Suid-Afrikaanse Tydskrif vir Natuurwetenskap en Tegnologie 2025; 44(1):17-19
South African Journal for Science and Technology 2025; 44(1):17-19
https://doi.org/10.36303/SATNT.2025.44.1.926E
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SATNT / SAJST
ISSN: 2222-4173 EISSN: 0254-3486
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ORIGINAL RESEARCH

Infrared analysis of $Al_xGa_{1-x}As$ Epilayers

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The use of Aluminium Gallium Arsenide ($Al_xGa_{1-x}As$) in optical device applications requires knowledge of the refractive index n of the ternary alloy as a function of wavelength or wavenumber and Al molar fraction x. Infrared spectroscopy was used to determine both the band gap E_g and the interference fringes to calculate the epilayer thickness of $Al_xGa_{1-x}As$ samples. Two formulas proposed to calculate the refractive index of $Al_xGa_{1-x}As$ are evaluated from the layer thickness results.

Keywords: $Al_xGa_{1-x}As$, refractive index, FTIR, layer thickness

Infrarooi analise van $Al_xGa_{1-x}As$-epilagies: Die gebruik van aluminium gallium arsenied ($Al_xGa_{1-x}As$) in optiese toestel toepassings vereis dat die brekingsindeks n van die ternêre legering as 'n funksie van golflengte of golfgetal en die Al-molfraksie x bekend moet wees. Infrarooi spektroskopie is gebruik om beide die bandgaping E_g en die interferensiepatrone te bepaal om die epilaagdikte van $Al_xGa_{1-x}As$-monsters te bereken. Twee formules wat voorgestel was om die brekingsindeks van $Al_xGa_{1-x}As$ te bereken, word aan die hand van die laagdikteresultate geëvalueer.

Sleutelwoorde (soektogte in Engels): $Al_xGa_{1-x}As$, refractive index, FTIR, layer thickness

Introduction

Aluminium Gallium Arsenide ($Al_xGa_{1-x}As$) alloys are used in high-speed, high-frequency microwave devices (Adachi, 1992), high electron mobility transistors (HEMT) (Lenka & Panda, 2009), quantum well infrared photodetectors (Billaha & Das, 2017) and other electro-optic devices. The refractive index of the utilised alloy of $Al_xGa_{1-x}As$ must be known in order to design the specific devices with given optical properties.

The present article reports an effortless way to obtain the band gap E_g and mole fraction x of $Al_xGa_{1-x}As$ ternary alloys of varying Al mole fraction. Results are then used to calculate the thickness of respective epilayers.

Theory

One of the earliest discussions of the refractive index of $Al_xGa_{1-x}As$ was a semi-empirical formulation by Afromowitz (Afromowitz, 1974):

$$(n^2 - 1) = E_d/E_0 + E^2(E_d/E_0^3) \quad (1)$$

where n is the refractive index and parameters E_0 and E_d are given in terms of the Al mole fraction x as:

$$E_0 = 3{,}65 + 0{,}871x + 0{,}179x^2 \quad (2)$$
$$E_d = 36{,}1 - 2{,}45x \quad (3)$$

while the band gap E_g of $Al_xGa_{1-x}As$ is given by:

$$E_g = 1{,}424 + 1{,}266x + 0{,}26x^2 \quad (4)$$

A method based on the real and imaginary parts of the dielectric function $\varepsilon(\omega) = n(\omega) + ik(\omega) = \varepsilon_1 + i\varepsilon_2$ and using the Kramers-Kronig transformation was introduced by Adachi to obtain the optical constants, including the refractive index (Adachi, 1985):

$$n(\lambda) = \sqrt{A_0\left[f(x) + \frac{f(x_{s0})}{2}\left(\frac{E_0}{E_0+\Delta_0}\right)^{\frac{3}{2}}\right] + B_0} \quad (5)$$

with

$$f(x) = \frac{2 - \sqrt{1+x} - \sqrt{1-x}}{x^2}$$
$$x = \frac{hc}{\lambda E_0}$$
$$x_{s0} = \frac{hc}{\lambda(E_0 + \Delta_0)}$$
$$A_0 = 6{,}3 + 19{,}0\,x$$
$$B_0 = 9{,}4 - 10{,}2\,x$$

which are fitted constants in terms of the Al mole fraction x.

$$E_0(x) = 1{,}425 + 1{,}155\,x + 0{,}37\,x^2 \text{ [eV]}$$

which is the fundamental band gap, while

$$E_0(x) + \Delta_0(x) = 1{,}765 + 1{,}115\,x + 0{,}37\,x^2 \text{ [eV]}$$

is the spin-orbit splitting energy, *h* is Planck's constant, *c* is the speed of light, λ is the wavelength and hc/λ the photon energy.

