An anomaly in a formula to calculate the refractive index of $Al_xGa_{1-x}As$

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Abstract. A formula to calculate the refractive index n of $Al_xGa_{1-x}As$ was proposed by Adachi in 1985. **The T**here are two equations for the calculation of the band gap, namely for the mole fraction $x \leq 0.45$ and for $0.45 \leq x \leq 1$. This article reports on an anomaly that occurs when the equation of the mole fraction to calculate the refractive index of $Al_xGa_{1-x}As$, and the subsequent use of the obtained refractive indexes to calculate the epilayer thickness of $Al_xGa_{1-x}As$ films.

1. Introduction

The ternary alloy $Al_xGa_{1-x}As$ is a useful material for both electronic and optical applications. Consequently, $Al_xGa_{1-x}As$ has been used in high-speed, high-frequency microwave devices [1,2], high electron mobility transistors (HEMT) [3], quantum well infrared photo detectors [4], and other electro-optic devices. In order to design and manufacture opto-electronic devices with the required optical properties, the refractive index of the applicable material must be known. The refractive index n is a function not only of the wavelength λ, but also the mole fraction x of the alloy in the case of ternary semiconductor alloys [5]. A relationship exists between the band gap E_g of a semiconductor and the mole fraction x [6] as well as the refractive index n and the band gap [7]. This leads to the advantage of the experimental determination of the band from the point of inflection of an infrared reflectance spectrum [8] from which the mole fraction x and thus the refractive index can then also be calculated. It is to be noted that the band gap E_g of $Al_xGa_{1-x}As$ changes from direct to indirect at a mole fraction of $x \leq 0.45$ [1,9] (Figure 1).

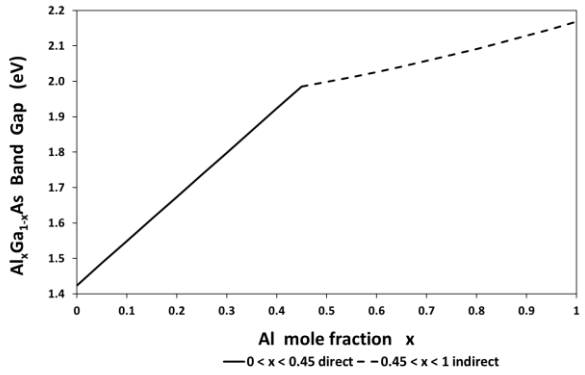

Figure 1 Band gap of $Al_xGa_{1-x}As$ as function of Al mole fraction x

A formula to calculate the refractive index of $Al_xGa_{1-x}As$ was proposed by Adachi in 1985 [1]:

$$n(\lambda) = \sqrt{A_0\left[f(x) + \frac{f(x_{so})}{2}\left(\frac{E_0}{E_0+\Delta_0}\right)^{\frac{3}{2}}\right] + B_0} \quad (1)$$

$$(x) = \frac{2 - \sqrt{1+x} - \sqrt{1-x}}{x^2}$$

$$x = \frac{hc}{\lambda E_0}$$

$$x_{so} = \frac{hc}{\lambda(E_0 + \Delta_0)}$$

The parameters A_0 = 6.3 + 19.0x and B_0 = 9.4 - 10.2x are fitting parameters in terms of the Al mole fraction x (see Reference [1]). $E_0(x)$ = 1.425 + 1.155 x + 0.37 x^2 eV is the fundamental band gap. $E_0(x) + \Delta_0(x)$ = 1.765 + 1.115 x + 0.37 x^2 eV includes the spin-orbit splitting energy $\Delta_0(x)$, h is Planck's constant, c is the speed of light, λ is the wavelength and hc/λ the photon energy.

The band gap energies presented in Figure 1 can readily be obtained from the two expressions proposed to provide for the direct and indirect band gap energies [9}:
For the mole fraction $0 \leq x \leq 0.45$, the direct band gap $E_g(x) = 1.424 + 1.247x$ (2)

In the indirect band gap where $0.45 < x < 1$, the band gap $E_g(x) = 1.9 + 0.125x + 0.143x^2$ (3)

The refractive index n for $Al_xGa_{1-x}As$ can hence be calculated using formula (1), taking into account the restrictions of equations (2) and (3).

2. Experimental Procedure and Data Analysis

AlxGa1-xAs samples with different thickness and Al mole fraction x was grown using organo-metallic vapor phase epitaxial (OMVPE). A Bruker 80V FTIR spectrometer was used to measure infrared reflectance spectra, with a Pike 10Spec specular reflectance attachment which allowed for near-normal incidence onto the samples. Fifty scans were acquired at a resolution of 4 cm^{-1} in the wavelength range 4,000 – 20,000 cm-1 (0.5 – 2.5 eV). The infrared (IR) reflectance spectra were then analyzed using the method proposed by Holtz et al. [8] to find the bandgap E_g. The bandgap was then used to calculate the Al mole fraction x for each sample from the appropriate equation (2) or (3), whereafter the refractive index was calculated from (1). Finally, the epilayer thickness for each sample is then calculated from the IR reflectance spectra and the parallel plate interference equation of Reizman [9]:

$$1/d = (2/p)[n_2/\lambda_2 - n_1/\lambda_1] \quad (4)$$

where n_1 and n_2 are refractive indexes calculated at the specific wavelengths λ_1 and λ_2 where the interference minima occur on the reflectance spectrum under consideration (Figure 2).

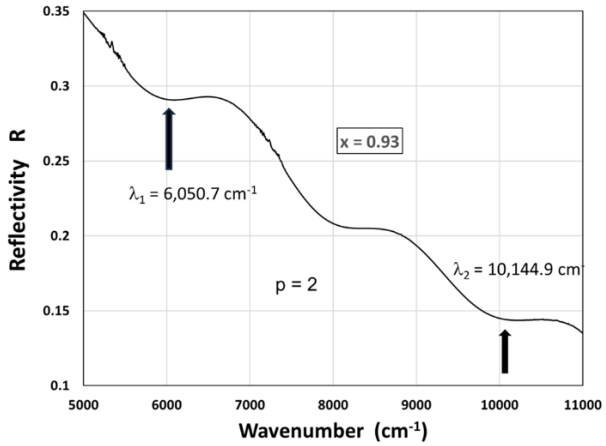

Figure 2 The infrared reflectance spectrum from an $Al_xGa_{1-x}As$ sample with Al mole fraction x = 0.93 and two minima (p =2) at wavenumber values as indicated. The negative slope of the spectrum is due to surface roughness.

The mole fraction x = 0.93 equates a band gap Eg = 2.14. An anomaly arises when equations (2) and (3) are used to calculate the refractive indexes for the same bandgap Eg (= 2.14 in this example). While different values for the refractive indexes from the equations (2) and (3) are obtained, calculated thicknesses of the epilayer only differ in the 3rd decimal (Table 1), even though the "wrong" equation (2) was used in the calculations.

Table 1 Results from equations (1) and (2).

	n_1	n_2	Film Thickness (μm)
$x \leq 0.45$ (equation 2)	2.962	3.022	0.785
$0.45 \leq x \leq 1$ (equation 3)	2.950	3.012	0.787

3. Concluding Remark

An interesting anomaly arises when use is made of the incorrect expression for the Al mole fraction x for a specific band gap E_g of an $Al_xGa_{1-x}As$ ternary alloy. Incorrect refractive index n as function of wavenumber (or wavelength) is obtained, yet when the refractive indexes are used to calculate epilayer thicknesses, the thicknesses only differ in the 3rd decimal place.

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