Refractive index and birefringence of In_xGa_{1-x}N films grown by MOCVD^{*}

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The refractive index and birefringence of $In_xGa_{1-x}N$ films grown on GaN layers were measured by prism coupling used in conjunction with multilayer optical waveguide analysis. Samples with x = 0.036, 0.049, 0.060, and 0.066 were examined at the separate wavelengths of 442, 457.9, 476.5, 488, 514.5, 532, and 632.8 nm. The In fraction x was determined by Rutherford backscattering spectroscopy. Separate measurements of the film thicknesses were performed by cross-sectional field-emission scanning electron microscopy (FESEM). Film thickness information was required in order to constrain the numerical simulation used to solve for the ordinary (n_o) and extraordinary (n_e) refractive indices. We found that n_o is a weak function of both x and wavelength for the InGaN layers and could only be well distinguished from GaN (x = 0) for the two shortest wavelengths used. On the other hand, n_e for the InGaN layers was resolved from GaN for all the wavelengths and x values. The measurements for n_e are limited by optical scattering observed at the shortest wavelengths and the higher values of x. Cross-sectional FESEM reveals that a source of this scattering is most likely triangular pits at the InGaN/GaN upper interface.

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1 Introduction

Measurements of refractive index and birefringence of $Al_xGa_{1-x}N$ and $In_xGa_{1-x}N$ compounds are important for the design of LED and laser devices. A number of papers reporting refractive index studies of $Al_xGa_{1-x}N$ have appeared ([1] and references therein) but there are comparatively few reports of refractive index measurement for $In_xGa_{1-x}N$ [2]. In many cases of engineering interest, the refractive indices of $In_xGa_{1-x}N$ films with x < 0.1 are required. In order to perform these measurements, test structures are needed with thick InGaN layers. These $In_xGa_{1-x}N$ layers were grown on top of $1-2 \mu m$ thick GaN films. This imposes restrictions on the $In_xGa_{1-x}N$ layer thickness, and typical thicknesses are roughly 300 nm. Further, the $In_xGa_{1-x}N$ layers are "capped" with a roughly 20 nm thick GaN film to protect the InGaN film during cooling. This results in a multilayer test structure where the dominant film constituent is GaN. For a transparent growth substrate such as sapphire, use of spectroscopic ellipsometry can be problematic because of complications arising from reflections from the bottom side of the substrate [3]. In these situations it is convenient to treat the multilayer GaN/In Ga_N/substrate composite as an

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optical waveguide and calculate the refractive index of the $In_xGa_{1-x}N$ layer from measurements of optical waveguide modes supported by the multilayer film.

2 Test structure growth and characterization

All samples were grown by metal-organic chemical vapor deposition (MOCVD) on c-plane sapphire substrates. A schematic of the sample structure is illustrated in Fig. 1. The In fractions x for the samples denoted by D, E, F, and G were measured using Rutherford backscattering spectroscopy (RBS) using a 2 MeV He⁺⁺ beam. The respective values of x were determined to be: 0.036, 0.049, 0.060, and 0.066 using a 4-layer model fit. The uncertainty in x for samples D and E is estimated to be \pm 0.001 and the uncertainty in x for samples F and G is approximately \pm 0.003.

Fig. 1 Schematic of a test structure for refractive index measurements of $In_sGa_{1-x}N$. The measured layer thicknesses for L_1 , L_2 , and L_3 are given in Table 1. The structure serves as an optical waveguide that constrains guided modes between the GaN/sapphire interface at the bottom and the GaN/air interface at the top. The relative thicknesses of the layers shown are not to scale.

GaN "cap" (~ 20 nm)	L
In _x Ga _{1-x} N	L_2
undoped GaN	L ₃
sapphire	

triangular pits



Table 1 Comparative thickness measurements (in micrometers) of the cap (L_1) , InGaN (L_2) , and undoped GaN (L_3) layers. The estimated uncertainty for the FESEM measurements \pm 20 nm. The RBS estimated thicknesses of L_2 are consistently lower than those obtained by FESEM due to the assumption that the density of the InGaN layer is equal to that of GaN. FESEM cannot separately measure the GaN cap layer thickness L_1 and a value of 20 nm, in good agreement with RBS estimates, is assumed from the established calibration of the film growth rate.

sapphire

	RBS			FESEM	
Sample	Х	L	L ₂	$L_{1} + L_{2}$	$L_1 + L_2 + L_3$
D	0.036	0.020	0.292	0.320	1.740
E	0.049	0.020	0.298	0.380	2.030
F	0.060	0.020	0.309	0.410	1.720
G	0.066	0.018	0.303	0.350	1.800

Direct measurements of the GaN and $In_xGa_{1,x}N$ layer thicknesses were necessary in order to constrain the solution range in thickness for the simulation codes used to calculate the refractive indices of the $In_xGa_{1,x}N$ layers. These thickness measurements were made by cross-sectional field-emission scanning electron microscopy (FESEM) and RBS. In computing the film thickness using RBS, the density of GaN of 8.9×10^{22} was assumed for both the GaN and the $In_xGa_{1,x}N$ layers. An example FESEM crosssectional image of sample G (x = 0.066) is shown in Fig. 2. The results of comparative thickness measurements made by RBS and FESEM analysis are given in Table 1.

