# Energy gap versus alloy composition and temperature in $Hg_{1-x}Cd_xTe$[a)]

G. L. Hansen, J. L. Schmit, and T. N. Casselman
*Honeywell Corporate Technology Center, Bloomington, Minnesota 55420*

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We have used the data from 22 different studies to derive a new empirical expression for the energy band gap ($E_g$) of $Hg_{1-x}Cd_xTe$: $E_g = -0.302 + 1.93x + 5.35(10^{-4})T(1-2x) - 0.810x^2 + 0.832x^3$. This expression is valid over the full composition range and for temperatures from 4.2 to 300 K. The standard error of estimate is 0.013 eV, which is at least 15% better than that of previously reported expressions.

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The development of mercury-cadmium telluride infrared detectors requires an accurate expression relating the energy band gap ($E_g$) to the mole fraction of cadmium ($x$) and temperature ($T$). Several such expressions have been presented in the literature,[1-5] each for a restricted range of $x$ and $T$. In this work we present a new empirical expression for $E_g(x,T)$ which has been fitted to energy gap data from a variety of sources covering the ranges $0 \leqslant x \lesssim 0.6$ (plus $x = 1$) and $4.2 \lesssim T \lesssim 300$ K.

The data used in the fitting of this expression were obtained from both optical absorption[1-3,6] and magneto-optical experiments.[4,7-20] The results of Ref. 6 are given in Table I.

The studies used various methods to determine $x$. Finkman and Nemirovsky[3] estimated a value for the energy gap from the $\alpha = 1000$ cm$^{-1}$ point on optical transmission curves. They used $x$ as stated by the vendor Cominco. Cominco, in turn, determined $x$ by optical transmission cutoff calibrated against the destructive chemistry of $Hg_{1-x}Cd_xTe$ wafers. Scott[2] defined $E_g$ as the $\alpha = 500$ cm$^{-1}$ point on optical transmission curves, and determined the composition from the density assuming a linear relationship. Schmidt and Stelzer[1] determined $E_g$ from the detector cutoff at half-peak value. The detectors were 10 $\mu$m thick; thus, the peak response is equivalent to $\alpha = 1000$ cm$^{-1}$ and the half-peak value should approximate the $\alpha = 500$ cm$^{-1}$ point on the absorption edge. They determined the composition by measuring density $\rho$, using the expression[21]

$$x = 3.628 - 0.44924\rho.$$

The four lowest $x$ samples of Schmit and Stelzer's original eight were deleted from the present work because of the presence of mercury inclusions. The energy gap for the diodes of Tobin and the photoconductors of Rawe (Table I) was determined from the 50% point ($\alpha \approx 500$ cm$^{-1}$) of the detector cutoff, and composition was determined from density.

It should be noted in all cases that what is actually measured by optical absorption techniques is cutoff energy $E_{co}$ rather than the energy band gap itself. However, despite the different cutoff criteria used the optical data are consistent with the magneto-optical measurements, and $E_g$ can be safely associated with $E_{co}$.

The magneto-optical data represent the most recent results of this technique. For the magneto-reflective results of Weiler,[4] we used values of $x$ as determined by Micklethwaite, who used transmission cut on.[22] Reine also remeasured $x$ for the Weiler's samples using a density technique[23] resulting in shifts of $x$ from $+0.01$ to $+0.035$ compared to Weiler's values. We feel that Micklethwaite's data are the most accurate of the three measurements. It should be emphasized that of all the magneto-optical data, we have only shifted Weiler's values of $x$ because we possessed the additional measurements on her samples; this does not imply the superiority of the $x$ measurements in other studies cited here.

Two studies provide the extremes of $x$: optical measurements of CdTe by Spitzer and Mead,[24] and magnetotransmission data from Dobrowolska *et al.*[25] for the HgTe point.

The fitting procedure involved first calculating, by means of linear regression, the slope of $E_g$ versus $T$ for each of the 22 samples which had temperature dependent data. Using the resulting set of linear functions, $\delta E_g/\delta T$ was determined as a function of $x$ by a second linear least squares fit (Fig. 1):

$$\frac{\delta E_g}{\delta T} = -1.08(10^{-3})x + 5.35(10^{-4}). \tag{1}$$

Normalized to $T = 80$ K, the following relation

$$E_g(x,80) = E_g(x,T) - (T-80)\frac{\delta E_g}{\delta T}, \tag{2}$$

resulted in an average value of $E_g$ for each sample at 80 K.

