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An assessment of some theoretical models used for the calculation of the refractive index of $In_XGa_{1-x}As$

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ABSTRACT

Theoretical models used for the determination of the refractive index of $In_XGa_{1-X}As$ are reviewed and compared. Attention is drawn to some problems experienced with some of the models. Models also extended to the mid-infrared region of the electromagnetic spectrum. Theoretical results in the mid-infrared region are then compared to previously published experimental results.

1. Introduction

InGaAs structures have attracted attention for use in optical devices such as laser diodes [1], photo detectors [2] and optical modulators [3]. The InGaAs-based alloys have higher electron transport properties than GaAs, and the room temperature band gap of the material lends itself to applications in the field of infrared LED's and detectors [4–6].

One of the important properties of any optical material is the refractive index, n, of such material. Consequently, this parameter has been determined or measured for just about all materials currently known. However, there are still some materials for which this parameter is not known throughout the whole of the electromagnetic spectrum. One example is $In_xGa_{1-x}As$: a review of literature available on the optical properties of $In_xGa_{1-x}As$ reveals that the refractive index of this material is known mainly in the visible and ultraviolet region (0.5 – 6 eV = 2480 – 207 nm = 4033 – 48395 cm^{-1}) of the spectrum [7–21]. Only four papers reported on work done in the infrared region, reporting on the dielectric parameters determined by infrared reflectance or the refractive index [14,18,19,21].

The current investigation reports on an assessment of some theoretical models proposed for the calculation of the refractive index of $In_xGa_{1-x}As$. A comparison is made between values of the refractive indices obtained by the various models in the nanometer range of the electromagnetic spectrum to determine the most appropriate model. Subsequently, the theoretical models that were investigated are extended to the mid-infrared region (4000 – 200 cm^{-1} = 0.5 – 0.025 eV) of the spectrum. As part of the assessment, a comparison of the theoretically calculated values and previously obtained experimental values for the refractive index of some samples of $In_xGa_{1-x}As$ in the mid-infrared region is made.

2. Theory

2.1. Single oscillator model

One way to calculate the refractive index is based on the single oscillator model of Wemple and DiDomenico [7,22]:

$$n^2 - 1 = E_0E_d/(E_0^2 - (h\nu)^2) \quad (1)$$

where E_0 is the energy of the oscillator in the intrinsic absorption region, E_d is the dispersion energy and hυ the energy of the incident radiation. Values for E_0 and E_d for $In_xGa_{1-x}As$ were determined by Tagaki [7], as being

$$E_0 = 3.65 - 2.15x \quad (2)$$

$$E_d = 36.1 - 19.9x \quad (3)$$

where x is the fraction of indium content.
E_0 can also be calculated from the band gap energy E_g by [7,23]:

$$E_0 = 0.94 + 1.90E_g \quad (4)$$

The band gap E_g is given by [20] as

$$E_g = E_{gGaAs} - 1.501x + 0.436x2 \quad (5)$$

with $Eg_{GaAs} = 1.424eV$ at room temperature.

Note that Nahory and co-workers reported slightly different band gap energy equations for $In_xGa_{1-x}As$ [24].

$$E_g = 1.425 - 1.337x + 0.270x^2 \quad (6)$$

And also as [25].

$$E_g = 0.36 + 0.629x + 0.436x^2 \quad (7)$$

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A further two formulae was provided by Jain et al. [26,27], namely

$$E_g = 0.\,36 + 1.\,064x \tag{8}$$

$$E_g = 0.\,354 + 0.\,576x + 0.\,475x^2 \tag{9}$$

On the other hand, Wemple et al. [28] reported the following relation for E_0 for III-V and II-IV-V_2 materials:

$$E_0 = 2.\,84 + 0.\,64E_g \tag{10}$$

Note also that it was pointed out by Nojima and Asahi [9], that the expressions for E_0 and E_d are growth method dependent for multi-quantum-well structures, with molecular beam epitaxy (MBE) and metalorganic molecular beam epitaxy (MOMBE) having different expressions to those for liquid-phase epitaxy (LPE) and vapour phase epitaxy (VPE). Unfortunately they only provided relations for MBE/MOMBE growth, viz.

$$E_0 = 2.\,21x + 2.\,02 \tag{11}$$

$$E_d = 13.\,2x + 20.\,9 \tag{12}$$

2.2. Modified single oscillator model

An improved equation for the refractive index of $In_xGa_{1-x}As$ was obtained from the work of Afromowitz [23], based on the model of Wemple and DiDomenico [22], by Takagi [7]:

$$n^2\text{–}1 = E_d/E_0 + Ed_d/E_0{}^3(h\upsilon)^2 + \eta/\pi\,(h\upsilon)^4 ln\,[2E_0^2 - E_g^2 - (h\upsilon)^2/(E_g^2 - (h\upsilon)^2)] \tag{13}$$

$$\text{with}\eta = \pi E_d/[2E_0^3(E_0^2 - E_g^2)] \tag{14}$$

E_0, E_d, E_g and $h\upsilon$ have the same meaning as in Section 2.1.

