

Short Communication

Polarized Infrared Reflectance Studies for Wurtzite $\text{In}_{0.10}\text{Ga}_{0.90}\text{N}$ Epilayer on Sapphire Grown by MBE

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Polarized infrared (IR) reflectance studies of $\text{In}_{0.10}\text{Ga}_{0.90}\text{N}$ epilayer on sapphire substrate (Al_2O_3) grown by molecular beam epitaxy are presented. The features of the polarized IR reflectance spectra and the optical characteristics of $\text{In}_{0.1}\text{Ga}_{0.90}\text{N}$ were investigated. Based on the anisotropic dielectric function model, the experimental IR reflectance spectra were numerically fitted by the theoretical IR reflectance spectra. Room temperature polarized IR reflectance measurements were performed at an incident angle of 15° by using a Fourier transform infrared spectroscopy. Good agreement between the measured and calculated spectra has been obtained. From the fit of the experimental curve, the optical parameters at the center of Brillouin zone are determined for the $\text{In}_{0.1}\text{Ga}_{0.90}\text{N}$ epilayer.

Keywords: III-Nitrides, InGaN, polarized infrared spectroscopy.

1. INTRODUCTION

The group-III nitrides such as GaN, InN and $\text{In}_x\text{Ga}_{1-x}\text{N}$ solid solutions attract much attention for application in high-power, high-frequency and high-temperature electronics, electrochemical and optoelectronic devices. InN and its related alloys have attracted much attention of both theoretical and experimental scientists in recent years [1-3]. Among InN ternary alloys, the $\text{In}_x\text{Ga}_{1-x}\text{N}$ ternary system is especially interesting because it is the most important and indispensable material used for the active layer in blue and green light emitting diodes and lasers [4-6]. The InGaN ternary system offers band gap tunability covering the whole visible spectral range [7,8].

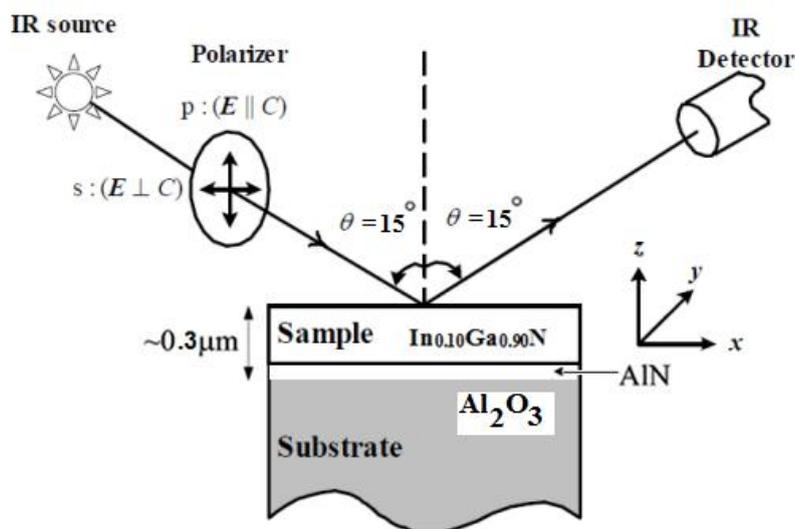
In order to further engineer these alloys and related optoelectronic and electrochemical devices, it is necessary to work on the fundamental properties of these materials. The infrared optical response

of these alloys is important for the determination of crystal quality and phonon properties. Consequently, it is important for the designing of the photonic and chemical devices.

Despite recent significant progress in InGaN technology, however, the fundamental physics related to the InGaN materials have not been well developed. To date, the study of optical phonon mode by infrared (IR) reflectance of InGaN is still in the early stage [9]. In order to contribute to the understanding of the fundamental properties of this material, the polarized IR reflectance studies of ternary $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ epilayers grown on AlN buffer layer on sapphire substrate (Al_2O_3) by molecular beam epitaxy (MBE) are investigated experimentally by using Fourier transform infrared (FTIR) spectroscopy and theoretically by using the anisotropic dielectric function model. Through this study, complete sets of Brillouin zone (BZ) center reststrahlen parameters of the epilayers involved are obtained. Also, in the present work, we aim to investigate the fundamental optical properties of the ternary $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ samples. In addition, no agreement has been made as to whether the ternary $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ phonons can be classified as having one-mode [10], two-mode [11-13], or mix-mode behaviour. Thus, the current experimental study addresses a few of the issues related to phonon modes.

2. EXPERIMENT DETAILS

The sample used in this study was an epilayer of $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ ternary nitride grown on a *c*-plane (0001) sapphire substrate, with an AlN buffer layer using plasma assisted molecular beam epitaxy (PA-MBE) technique.



s: the electric field vector (*E*) is perpendicular to the plane of incidence
p: the electric field vector (*E*) is parallel to the plane of incidence

Figure 1. Schematic diagram of the $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ / AlN / Al_2O_3 (0001) cross-section and the beam geometry of the polarization measurements.

