INTRINSIC CARRIER CONCENTRATIONS IN LONG WAVELENGTH HgCdTe BASED ON THE NEW, NONLINEAR TEMPERATURE DEPENDENCE OF $E_g(x,T)$ †

D. G. Seiler*, J. R. Lowney*, C. L. Littler**, and I. T. Yoon**
*Semiconductor Electronics Division, National Institute of Standards and Technology, Gaithersburg, MD 20899
**Department of Physics, University of North Texas, Denton, TX 76203

Abstract

Intrinsic carrier concentrations of narrow-gap $Hg_{1-x}Cd_xTe$ alloys ($0.17 \leq x \leq 0.30$) have been calculated as a function of temperature between 0 and 300 K by using the new nonlinear temperature dependence of the energy gap obtained previously by two-photon magneto-absorption measurements for samples with $0.24 \leq x \leq 0.26$. We report here experimental values for $E_g(x,T)$ for samples with $x = 0.20$ and 0.23 obtained by one-photon magneto-absorption measurements. These data confirm the validity of the new $E_g(x,T)$ relationship for these x values. In this range of composition and temperature, the energy gap of mercury cadmium telluride is small, and very accurate values are needed for the gap to obtain reliable values for the intrinsic carrier density. Large percentage differences exist between our new calculations and previous values for n_i at low temperatures. Even at 77 K, differences approaching 10 percent exist, confirming the importance of using the new n_i results for materials and device characterization and a proper understanding of device operation in long-wavelength materials.

Introduction

The intrinsic carrier concentration, n_i, of mercury cadmium telluride is an important quantity that must be known accurately for understanding and characterizing a wide variety of material and device properties. A great deal of effort has gone into calculating n_i from measured band parameters [1-3]. The calculations of Madarasz *et al.* [2] and Hansen and Schmit [1] are in reasonably good agreement, but are only as good as the values for the parameters that define them. The most important parameter that must be known is the band gap, which varies greatly with temperature T and composition x. Recently, two-photon magneto-absorption measurements [4] on samples of HgCdTe with $0.24 \leq x \leq 0.26$ were used to accurately determine the nonlinear temperature dependence of $E_g(T)$ for T <77 K, yielding a new $E_g(x,T)$ relation:

$$E_g = -0.302+1.93x-0.810x^2+0.832x^3+5.35\times10^{-4}(1-2x)(-1822+T^3)/(255.2+T^2), \quad (1)$$

where E_g is in eV, T in K, and $0.2 < x < 0.3$. For samples with 10-μm cutoff wavelengths (i.e., $x \approx 0.2$), the predicted maximum deviation of the new relation from that of Hansen, Schmit, and Casselman (HSC) [5] is approximately 3 to 4 meV at 10 to 12 K. Here we also report on further, experimental values of $E_g(x,T)$ for samples with $x = 0.201$ and $x = 0.229$ that confirm the use of the new relationship for lower x-value samples.

We have calculated the intrinsic carrier density, n_i, as a function of T between 0 and 300 K and as a function of x between 0.17 and 0.30 for use in materials-characterization studies and for the prediction of device operation. The model we have used to determine the nonparabolicity of the conduction band is Kane's three-band $k \cdot p$ model [6]. This

† Contribution of the National Institute of Standards and Technology; not subject to copyright.

model has also been used in the most recent calculation of n_i, which was performed by Madarasz *et al.* [2]. Their calculation was an improvement on earlier work [1,3,7] by not making any approximations other than those inherent in the $k \cdot p$ theory itself. We have used full Fermi-Dirac statistics and a momentum matrix element that did not vary with composition or temperature over our range of calculations. The results show values of n_i that differ from those of Refs. [1] and [2] by more than an order of magnitude at 5 K for all x-values studied. Differences approaching 10 percent occur even at 77 K for samples throughout the compositional range studied. Thus, it is important to include the nonlinear temperature dependence of the energy gap of $Hg_{1-x}Cd_xTe$ when modeling the low temperature operation of long-wavelength detectors.

Theory

Our calculations follow the general outline of Madarasz *et al.* [2] except that the band-gap dependence given by the HSC relation is used in Ref [2]. As in Madarasz *et al.* [2], the theory of Kane [6] was used to calculate the $E(k)$ relation for the conduction band of mercury cadmium telluride. This method uses $k \cdot p$ perturbation theory to calculate the conduction band in the vicinity of the Γ point. Interactions with the light-hole and split-off valence bands are included. To first order the conduction band does not interact with the heavy-hole band, and therefore, this band is not included. The value of Δ, the energy of the split-off band, is taken to be 1 eV [8], and the value of P, the momentum matrix element, to be 8.49×10^{-8} eV cm [8]. Madarasz *et al.* [2] vary the value of P with composition by a few percent to obtain better agreement with measured effective masses. However, we have kept P constant in order to deal directly with the effect of the nonlinearity of the temperature dependence of the energy gap and because any effective variation in P is very small over our range of x.