Finally, a nonlinear least squares fit to these data, plus

TABLE I. Tobin and Rawe data $T = 80$ K.[6]

| Study | $x$ (Mole fraction) | $E_{co}$ (eV) at $T = 80$ K |
|---|---|---|
| Tobin data (photodiodes) | 0.199 | 0.0873 |
| | 0.202 | 0.0867 |
| | 0.205 | 0.0879 |
| | 0.206 | 0.0899 |
| | 0.208 | 0.0961 |
| | 0.210 | 0.0992 |
| | 0.213 | 0.1033 |
| Rawe data (photoconductors) | 0.199 | 0.0790 |
| | 0.204 | 0.0867 |
| | 0.205 | 0.0919 |
| | 0.206 | 0.0912 |
| | 0.207 | 0.0925 |
| | 0.209 | 0.0939 |
| | 0.210 | 0.1008 |
| | 0.211 | 0.1016 |
| | 0.216 | 0.1097 |

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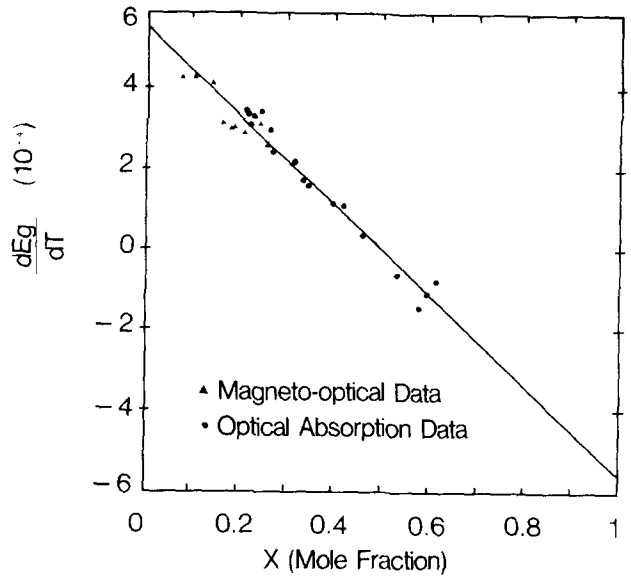


FIG. 1. The fitted slope of energy gap with respect to temperature as a function of $x$ (solid line), and data from the indicated studies. Optical and magneto-optical samples are shown for which there is temperature dependence.

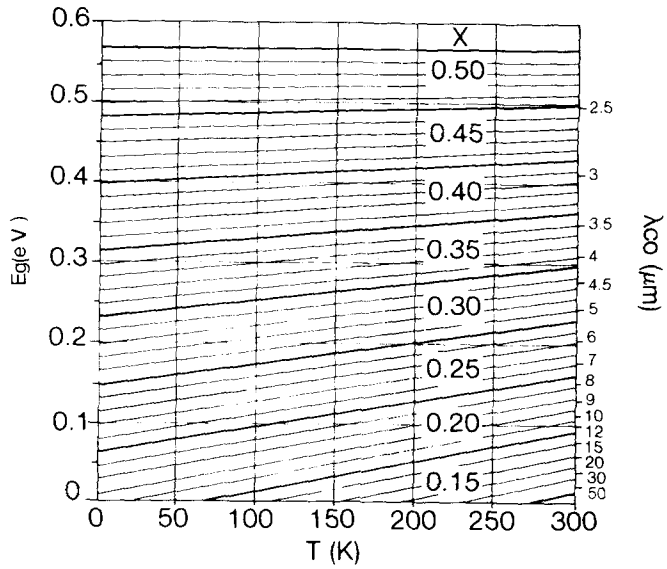


FIG. 3. $E_g$ vs $T$ for various values of $x$ calculated from Eq. (3).

the non-temperature-dependent data gave the following expression

$$E_g(x,T) = -0.302 + 1.93x + 5.35(10^{-4})T(1-2x) - 0.810x^2 + 0.832x^3. \quad (3)$$

The dependence of $E_g$ on $x$ in the region $(0.2 < x \lesssim 0.6)$ is approximately linear; however, a cubic expression was needed to represent the full range (Figs. 2 and 3). However, it must also be noted that the true $x$ dependence of $E_g$ for $x \gtrsim 0.6$ is conjectural.

