×10^3	2.49×10^3	1.55×10^3
0.8	1.6×10^3	1.44×10^3	1.16×10^3
1.0	1.04×10^3	9.22×10^2	1×10^3

of other scattering mechanisms, we have considered the effects of deformation potential acoustic, ionized impurity, and electron-hole scattering. Inclusion of these scattering processes requires the addition of two terms $\nu_{ac}g(E)$ and $\nu_{imp}g(E)$ to the left-hand side of Eq. (3). The effect of electron-hole scattering has been estimated by using the same expression as that for impurity scattering. Expressions for the scattering rates ν_{ac} and ν_{imp} were obtained from Refs. 12 and 16, respectively.

The values assumed for the acoustic deformation potential constant (E_1) and the elastic stiffness constant (C_1) were, respectively, 9.5 eV and 6.97×10^{10} N/m². These values are the same as in CdTe.¹⁴ Variation of E_1 and C_1 with x has not been considered. The effect of the uncertainty in the values of E_1 and C_1 on mobility would not be significant since acoustic scattering contributes only a small percentage to the total scattering.

Contribution of the ionized impurity scattering has been included by assuming the sample to be uncompensated and taking the ionized donor concentration¹ as 2×10^{15} cm⁻³. This assumption gave fairly good agreement with the experimental data at low temperatures. For $x \geq 0.4$, the intrinsic carrier concentration n_i becomes¹⁰ less than 3×10^{14} cm⁻³, so that the electron-hole scattering is insignificant compared with ionized impurity scattering for such compositions and has been neglected. At $x=0.2$, however, the effect of electron-hole scattering would be significant since n_i is about 2×10^{16} cm⁻³ which is much larger than the donor concentration. The mobility at $x=0.2$ was, therefore, computed by putting the concentration of charged scattering centers at 2×10^{16} cm⁻³.

In column III of Table II we have shown the mobility values when the influences of acoustic, ionized impurity, and electron-hole scattering are considered in addition to those of polar-mode scattering and band nonparabolicity. It is found that the incorporation of other scattering mechanisms together with polar scattering slightly improves the agreement between theory and experiment. The agreement is comparatively poor at $x=0.4$ and 0.6, but is good for higher and lower values of x .

In order to determine if the discrepancy between the calculated and the measured mobilities for intermediate values of x can be attributed to excess impurity scattering, we have recalculated the mobility at $x=0.4$ using a compensation ratio of 5. However, the mobility is then found to be reduced by only 5.8%, showing the ineffectiveness of the impurity scattering.

We find that the electron mobility in Hg_{1-x}Cd_xTe at room temperature is mostly determined by the polar optical phonon scattering. The calculated values of polar-scattering-limited mobility including the effect of nonparabolicity agree with the experimental results to within a factor of 1.6 for $x=0.2$ and 0.8. In calculating the polar-scattering-limited mobility, we have used extrapolated values of effective mass and of the dielectric constants. The remaining discrepancy between the experimental and our calculated values for $x=0.2$ and 0.8 may be attributed to the inaccuracy of these extrapolated values. On the other hand, the discrepancies at $x=0.4$ and 0.6 are larger, being about a factor of 2. This larger discrepancy may be due to the assumption of the dispersion relation (1) for the inclusion of the effect of nonparabolicity. We should note that this relation is valid when the spin-orbit splitting energy Δ is either much larger or smaller than the energy gap E_g . The former condition² is obeyed at $x=0.2$ and the latter¹⁴ at $x=1$, and we may, hence, expect that for intermediate values of x Δ may be comparable to E_g and the assumed dispersion relation would not be fully applicable. The use of this dispersion relation may have introduced errors to cause larger discrepancy at $x=0.4$ and 0.6.

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