The band gap E_g of $Al_xGa_{1-x}As$ can readily be obtained from the minimum in the infrared reflectance spectra (Holtz et al., 2001). This minimum or inflection point is due to the fact that energy is absorbed from the incident infrared radiation by the energy

gap between the valence and conduction band of the material. This results in a decrease in the reflected intensity. The Al mole fraction x can then be calculated from the measured band gap E_g using the applicable formula (Adachi, 1985):

$$0<x<0{,}45 \qquad E_g = 1{,}424 + 1{,}247x \qquad (6)$$

$$0{,}45<x<1 \qquad E_g = 1{,}9 + 0{,}125x + 0{,}143x^2 \qquad (7)$$

Infrared reflectance spectra can also be used to calculate the epilayer thickness d of a sample with a parallel plate structure from (Reizman, 1965):

$$1/d = (2/p)[n_2/\lambda_2 - n_1/\lambda_1] \qquad (8)$$

where p is the number of minima between wavelengths λ_1 and λ_2 and n_1 and n_2 are the refractive index at λ_1 and λ_2.

Experimental results

$Al_xGa_{1-x}As$ epilayers with various aluminium concentrations were prepared using organo-metallic vapour phase epitaxial (OMVPE) deposition. 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. An average was obtained for 50 scans acquired at a resolution of 8 cm^{-1} in the wavelength range of 0,5–50eV. The band gap E_g and Al mole fraction were then measured and calculated, whereafter the layer thickness of the relevant sample was calculated.

The results of the measured E_g, the associated Al mole fraction x and the epilayer thicknesses calculated from the equations proposed by Afromowitz [4] and Adachi [5] are presented in Table I (Afromowitz, 1974; Adachi, 1985). The band gap for GaAs = 1,43 eV and that for AlAs = 2,16 eV. As more Al is added to the alloy, the band gap will increase according to Vegard's law as the alloy becomes more like AlAs.

The layer thicknesses presented in Table I for both the Afromowitz and Adachi formulations yield values, which either agree or differ in the 2nd decimal place with a maximum error of ~1%. It can therefore be concluded that both formulas yield the same epilayer thickness for $Al_xGa_{1-x}As$ alloys.

Conclusions

The infrared analysis of $Al_xGa_{1-x}As$ ternary alloys is a quick and straightforward technique which enables the determination of band gap, Al mole fraction and epilayer thicknesses from a single reflectance spectrum of $Al_xGa_{1-x}As$ semiconductor samples.

Table I: Band gaps, mole fractions and epilayer thicknesses of samples evaluated

Sample	IR minimum reflectance (cm^{-1})	Band gap E_g (eV)	Al-mole fraction x	Layer Thickness (μm)	
				Afromowitz	Adachi
A	13716,3	1,70	0,22	2,63	2,62
B	14603,8	1,81	0,31	1,06	1,06
C	15330,0	1,90	0,38	1,08	1,07
D	17264,0	2,14	0,93	0,66	0,66

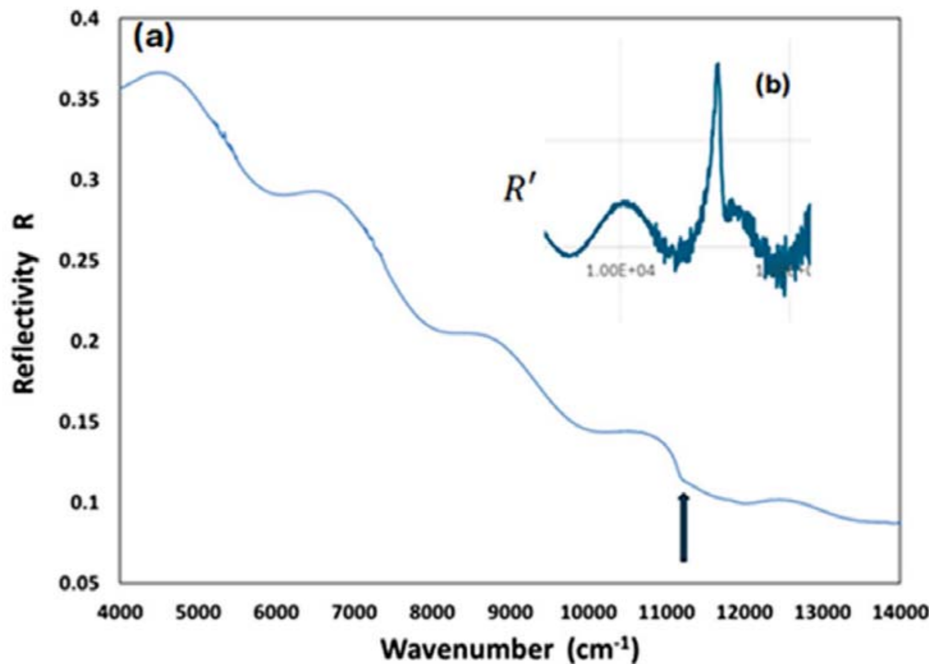

Figure 1: (a) An example of an infrared reflectance spectrum showing interference fringes, with the arrow indicating the inflection where the band gap E_g is measured, confirmed by the first derivative in (b).

Acknowledgements

Funding provided by the National Research Foundation (NRF) is gratefully acknowledged. Any opinion, findings and conclusions or recommendations expressed in this article are those of the authors, and therefore the NRF does not accept liability in regard thereto. Helpful discussions and the supply of samples by Prof MC Wagener and Dr JH O'Connell for assistance with the first derivative processing is acknowledged. The authors would also like to extend their gratitude to Prof SWP Engelbrecht for making his facilities available for part of the investigation.

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