2.3. Sellmeier model

The refractive index of a material may also be established from the Sellmeier equation [29]:

$$n^2(\lambda) = 1 + B1\lambda^2/(\lambda^2 - C_1) + B_2\lambda^2/(\lambda^2 - C_2) + B_3\lambda^2/(\lambda^2 - C_3) \tag{15}$$

where $B_{i=1,2,3}$ and $C_{i=1,2,3}$ are Sellmeier coefficients which are experimentally determined. A more general form of the above equation is used in the case of semiconductor materials [30], viz.

$$n^2(\lambda) = A + B_1\lambda^2/(\lambda^2 - C_1) + B_2\lambda^2/(\lambda^2 - C_2) \tag{16}$$

where the coefficient A is taken as an approximation of the short-wavelength absorptions to the refractive index. For $In_xGa_{1-x}As$, the Sellmeier equation is given at room temperature by [20]:

$$n = [A + B/\{1\text{–}(C.\,E_{GaAs}/\lambda\,E_g(x))^2\}]^{1/2} \tag{17}$$

where x is the In fraction, λ is the wavelength in μm, and the empirical coefficients $A = 8.950$, $B = 2.054$, $C = 0.6245$ and E_g given by Eq. (5).

Refractive index calculations using Eq. (17) have only been performed in the nanometre range of wavelengths for $In_xGa_{1-x}As$ [20].

2.4. Dielectric function model

Another way of determining the refractive index n for $In_xGa_{1-x}As$ based on the real part of the dielectric constant ε', was proposed by Alam et al. [19]:

$$n = \sqrt{(\varepsilon')} \tag{18}$$

where the real part of the dielectric constant ε' is given as function of frequency υ by Adachi [31]:

$$\varepsilon'(\upsilon) = A\{f(\chi) + ½[E_0/(E_0 + \Delta_0)]^{1/2} f(\chi_s)\} + B \tag{19}$$

$$\text{Where} f(\chi) = \chi^{-2}[2 - (1+\chi)^{1/2} - (1-\chi)^{1/2}] \tag{20}$$

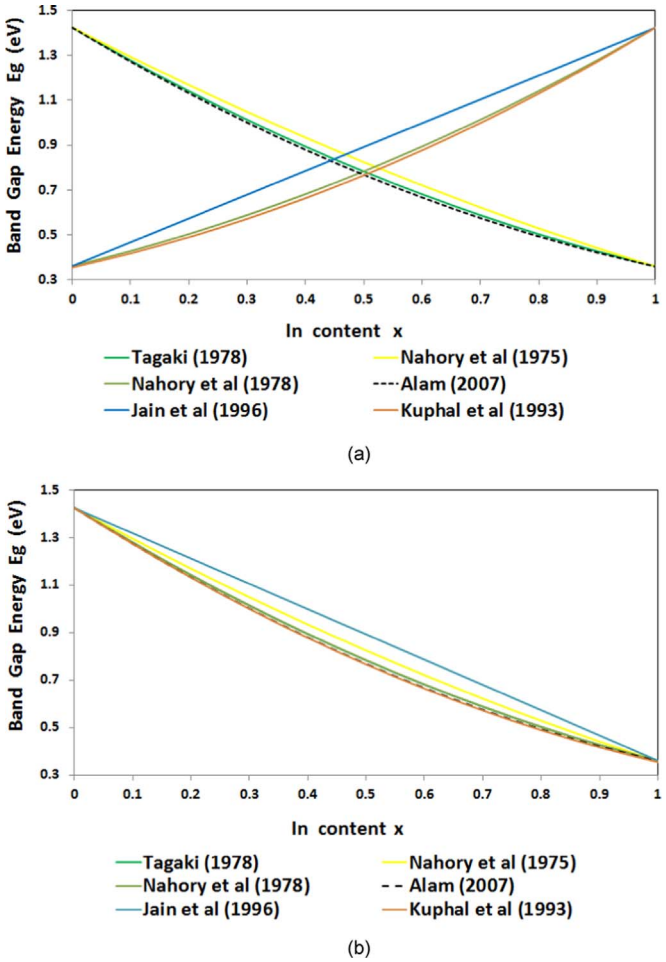

Fig. 1. (a) Calculated values of the band gap energy E_g according to the various proposed theoretical models and (b) corrected plot of band gap energy Eg as function of In content.

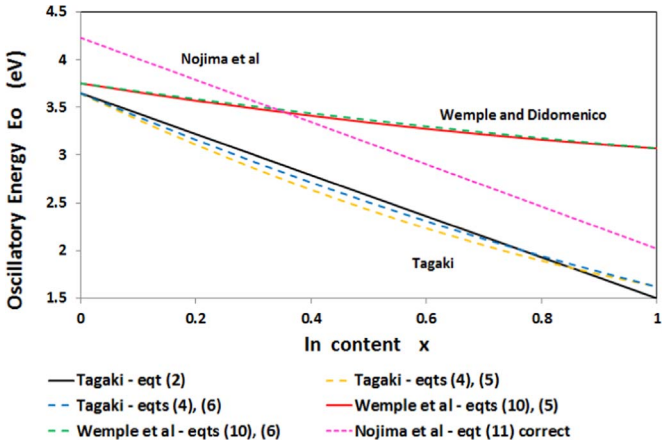

Fig. 2. Oscillator energy E_0 as function of In doping content x, according to the various proposed models.

$$\chi = \hbar\upsilon/E_0 and \chi_s = \hbar\upsilon/(E_0 + \Delta_0) \tag{21}$$

$$\text{with} E_0 = 1.\,424 - 1.\,56x + 0.\,494x^2 \tag{22}$$

In the above, A, B and are Δ_0 are parameters established using linear interpolation between values provided by Adachi [19,31] for GaAs and InAs. In the present study, the following relations were hence used:

$$A = 4.\,93x + 9.\,29 \tag{23}$$