The thickness of the $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ epilayer as measured by Filmetrics F20-VIS is 0.12 μm. Room temperature *s*- and *p*- polarized far IR reflectance measurements were carried out on the

In_{0.10}Ga_{0.90}N sample by using a Fourier transform IR spectrometer (Spectrum GX FTIR, Perkin Elmer). A wire grid polarizer was used in the polarization measurements. The angle of the incident was set to 15° by using a variable angle reflectance accessory. An aluminum coating mirror is employed as reference standards. The measurements were taken at frequencies ranging from 400 to 1000 cm⁻¹. The spectra were recorded using 512 scans at a resolution of 4 cm⁻¹. Fig 1 shows the schematic diagram of the In_{0.1}Ga_{0.90}N /AlN/ Al₂O₃ (0001) cross-section structure and the beam geometry of the polarization measurements. Furthermore, we fit the reflectance spectra using the anisotropic dielectric function model.

3. THEORY

Dielectric properties greatly depend on the crystal symmetry. In this work, the curve fitting method is applied to extract all the important properties of the studied structure. The theoretical polarized IR reflectance spectra for the studied structure are calculated by using the standard transfer matrix formulation based on four layers model, i.e., air/ In_{0.1}Ga_{0.90}N/AlN/Al₂O₃ (0001). It is known that III-nitrides ternary crystallize preferentially in hexagonal wurtzite (α -) structure. For this study, we focused on the α -InGa_{0.90}N and an anisotropy model is used to simulate its surface polarization dispersion relations. For α -InGa_{0.90}N crystal with c -axis is parallel to the surface normal ($c_{\text{axis}} \parallel z$) and perpendicular to the propagation direction ($c_{\text{axis}} \perp x$), the dielectric function is given by [14]:

$$\varepsilon_j(\omega) = \varepsilon_{\infty,j} \left[\frac{\omega_{LOj}^2 - \omega^2 - i\omega\gamma_{LOj}}{\omega_{TOj}^2 - \omega^2 - i\omega\gamma_{TOj}} \right] \quad (1)$$

where $\varepsilon_{\infty,j}(\omega)$ is the high-frequency dielectric constant, ω_{LO} , ω_{TO} , γ_{LO} and γ_{TO} are respectively, the frequencies and phonon damping constants for LO and TO phonons in the j^{th} lattice mode. The subscript j stands for parallel (\parallel) and perpendicular (\perp) vibration modes with respects to the optical crystal axis, respectively. It is well known that the behaviour of phonon modes of the ternary alloys is complicated and are found to exhibit either one- or two-mode behaviour [15]. For a ternary alloy with the form of A _{x} B _{$1-x$} C, the expression for the $\varepsilon_{\parallel(\perp)}(\omega)$ is more complicated. The $\varepsilon_{\parallel(\perp)}(\omega)$ as a function of alloy composition x is given by [16].

$$\varepsilon(\mathbf{A}_x\mathbf{B}_{1-x}\mathbf{C})_{\parallel,\perp} = x\varepsilon(\mathbf{AC})_{\parallel,\perp} + (1-x)\varepsilon(\mathbf{BC})_{\parallel,(\perp)}, \quad (2)$$

where $\varepsilon(\mathbf{AC})_{\parallel(\perp)}$ and $\varepsilon(\mathbf{BC})_{\parallel(\perp)}$ are, respectively, the dielectric constants parallel and perpendicular to the optical for AC and BC binary compounds.

4. RESULTS AND DISCUSSION

Fig. 2 shows the room temperature experimental (dotted line) and theoretical (solid line) (a) s- and (b) p-polarized IR reflectance spectra for the air/InGa_{0.90}N/ /AlN/ Al₂O₃ (0001) in the range of 400-1000 cm⁻¹ at incident angle of 15°.

For the s-polarization, the reflectivity is depending only on ε_{\perp} of each layer. However, for the

p-polarization measurement, the reflectivity is depend on both ϵ_{\parallel} and ϵ_{\perp} , thus two set of phonon parameters are required to fit in the *p*-polarize IR reflectance spectra. The phonon parameters are adjusted until the theoretical give the best fit to the experimental spectra for both the *s*- and *p*-polarization measurements. The best fit parameters are listed in Table 1

