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Investigation of the absorption coefficient, refractive index, energy band gap, and film thickness for $Al_{0.11}Ga_{0.89}N$, $Al_{0.03}Ga_{0.97}N$, and GaN by optical transmission method

Naser M. Ahmed*, Zaliman Sauli, Uda Hashim, Yarub Al-Douri

School of Microelectronic Engineering, Universiti Malaysia Perlis, 02600, Jejawi, Kangar, Malaysia

Abstract

The design of optoelectronic devices fabricated from III-Nitride materials is aided by knowledge of refractive index and absorption coefficient of these materials .The optical properties of $Al_{0.11}Ga_{0.89}N$, $Al_{0.03}Ga_{0.97}N$, and GaN grown by MOVPE on sapphire were investigated by means of transmittance measurements .The optical transmission method is successfully used to determine the refractive index (n), absorption coefficient (α), film thickness and energy gap of three samples of film over the spectral range of (1-5 eV) .

Keywords: Absorption coefficient; Refractive index; Optical properties; III-Nitride energy band gap
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1. Introduction

III nitrides have been extensively studied in recent years because of their scientific and technological importance [1-3]. In particular, the $Al_xGa_{1-x}N$ alloy system covers a wide ultraviolet (UV) spectral range between the direct band gaps of 3.4 eV for GaN and 6.2 eV for AlN at room temperature, and is very attractive for short-wavelength optical applications such as UV light emitters and UV detectors, [4–6]. In addition, AlGaN alloys with small mole fractions are used to form strained hetero structures with GaN and InGaN in light emitting diodes and laser diodes and in GAN/AlGaN field-effect transistors (FETs). Therefore, it is important to know the fundamental band gap, refractive index, and thickness of GaN and $Al_xGa_{1-x}N$ epitaxial layer with a given mole fraction. The recent development of III-V optoelectronic devices such as blue light-emitting diodes (LEDs), blue lasers, and solar blind ultraviolet photodetectors shows that GaN and related compounds are technologically important.

The success of these optoelectronic devices is largely the result of recent improvements in material quality. This study was motivated by the relatively large variance in reported values of the absorption coefficient, refractive index, energy band gap, and thickness by using the techniques of transmission and reflection spectroscopy. Optical experiments provide a good way of examining the properties of semiconductors. Particularly measuring the absorption coefficient for various energies gives information about the band gaps of the material. Knowledge of these band gaps is extremely important for

*) For Correspondence, E-mail: naser@unimap.edu.my

understanding the electrical properties of a semiconductor, and is therefore of great practical interest. This work describes experiments of this kind using the techniques of transmission to study the properties of three thin semiconductor films (GaN/Sapphire, $Al_{0.03}Ga_{0.97}N$/Sapphire, $Al_{0.11}Ga_{0.89}N$/Sapphire).

2. Theoretical Background

Much of the information about the properties of materials is obtained when they interact with electromagnetic radiation. When a beam of light (photons) is incident on a material, the intensity is expressed by the Lambert-Beer-Bouguer law [7-9]:

$$I = I_0 \exp(-\alpha d) \tag{1}$$

If this condition for absorption is met, it appears that the optical intensity of the light wave, (I), is exponentially reduced while traveling through the film. If the power that is coupled into the film is denoted by I_0, gives the transmitted intensity that leaves the film of thickness d.
(α) Is called “absorption coefficient”. From (1) it follows that

$$\alpha = -\frac{1}{d}\ln\left(\frac{I}{I_0}\right) \tag{2}$$

It is clear that α must be a strong function of the energy hν of the photons . For hν < E_g (direct), no electron hole pairs can be created, the material is transparent and α is small. For hν ≥ E_g (direct), absorption should be strong. All mechanisms other than the fundamental absorption may add complications (e.g. "sub band gap absorption" through excitons), but usually are not very pronounced.

Optical transmission measurements were carried out to determine the film thickness, the wavelength dependence of the refractive index and optical absorption coefficient. The optical constants were determined from the optical transmission measurements using the method described by Swanepoel [10].

The transparent substrate has a thickness several orders of magnitude larger than (*d*) and has index of refraction (n) and absorption coefficient (α = 0). The index of refraction for air is taken to be n_0 =1.

The transmission spectrum can roughly be divided into four regions as shown in figure (1). In the transparent region (α=0) the transmission is determined by *n* and *s* through multiple reflections. In the region of weak absorption α is small and the transmission begins to decrease. In the medium absorption region α is large and the transmission decreases mainly due to the effect of α. In the region of strong absorption the transmission decreases drastically due almost exclusively to the influence of α.