The intrinsic carrier density is determined by solving the following equation, from Eq. (1) of Ref. [2], where energy is in Ry and length is in atomic units:

$$\frac{2\beta^{3/2}}{\pi^{1/2}} \left(\frac{m^*_{hh}}{m_0} \right)^{-3/2} e^{\eta} \times \int_{\beta E_g}^{\infty} \frac{\gamma^{1/2}(x/\beta) \frac{d\gamma(x/\beta)}{dx} dx}{1 + e^{(x-\eta)}} = 1, \tag{2}$$

where $\beta = 1/k_B T$, m^*_{hh} is the heavy hole mass, $\gamma = k^2$, $\eta = \beta E_F$, E_F is the Fermi energy, and k is the electron wavenumber. Note that the lower limit of the integral in Eq. (2) is the reduced band gap because the zero of energy is the top of the valence band. The heavy-hole mass is taken to be 0.55 as in Ref. [2]. The value of 0.55 was used by Madarasz *et al.* because it gives better agreement with experiment. This value is also within the range of uncertainty for the spatially averaged effective mass determined from Weiler's cyclotron resonance data [8].

The computation time for the integral in Eq. (2) can be significantly reduced by performing an integration by parts to remove the derivative from the integrand. The resulting equation is:

$$\frac{4\beta^{3/2}}{3\pi^{1/2}} \left(\frac{m^*_{hh}}{m_0} \right)^{-3/2} e^{\eta} \times \int_{\beta E_g}^{\infty} \gamma^{3/2}(x/\beta) f(x)(1 - f(x)) dx = 1, \tag{3}$$

where $f(x) = 1/(1 + e^{(x-\eta)})$, and $f(x)$ is the Fermi-Dirac distribution function.

The function $\gamma(x/\beta)$ is found by inverting Kane's secular equation which is cubic in energy and solving for γ. The resulting cubic equation for γ is solved directly. A Newton-iteration technique finds the value of η. Note that full Fermi-Dirac statistics have

been used for the conduction band while nondegenerate statistics have been used for the valence band because the valence-band edge is more than the required $4k_BT$ below the Fermi energy.

Once the Fermi energy is found, the intrinsic carrier density is computed by calculating either the hole or electron density. As in Eq. (2) of Ref. [2]:

$$n_i = p = \frac{(\pi\beta)^{-3/2}}{4}\left(\frac{m^*_{hh}}{m_0}\right)^{3/2} e^{-\eta}. \tag{4}$$

Results and Discussion

One-photon magneto-absorption data were taken at various wavelengths in order to extract accurate values for the band gap for a particular temperature. A modified Pidgeon-Brown energy-band model and a free exciton binding energy of 2 meV were used to determine E_g [9]. First we show comparisons between the energy gaps obtained from the data and the predictions of Eq. (1) for the energy gap as a function of composition x and temperature T. Figures 1(a) and (b) show the excellent agreement between predictions and experiment for the temperature dependence of the energy gap for samples with x=0.229 and 0.201. The slope of the curves of E_g-vs-T initially rises rapidly and then decreases slightly beyond about 20 K to reach the asymptotic value of the HSC relation at temperatures above about 100 K. The agreement between prediction and experiment is excellent. The agreement that has been obtained between Eq. (1) and data over the compositional range of 0.20 to 0.26 from this and our earlier work now gives us the confidence to use Eq. (1) to predict the intrinsic carrier density over the narrow-gap compositional range of 0.17 to 0.30.

The result of our n_i calculation between 4 and 100 K for x=0.17 is shown in Fig. 2a. We plot the logarithm of n_i for both Eq. (1) (solid) and the HSC relation (dotted). One can see that at 5 K the difference is more than an order of magnitude while the differences become small above 77 K. We show the percentage difference between n_i computed with our new relation and with the HSC relation, relative to the values computed with our new relation in Fig. 2b for the same composition. Even at 77 K the percentage difference is about seven percent. We show the same set of graphs in Fig. 3 for an x-value of 0.22. It is not possible to see the difference between our results and those based on the HSC relation directly in Fig. 3a because of the rapid variation of n_i with T. However, from the percentage differences given in Fig. 3b, one observes that the overall differences are similar to those of Fig. 2b, which shows that our relation is important throughout the long-wavelength region of mercury cadmium telluride. Similar results are also obtained for x=0.30.

The differences between the n_i results of Hansen and Schmit [1] and Madarasz *et al.* [2] are small in the range of x-values between 0.17 and 0.30. Part of the difference is due to the larger effective mass used in Ref. [2], which leads to an approximately fifteen percent increase in n_i. However, there are compensating effects due to the use of full Fermi-Dirac statistics in Ref. [2] that reduce the differences to generally less than ten percent. Thus, whether one compares the results from our calculations with either those of Refs. [1] or [2], the overall behavior is similar. At temperatures below about 50 K, our new relation gives significantly larger values of n_i than either previous one, while at temperatures above 77 K, the differences are small among all three sets of calculations. Analytic functions are being fit to the n_i curves for use in modeling.

