Empirical expressions for the alloy composition and temperature dependence of the band gap and intrinsic carrier density in $Ga_xIn_{1-x}As$

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The band gap and the intrinsic carrier concentration in a semiconductor are important material parameters needed in the interpretation of various experimental and theoretical data. In the present work, empirical expressions for both the parameters as a function of alloy composition x and temperature are proposed for $Ga_xIn_{1-x}As$. The calculated results for band gap are in close agreement with the available data, while the same for intrinsic concentration give fair agreement with the data at the two ends of the alloy composition.

I. INTRODUCTION

The intrinsic carrier concentration is an important material parameter for semiconductors. The knowledge of this concentration is required in various analyses,[1,2] a typical example being in the interpretation of the capacitance (C)-voltage (V) characteristics of metal-insulator-semiconductor (MIS) or p-n junction diodes. In ternary semiconductors, the intrinsic carrier concentration n_i is a function of the composition x and temperature T, since the band gap E_g is itself a function of both the variables. In many cases it is useful to obtain analytical expressions for n_i in terms of x and T. Such an expression has been obtained[3] for $Hg_xCd_{1-x}Te$, and has been used to obtain the C-V characteristics of $Hg_xCd_{1-x}Te$-based MIS structures which determines the doping and composition profiles.

$Ga_xIn_{1-x}As$ is an important ternary semiconductor that finds widespread application in various high-speed electronic and optoelectronic devices.[4] In order to interpret different data obtained for this material, the knowledge of $n_i(x,T)$ is necessary. Keeping this in view, we propose an empirical relation for n_i in $Ga_xIn_{1-x}As$ as a function of x and T. The expression for the band gap E_g, either as a function of x only[5,6] for fixed T, or as a function of T only[7] for fixed values of x are available. We first develop an empirical relation for E_g as a function of both x and T, in terms of the temperature-dependent band gap of the two constituents GaAs and InAs. It is, however, assumed that the band-gap bowing parameter c, defined in Eq. (1) below, is independent of temperature. Furthermore, the band gap versus temperature relation for $x=0$ and 1 is assumed to be expressed in terms of two parameters α and β that are obtained by a least-squares fit to the experimental data. The expression for $E_g(x,T)$ so obtained is found to give values in close agreement with the data available for GaInAs. Using this expression and assuming linear variation of the effective mass between $x=0$ and 1, the expression for $n_i(x,T)$ is then developed. The calculations are given in Sec. II. In Sec. III, the calculated values of $n_i(x,T)$ are presented and are compared with the available experimental data for the two extreme values of the alloy composition (i.e., for InAs and GaAs). The range of applicability of the expression is then examined. Section IV gives the conclusion of the present work.

II. CALCULATIONS

The variation in the band-gap energy E_g with composition of a ternary alloy $A_xB_{1-x}C$ is expressed as[8]

$$E_g(x) = a + bx + cx(1-x), \tag{1}$$

where a and $(a+b)$ are, respectively, the measured band gap at $x=0$ and $x=1$ and the last term depends on the bowing parameter c. Equation (1) may be rewritten for $Ga_xIn_{1-x}As$ as a function of x and T as follows[5]:

$$E_g(x,T) = E_g^{\mathrm{InAs}}(T) + [E_g^{\mathrm{GaAs}}(T) - E_g^{\mathrm{InAs}}(T)]x + 0.475x(1-x). \tag{2}$$

Using the expression[1] $E_g(T) = E_g(0) - [\alpha T^2/(T+\beta)]$, one may obtain from Eq. (2)

$$E_g(x,T) = E_g^{\mathrm{InAs}}(0) - \frac{\alpha^{\mathrm{InAs}}T^2}{T+\beta^{\mathrm{InAs}}} + \left[E_g^{\mathrm{GaAs}}(0) - \frac{\alpha^{\mathrm{GaAs}}T^2}{T+\beta^{\mathrm{GaAs}}} - E_g^{\mathrm{InAs}}(0) + \frac{\alpha^{\mathrm{InAs}}T^2}{T+\beta^{\mathrm{InAs}}}\right]x - 0.475x(1-x). \tag{3}$$

The values of $E_g(0)$, α, and β are given in Table I and using the values, we may write

TABLE I. Values of material parameters E_g, α, and β.

	E_g in eV 0 K	300 K	77 K	α ($\times 10^{-4}$)	β
GaAs	1.52[a]	1.42[a]	⋯	5.8[a]	300[a]
InAs	0.42[a]	0.36[a]	0.41[b]	4.19[a]	271

[a] See Ref. 1.
[b] See Ref. 12.