If the thickness *d* is uniform, interference effects give rise to the spectrum, shown by the full curve in Figure 1. These interference fringes can be used to calculate the optical constants of the film.

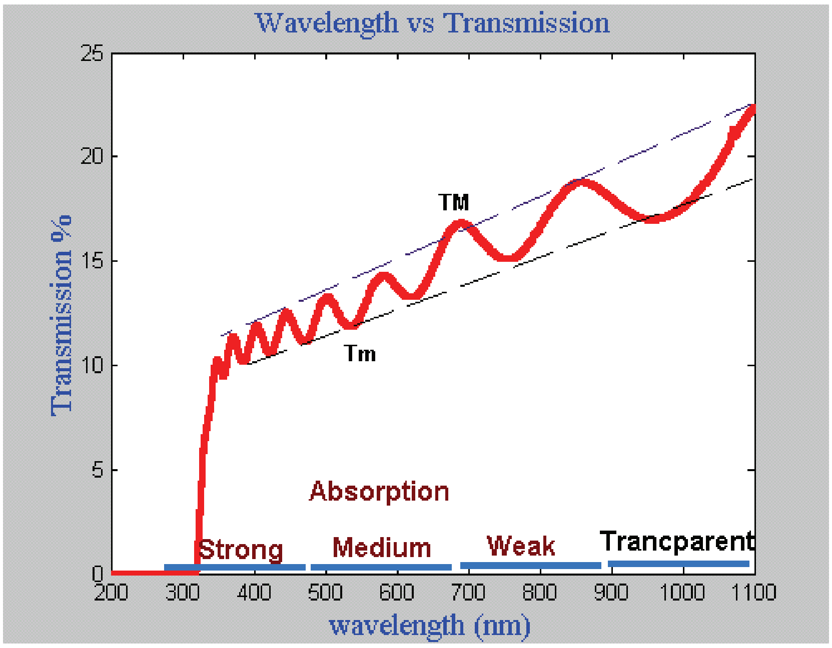

Fig. 1: Interference fringes of thin film transmission

3.Experimental Method

3(a) Refractive index and film thickness

The refractive index and thickness of a thin film can be calculated from a simple transmittance spectrum using the Swanepoel method [11]. This method can only be applied to thin films deposited on transparent substrates several orders of magnitude thicker than the film. When film thickness is uniform, interference effects give rise to the typical transmittance spectrum with successive maxima and minima (see Fig. 1). Practical application of this method entails, as a first step, the calculation of the maximum and minimum transmittance envelope functions, T_M (λ) and T_m (λ), *M m* respectively. From these functions the refractive index n (λ) can be obtained as [12]:

$$n = \left[N + \left(N^2 - S^2 \right)^{1/2} \right]^{1/2} \tag{3}$$

where

$$N = 2s \frac{T_M - T_m}{T_M T_m} + \frac{s^2 + 1}{2} \tag{4}$$

s being the refractive index of the substrate. Then, the film thickness can be obtained from the refractive index corresponding to adjacent extreme values, $n_1 = n\,(\lambda_1)$ and $n_2 = n\,(\lambda_2)$ through the following expression:

$$d = M \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_2 - \lambda_2 n_1)} \tag{5}$$

With M=1 for two adjacent maxima (or minima).

3(b) Determination of Band Gaps

The fundamental absorption is related to band-to-band or to exciton transition, which are subjected to certain selection rules [13]. The transitions are classified into several types, according to the band structure of a material. The relation between absorption coefficient and optic band gap for direct transition (k=0) is given by Tauc equation [14]:

$$\sqrt{\alpha h\nu} = B\left(h\nu - E_g^{opt}\right) \tag{6}$$

And for indirect transition ($k \neq 0$) the relation becomes

$$\alpha(h\omega)\,\alpha\,\frac{\left(\hbar\omega - E_{gap}\right)^2}{\hbar\omega} \tag{7}$$

From the graph of $(\alpha h\nu)^{1/2}$ versus $h\nu$ one obtains E_g and B parameters. B is also a useful diagnostic of the material since it is inversely proportional to the extent of the tail state (ΔE) at conduction and valance band edges.