3 Optical characterization

The samples were examined by prism-coupled optical waveguide methods in a fashion that has been described in detail elsewhere [1]. A brief description of the procedure is given here. Light is coupled into the guided modes of the multilayer film using a prism coupler apparatus as illustrated in Fig. 3. At specific launch angles with respect to the prism normal, TE modes (polarization parallel to the film plane) or TM modes (polarization perpendicular to the film plane) may be launched into the film. Typically, because of optical scatter, launching into a single mode will excite the entire spectrum of guided modes supported by the film, usually 10 to 15 modes for the samples and conditions described here. A guided mode propagates as a plane wave in the multilayer media and has an effective refractive index that is bounded on the high end by the maximum refractive index of the multilayer film and on the low end by the refractive index of the sapphire substrate. By measuring the launch (or exit) angles of modes with respect to the prism normal n, and knowing the prism refractive index and apex angle γ , the effective refractive indices may be separately computed for both the TE and TM modes [1]. With this information in hand, one may then solve a transcendental equation describing TE modes via graphical or least-squares methods in order to calculate the ordinary refractive index n_0 of the InGaN layer. Similarly, with the ordinary index now established, one may use this as input into a second transcendental equation describing TM modes in order to calculate the extraordinary refractive index n_{e} of the InGaN layer. These equations may be derived in a manner similar to that presented for the simpler single-layer birefringent waveguide films of reference [1].

Fig. 3 Schematic of apparatus used to launch and analyze guided modes in the samples. A rutile prism with apex angle γ and optic axis perpendicular to the page is weakly clamped on the surface of the sample. Laser light at a fixed wavelength is launched into (for example) mode # 1 by directing it into the prism at an angle $\alpha_1^{\ i}$ with respect to the prism face normal n as illustrated. Mode #1 is excited and out-coupled by the prism and illuminates the screen at a location coincident with the exit path of the launch beam. Because of optical scattering, it is common to observe several guided modes simultaneously excited even if the launch condition is optimized for one particular mode. The modes fall at locations d_i on the screen as illustrated.



In the single-layer birefringent waveguide theory, one may calculate the film index, birefringence, and thickness armed only with the effective indices of refraction of 2 TE and 2 TM modes. For the present case that is concerned with 3-layer birefringent GaN/InGaN/GaN optical waveguides on sapphire substrates, the solution codes will not converge to unique values of refractive index and thickness for the InGaN layers unless the constituent layer thicknesses are constrained by separate measurements and the refractive index and birefringence of the GaN layers are known beforehand. Our solution procedure is as follows: (i) For a given test wavelength calculate the effective indices of the observed TE and TM modes; (ii) using the GaN refractive index data from reference [1] along with the measured TE effective index data as input, and taking $L_1 = 20$ nm, iteratively solve for the ordinary refractive index of the InGaN layer and thicknesses L_2 and L_3 , with the range of the thickness variation constrained by the estimated uncertainty in the FESEM thickness measurements; (iii) repeat the process for TM modes using as input the corresponding values of measured TM effective indices, the value of n_e for GaN, and computed values of n_0 for the InGaN layer. The results of this analysis are illustrated in Fig. 4 (a, b).



Fig. 4 (a) Ordinary refractive index of $In_x Ga_{1-x}N$ for the wavelengths indicated. The values for x were given earlier. Refractive index values for GaN (x = 0) are taken from Ref. [1].

4 Discussion and conclusions



Fig. 4 (b) Extraordinary refractive index of $In_xGa_{1-x}N$ over the same wavelength and x values as used in (a).

The results indicate that n_0 for $\ln_{x}Ga_{1,x}N$ is a comparatively weak function of x. Indeed, over the samples studied the ordinary index is only well resolved from that of GaN for the two shortest wavelengths considered. This observation is corroborated by similar measurements reported by Akasaki and Amano [2]. The trend in n_e with composition and wavelength for $In_xGa_{1-x}N$ is much better resolved but measurements performed on samples F and G were hampered by excessive optical scattering observed at the two shortest wavelengths. Indeed, we note that the presence of triangular pits (common for such layers) as illustrated in Fig. 2 could contribute to such scattering. Optical absorption measurements were not performed on these samples, however room temperature photoluminescence reveals apparent band-tail emission extending to roughly 450 nm in samples F and G. If this is also accompanied by absorption then the refractive index measurements on these samples at 442 nm (or shorter) could be corrupted since optical absorption was not considered in the theoretical modelling. It appears that the comparatively large error bars given in Fig. 4 (a, b) are the consequence of the inherent uncertainty of the thickness measurements of the layers – approximately ± 20 nm for the combined thicknesses $L_1 + L_2 \pm 20$ nm for L_3 , and the uncertainty in the refractive index of GaN [1]. More precise measurements of layer thicknesses by use of XRD and cross sectional TEM are in process in efforts to reduce the computed uncertainty for the InGaN refractive indices. Reduced uncertainty can also be expected if it eventually becomes practical to fabricate samples with thicker InGaN layers (by roughly a factor of 2 or 3). In this way the InGaN layer would serve a stronger waveguiding role rather than being essentially a perturbation on the waveguide character of the dominating GaN layer L₃.

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