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$$E_g(x,T) = 0.42 + 0.625x - \left(\frac{5.8}{T+300} - \frac{4.19}{T+271}\right) 10^{-4}T^2x - \frac{4.19\times 10^{-4}}{T+271} T^2 + 0.475x^2. \quad (4)$$

It seems worthwhile at this stage to examine the validity of the expression given above in the light of the available experimental data.[5,7,8] Table II compares the data of $E_g(0.47,T)$ obtained from Eq. (4) with the available data reported by different workers. Table III gives the results for $E_g(x, T = 2\text{ K})$ for $0.45 \leqslant x \leqslant 0.48$. The comparison indicates that the above relation is perfectly satisfactory.

To obtain the expression for the intrinsic carrier density, we note that the electron density in the conduction band is[3,9]

$$n = 2\left(\frac{m_e(0)k_BT}{2\pi\hbar^2}\right)^{3/2} F(\epsilon,\eta), \quad (5)$$

$$F(\epsilon,\eta) = \frac{2}{\pi^{1/2}}\int_0^\infty \frac{\phi^{1/2}(1+\phi/\epsilon)^{1/2}(1+2\phi/\epsilon)}{\exp(\phi-\eta)+1} d\phi, \quad (6)$$

where $\eta = (E_f - E_g)/k_BT$, $\phi = [E_c(k) - E_g]/k_BT$, and $\epsilon = E_g/k_BT$. In the above, $m_e(0)$ is the effective mass of the conduction-band electrons at $k = 0$, F is the Fermi–Dirac integral for a nonparabolic band, η, ϕ, and ϵ are the reduced energies, the energy being measured from the top of the valence band, k_B is the Boltzmann constant, $\hbar$ is Planck constant divided by 2π, E_f and E_c, are respectively, the Fermi energy and the energy in the conduction band. The hole density may be expressed as

$$p = \left(\frac{m_{dh}k_BT}{\pi\hbar^2}\right)^{3/2} \frac{1}{\sqrt{2}} \exp[-(\epsilon+\eta)], \quad (7)$$

where m_{dh} is the density-of-states mass for the valence band given by

$$m_{dh}^{3/2} = m_{\rm lh}^{3/2} + m_{\rm hh}^{3/2}, \quad (8)$$

lh and hh refer to the light hole and heavy hole, respectively. The intrinsic reduced Fermi energy η_i may be found by equating Eqs. (5) and (7), so that

$$m_e(0)^{3/2}F(\epsilon,\eta_i) = m_{dh}^{3/2}\exp[-(\epsilon+\eta_i)]. \quad (9)$$

Over a wide range of temperature (0–500 K), $\epsilon > 2$, $\eta < -2$ for $Ga_xIn_{1-x}As$, so that the approximation[9]

TABLE II. Comparison of the band-gap energy in $Ga_xIn_{1-x}As$ at different temperature (T) for a fixed composition ($x = 0.47$) with the present work.

	Values of band-gap energy $E_g(x,T)$ in eV			
	Towe[a]	Pearsall[b]	Goetz *et al.*[c]	Present work
$E_g(0.47,0)$	0.820	0.812	0.813 (2 K)	0.819
$E_g(0.47,77)$	0.802	0.789	⋯	0.809
$E_g(0.47,300)$	0.7305	0.750	⋯	0.735

[a] See Ref. 7.
[b] See Ref. 8.
[c] See Ref. 5.

TABLE III. Comparison of the band-gap energy (E_g) in $Ga_xIn_{1-x}As$ at different composition (x) for a fixed temperature (2 K) with the present work.

$E_g(x,T)$	$E_g(0.45,2)$ (eV)	$E_g(0.46,2)$ (eV)	$E_g(0.47,2)$ (eV)	$E_g(0.48,2)$ (eV)
Goetz *et al.*[a]	0.7918	0.8025	0.8133	0.8241
Present work	0.7974	0.8080	0.8187	0.8294

[a] See Ref. 5.

$$F(\epsilon,\eta) = e^\eta\left(1 + \frac{3.75}{\epsilon} + \frac{3.2812}{\epsilon^2} - \frac{2.4609}{\epsilon^3}\right) \quad (10)$$

is valid. Thus from Eqs. (9) and (10), one gets

$$e^{\eta_i} = \left(\frac{m_{dh}}{m_e(0)}\right)^{3/4} \times \frac{\exp(-\epsilon/2)}{(1 + 3.75/\epsilon + 3.2812/\epsilon^2 - 2.4609/\epsilon^3)^{1/2}}. \quad (11)$$

Putting Eq. (11) in Eq. (7), we may write

$$n_i(x,T) = \left(\frac{k_BT}{\pi\hbar^2}\right)^{3/2} \frac{1}{\sqrt{2}}[m_{dh}m_e(0)]^{3/4}e^{-\epsilon/2} \times\left(1 + \frac{3.75}{\epsilon} + \frac{3.2812}{\epsilon^2} - \frac{2.4609}{\epsilon^3}\right)^{1/2}. \quad (12)$$