4. Results and Discussion

4(a) Results of Transmission/Reflection measurements:

In this section we will present the results of our transmission and reflection measurements

4(b) Transmission

Figure 2 shows the transmission of (GaN/Sapphire, $Al_{0.03}Ga_{0.97}N$/sapphire, $Al_{0.11}Ga_{0.89}N$ /sapphire) as a function of the wavelength. The thickness of the film is determined by using filmetric system were 4221 nm for GaN, 764 nm for $Al_{0.11}Ga_{0.89}N$ and 736 nm for $Al_{0.03}Ga_{0.97}N$ as shown in table (1) .The transmittance curves show that for high energies (lower wavelengths) there is no transmission because all the light is absorbed. For low energies (higher wavelengths) however there are no appropriate electronic transitions possible so transmission is very high in this range. . The energy at which absorption starts seems to be characteristic for each material: For GaN it corresponds to the direct band gap at 3.4 eV. For low energies we observe thin film interference effects resulting from the overlaying of light that is reflected on both sides of the thin film. In figure 3 we can see the strong absorption for different samples viz for GaN at λ=364 nm that mean E_g=3.406593 eV, $Al_{0.03}G_{0.97}N$ at λ=345 nm (E_g=3.594203 eV), and for $Al_{0.11}G_{0.89}N$ at λ=320 nm (E_g=3.875 eV).

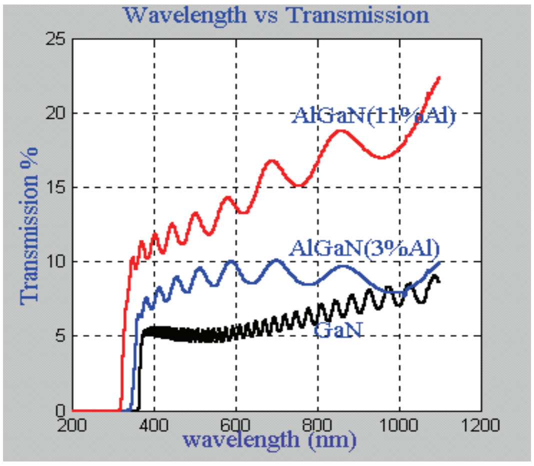

Fig. 2: Transmission data for $Al_xGa_{1-x}N$

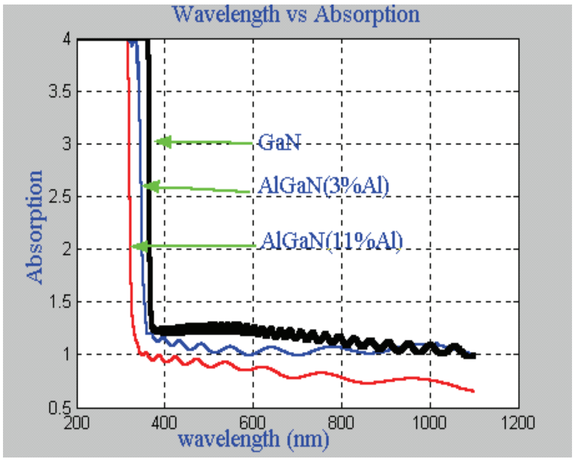

Fig. 3: Absorption experimental result from spectrophotometer for $Al_xGa_{1-x}N$

4(c) Refraction indices

The method to determine the optical constants is based on parabolic procedure of adjacent maximum (T_M) and minimum (T_m) and by using the equations (5 and 6) we can see the relation between energy and refractive index as shown in figure 4.

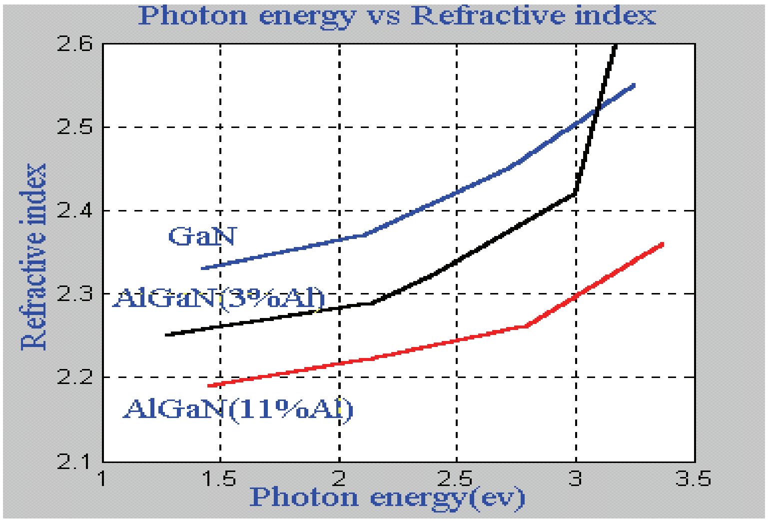

Fig. 4: Index of refraction as a function of photon energy for $Al_xGa_{1-x}N$

4(d) Thickness of the semiconductor films

The thickness of the prepared films has been determined experimentally using FILMETRIC device and also it has been calculated from the transmission curves of Fig 2 using equation (5). A comparison of the results is shown in Table 1.