The agreement between the empirical expression in Eq. (3) and the data is quite good, and is an improvement over that of other empirical expressions for $E_g$. The comparisons in Table II show the quality of fit over the full range of $x$ (0 to 0.6) and $T$ (4.2–300 K), even though several of the expressions listed were not meant to be extended to this range. Further calculations show that the new expression provides a 15% improvement in standard error over that of the Finkman-Nemirovsky equation within its specified range of $0.205 \leqslant x \leqslant 0.220$. Similarly, the new expression gives an improvement of about 60% in the standard error over that of the expression of Weiler within its specified range of $x < 0.3$ and $T < 100$ K.

The fit of the new expression at the extremes of $x$ also appears to be good, especially since the data were not well grouped. At $x = 0$ the curve passes within 0.009 eV of the measured HgTe point of Dobrowolska *et al.* ($E_g \approx -0.254$ at $T = 80$ K). At $x = 1$, the expression yields a value of $E_g$ within 0.005 eV of the gap for CdTe[22] ($E_g \approx 1.6$ at $T = 80$ K).

There are several possible sources of error. Among these are the different choices of $\alpha$ at which cutoff is determined, as well as the difference between energy cutoff and energy gap. Also, different measurement techniques used by the 22 studies cited here are undoubtedly a source of error. The range in the $x$ value is critical in small band gap

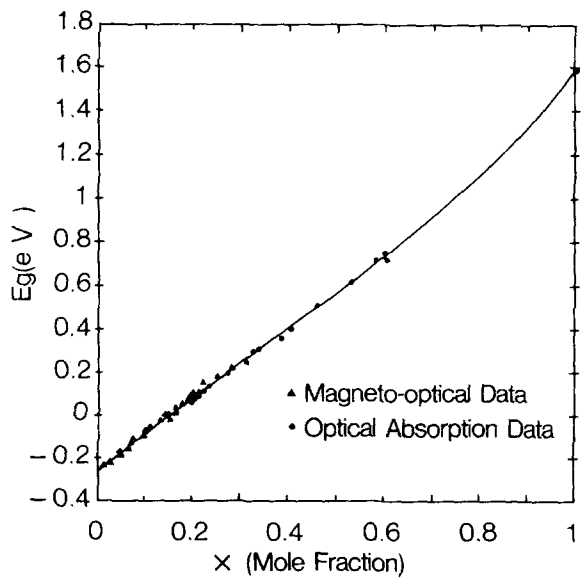


FIG. 2. The new expression on a plot of energy gap vs composition for $T = 80$ K. Also shown are the complete data used to fit the relation. The fit is nearly linear for $0.1 < x < 0.7$. A conjectural cubic dependence includes the CdTe point.

TABLE II. Comparison of energy gap expressions for $0 \leqslant x \leqslant 1$ and $4.2 \leqslant T \leqslant 300$.

| Study | Average deviation $\overline{\Delta E_g}$ (eV) | Standard error of estimate (eV) |
|---|---|---|
| This work | −0.001 | 0.013 |
| Scott[2] | −0.006 | 0.018 |
| Schmit and Stelzer[1] | 0.015 | 0.021 |
| Weiler[19] | 0.032 | 0.042 |
| Finkman and Nemirovsky[3] | 0.022 | 0.042 |
| Wiley[5] | 0.042 | 0.051 |

$Hg_{1-x}Cd_xTe$; a typical $x$ variance of $\pm 0.003$ near $x = 0.2$ results in an $E_g$ variance of $\pm 0.005$ eV, which is 6% of the band gap at 80 K. An error in temperature measurement is less important. A reasonable variance in $T$ of $\pm$ 1K gives an $E_g$ variance of $\pm 0.0003$ eV, only 0.004 of the bandgap at 80 K. The new expression is a compromise; a more definitive expression must await the refinement of methods for measuring $x$.

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