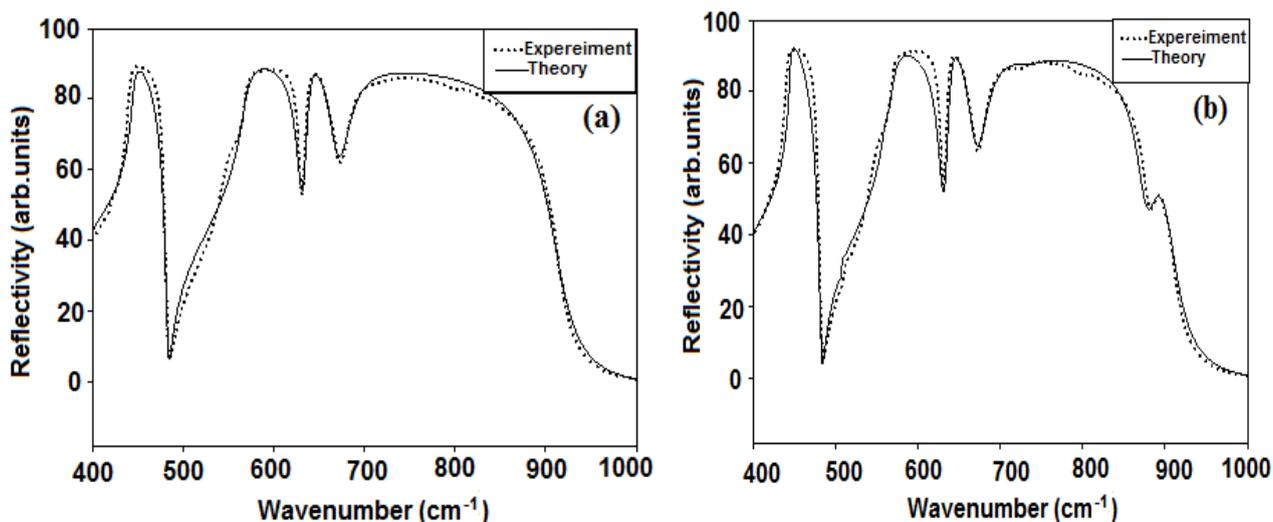


Figure 2. Room temperature (a) *s*- and (b) *p*-polarized IR reflectance spectra of In_{0.10}Ga_{0.90}N measured at angle of incidence of 15°. The solid line and dotted line indicate the theoretical and experimental IR reflectance spectra, respectively.

Table 1. Best fit parameters obtained from the theoretical modeling of the *s*- and *p*-polarized IR reflectance spectra for In_{0.1}Ga_{0.90}N epilayer grown by MBE.

	ϵ	ϵ_{∞}	ω_{LO} (cm ⁻¹)	ω_{TO} (cm ⁻¹)
GaN	\perp	5	741	564
	\parallel	4.94	734	532
AlN	\perp	4.53	917	675
	\parallel	4.72	891	610
InN	\perp	5	593	476
	\parallel	6	586	447
Al ₂ O ₃	\perp	3.077	388	385
			482	446
			630	575
			884	633.5
			905	
	\parallel	3.072	506	400
			877	587

The numerical fitting was set at high phonon damping constant in order to obtain the best fitting. From Figure 2, it can be seen that the theoretical spectra are in good agreement with the

experimental spectra and with other reported results [17-19]. From the IR measurements with s- and p-polarization, purely transverse optical $E_1(\text{TO})$ and longitudinal optical $A_1(\text{LO})$ phonon modes were observed, with the phonon propagation direction being perpendicular and parallel to the crystal axis, respectively.

Due to the superimposed of the films (InGaN and AlN) reststrahlen bands with that of Al_2O_3 substrate, the features caused by the films cannot figure out clearly. Nevertheless, as shown in Figure 2(b), three pronounced dips at 506.5 cm^{-1} , 730 cm^{-1} and 881 cm^{-1} can be clearly seen which indicated the LO mode of Al_2O_3 substrate, GaN-like [$A_1(\text{LO})$] and the Al_2O_3 substrate respectively. The appearance of these peaks is due to Berreman effect [20, 21].

5. CONCLUSIONS

The optical parameters of $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}/\text{AlN}/\text{Al}_2\text{O}_3$ (0001) have been obtained by numerical fitting to experimental data of the FTIR spectra. The best fitting was obtained at high phonon damping constant. From the IR measurements with s- and p-polarization, purely transverse optical $E_1(\text{TO})$ and longitudinal optical $A_1(\text{LO})$ phonon modes were observed, with the phonon propagation direction being perpendicular and parallel to the crystal axis, respectively. We have measured and calculated infrared reflection spectra obtained within the phonon region of InGaN, and AlN heterostructures on sapphire. Due to the strong reflection of the substrates, the otherwise forbidden LO modes could be observed in off-axis reflection. Individual optical phonon modes could be observed and attributed to the AlN buffer layer of the InGaN alloy films, also, three pronounced dips at 506.5 cm^{-1} , 730 cm^{-1} and 881 cm^{-1} can be clearly seen which indicated the LO mode of Al_2O_3 substrate, GaN-like [$A_1(\text{LO})$] and the Al_2O_3 substrate respectively.

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