Table 1.

Sample	$\lambda 1$ nm	$\lambda 2$ nm	d(nm)	Filmetric thickness result (nm)
$Al_{0.03}Ga_{0.97}N$	1100	869	1055.3	**736.9**
	700	586	837.828	
	513	456	891.971	
	414	382	1045.6	
$Al_{0.11}Ga_{0.89}N$	$\lambda 1$ nm	$\lambda 2$ nm	d(nm)	Filmetric thickness result (nm)
	1100	851	896.15	**764.2**
	684	578	873.85	
	499	443	895.763	
	401	368	976.873	
GaN	$\lambda 1$ nm	$\lambda 2$ nm	d(nm)	Filmetric thickness result (nm)
	1085	1021	4809.5	**4221**
	972	926	15071	
	884	842	4947.4	
	776	719	1969.8	
	694	671	4953.4	
	649	628	4789.1	
	611	592	2935.6	
	577	561	2935.6	
	547	533	2865.3	
	520	508	6267.4	
	497	486	5907.3	
	413	396	3542.3	
	391	386	9119.6	
	382	378	11563	

4(e) Determination of Band Gaps and Absorption coefficients

The absorption coefficient and optical band gap *Eg* were determined for each sample, and shown as a function of photon energy in figure (5). Figure (6) shows the dependence of band gap on Al fraction (x) for $Al_xGa_{1-x}N$ we note that increasing Al fraction causes increasing in energy gap.

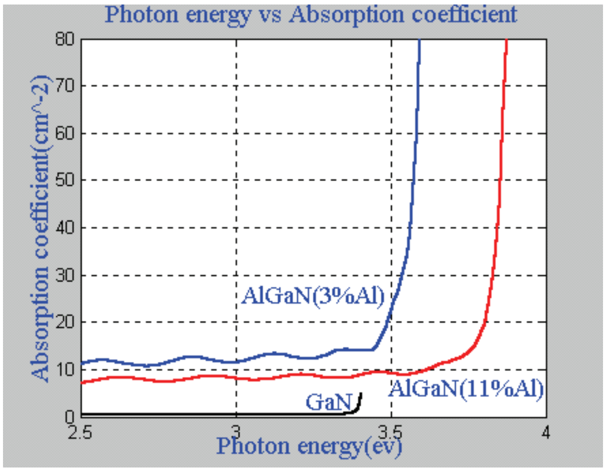

Figure 5. Square of the optical absorption vs. energy.

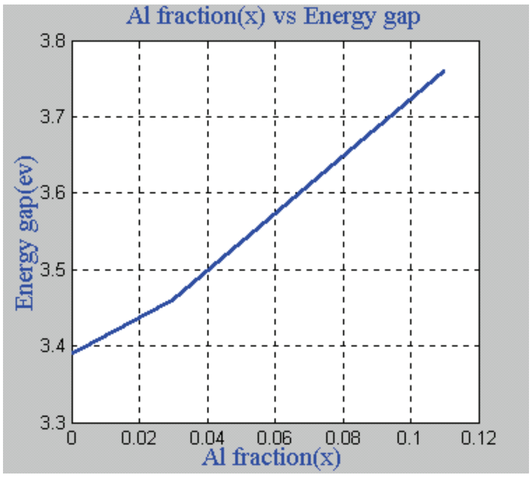

Figure 6. Dependence of band gap on photon Al fraction (x) for $Al_xGa_{1-x}N$

Conclusion

We have described an optical method for measurement of optical properties of $Al_xGa_{1-x}N$ film, which uses total reflectance of the thin film at a wavelength range (300-1100nm). In other measurements, we have made some preliminary comparisons between the thickness measured by this technique and other techniques. Our results showed the transmission increased and refractive index decreased with increasing Al mole fraction. GaN shows low absorption below its band gap at 3.4 eV.

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