These results have important implications for HgCdTe material characterization and device operation. In device operation it is usually necesary to compute diffusion currents

for minority carriers, which depend on n_i^2. Recombination is also sensitive to n_i with radiative and Auger recombination varying as n_i^2. A quantity of great importance to the operation of infrared detectors, the resistance-area product R_0A, also depends on n_i^2. Tunneling currents and impact ionization depend exponentially on the energy gap so that there is a definite need to use Eq. (1) in expressions for these quantities, especially at low temperatures. The reason that such quantities depend so critically on the value of E_g at low temperatures is that the thermal energy, k_BT, is so small.

Conclusions

We have computed the intrinsic carrier density of $Hg_{1-x}Cd_xTe$ for x between 0.17 and 0.30 as a function of temperature between 4 and 300 K. A new and highly accurate relation for the energy gap has been used, which was determined from one- and two-photon magneto- absorption spectroscopy. These data are presented in this and earlier work. Kane's theory has been used to treat the nonparabolicity of the conduction band. The results of the calculations show the need to include the nonlinearity of the temperature dependence of the energy gap, even though the nonlinearities are only several millivolts. Therefore, our new relation for the energy gap has important consequences in HgCdTe material characterization and device operation at temperatures below 77 K.

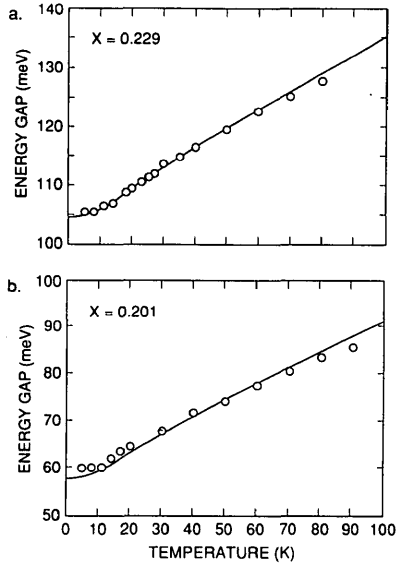

Figure 1. a.) Energy gap of sample with $x = 0.229$ as a function of temperature. The fit by our new relation with $x = 0.2285$ is the solid line. b.) Energy gap of sample with $x = 0.201$ as a function of temperature. The fit by our new relation is the solid line.

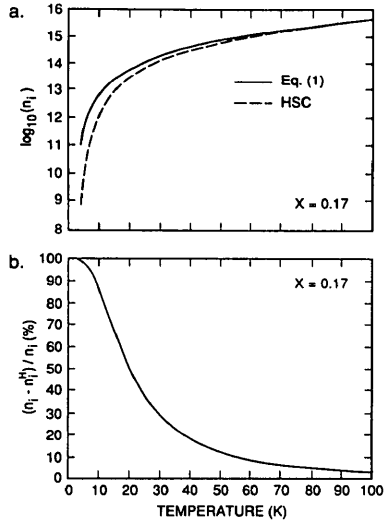

Figure 2. a.) Logarithm of the intrinsic carrier density, n_i, (cm^{-3}) as a function of temperature for $x = 0.17$. The solid line is with our new relation and the dotted line is with the HSC relation. b.) The percentage difference between n_i from our new relation and n_i^H from the HSC relation, relative to our new relation.

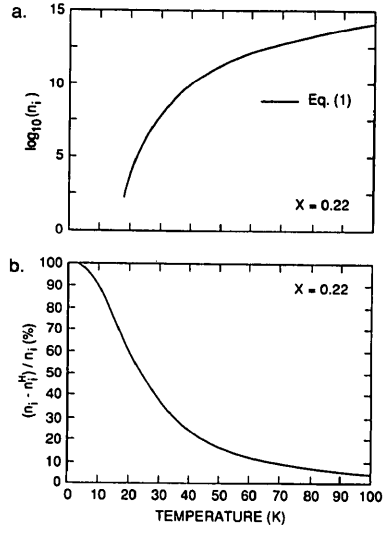

Figure 3. a.) Logarithm of the intrinsic carrier density, n_i, (cm^{-3}) as a function of temperature for $x = 0.22$. The solid line is with our new relation. b.) The percentage difference between n_i from our new relation and n_i^H from the HSC relation, relative to our new relation.

References

1. G. L. Hansen and J. L. Schmit, *J. Appl. Phys.* 54, 1639 (1982).
2. F. L. Madarasz and F. Szmulowicz, *J. Appl. Phys.* 58, 2770 (1985).
3. Y. Nemirovsky and E. Finkman, *J. Appl. Phys.* 50, 8107 (1980).
4. D. G. Seiler, J. R. Lowney, C. L. Littler, and M. R. Loloee, *J. Vac. Sci. Technol. A* 8, 1237 (1990).
5. G. L. Hansen, J. L. Schmit, and T. N. Casselman, *J. Appl. Phys.* 53, 7099 (1982).
6. E. O. Kane, *J. Phys. Chem. Solids* 1, 249 (1957).
7. J. L. Schmit, *J. Appl. Phys.* 41, 2876 (1970).
8. M. H. Weiler, *Semiconductors and Semimetals*, edited by Willardson and Beer (Academic, New York, 1981), Vol. 16, p. 119.
9. D. G. Seiler, C. L. Littler, M. R. Loloee, and S. A. Milazzo, *J. Vac. Sci. Technol. A* 7, 370 (1989).