We employ the linear interpolation scheme[6] to relate the effective mass and the composition, i.e.,

$$m(Ga_xIn_{1-x}As) = m(\text{InAs}) + [m(\text{GaAs}) - m(\text{InAs})]x \quad (13)$$

and using the mass values given,[11,12] we get finally

$$n_i(x,T) = 4.8327\times 10^{15}[(0.41+0.09x)^{3/2} + (0.027+0.047x)^{3/2}]^{1/2}\times(0.025+0.043x)^{3/4} \times\left[T^{3/2}e^{-\epsilon/2}\left(1 + \frac{3.75}{\epsilon} + \frac{3.2812}{\epsilon^2} - \frac{2.4609}{\epsilon^3}\right)^{1/2}\right]. \quad (14)$$

III. RESULTS

The values of the intrinsic carrier density in $Ga_xIn_{1-x}As$ as a function of composition x obtained from Eq. (14) are plotted in Fig. 1 for several values of temperature T.

To the best of our knowledge, there are no published experimental data on the intrinsic carrier concentration of $Ga_xIn_{1-x}As$ in the useful range of composition, i.e., $x = 0.47$. In view of this, we compare the values of $n_i(x,T)$ obtained from Eq. (14) for two extreme values of x with the reported data for InAs and GaAs at several temperatures. The values are entered in Table IV. A comparison indicates that the present values agree with the data for GaAs quite well. However, our values are somewhat larger than the values quoted for InAs. The uncertainties in the values of the

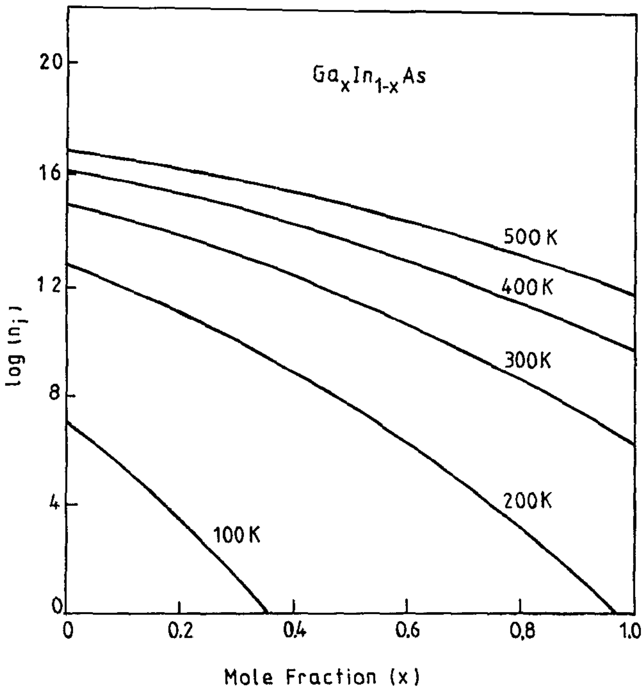

FIG. 1. Variation of intrinsic carrier concentration $n_i(x,T)$ in $Ga_xIn_{1-x}As$ with alloy composition (x) at different temperatures.

effective mass and the warping of the valence bands may be the sources of this discrepancy. In order to verify the correctness of our values, experimental data should be available. We hope that the present work will stimulate activity in this direction.

IV. CONCLUSIONS

In conclusion, we have developed empirical expressions for the composition and temperature dependence of the band gap and intrinsic carrier density in GaInAs. The expression for band gap gives satisfactory values that agree with available data. The correctness for the expression for n_i cannot be tested for GaInAs, because of lack of data; however, it yields correct values for GaAs, and values of the same order for InAs, as reported by other workers.

TABLE IV. Comparison of the available intrinsic carrier concentration (n_i) at the two extreme ends of $Ga_xIn_{1-x}As$ with the present work at 300, 400, and 500 K.

	GaAs (cm^{-3})			InAs (cm^{-3})		
	300 K ($\times 10^6$)	400 K ($\times 10^{10}$)	500 K ($\times 10^{12}$)	300 K ($\times 10^{15}$)	400 K ($\times 10^{16}$)	500 K ($\times 10^{17}$)
Available data (n_i)	1.79[a] 2.38[c]	0.6[a]	0.82[a]	0.57[b]	0.85[b]	0.52[b]
Present work (n_i)	1.95	0.602	0.839	0.988	1.45	0.83

[a] See Ref. 1.
[b] See Ref. 13.
[c] See Ref. 10.

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