

Optical characterization of $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys

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Abstract

InGaN layers were grown by molecular beam epitaxy (MBE) either directly on (0 0 0 1) sapphire substrates or on GaN-template layers deposited by metal-organic vapor-phase epitaxy (MOVPE). We combined spectroscopic ellipsometry (SE), Raman spectroscopy (RS), photoluminescence (PL) and atomic force microscopy (AFM) measurements to investigate optical properties, microstructure, vibrational and mechanical properties of the InGaN/GaN/sapphire layers.

The analysis of SE data was done using a parametric dielectric function model, established by in situ and ex situ measurements. A dielectric function database, optical band gap, the microstructure and the alloy composition of the layers were derived. The variation of the InGaN band gap with the In content (x) in the $0 < x \leq 0.14$ range was found to follow the linear law $E_g = 3.44 - 4.5x$.

The purity and the stability of the GaN and InGaN crystalline phase were investigated by RS.

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1. Introduction

In the last years, the development of blue light-emitting diodes has attracted a great deal of research activity on GaN-based III–V nitrides. Among them the most interesting for optoelectronic applications is the $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloy, whose band gap covers a wide spectral range, from infrared (0.7 eV [1]) to UV (GaN-3.6 eV) [2]. High quantum efficiency was also reported, by using these layers as active media in optoelectronic devices [3].

One can find in the literature optical studies on hexagonal (wurtzite) epitaxial $\text{In}_x\text{Ga}_{1-x}\text{N}$ such as optical absorption [2,4], electron energy loss spectroscopy [5], optical transmission [6], photoluminescence [7–9], photoreflectance [10], spectroscopic ellipsometric measurements [11,12], Raman spectroscopy [13] as well as theoretical studies with some disagreements in the resultant band gap energies and their strain dependence.

The quality of the $\text{In}_x\text{Ga}_{1-x}\text{N}$ epitaxial layers is known to be significantly improved by the existence of MOVPE GaN-template layers [5,14,15]. However, it is also known that it is

very difficult to grow $\text{In}_x\text{Ga}_{1-x}\text{N}$ with In composition above 0.4 due to the large lattice mismatch (11–13% and even more) between wurtzite GaN and InN, leading to a compressive strained layer. Moreover, it is possible that the thickness of the MOVPE GaN-template layer influences the optical properties of InGaN layers grown on it [5].

In order to improve the optical and structural properties of InGaN layers and to reduce the stress in an effective way, suitable techniques for in situ growth monitoring are required. Compared to reflection measurements SE has the advantage of sensitivity to layer thicknesses of a few nanometers, typical for quantum wells.

Raman spectroscopy has been extensively used to study III–V-nitrides stress [16]. This is an important factor that alters the energy band structure and influences the vibrational properties.

2. Experimental

2.1. Preparation of the layers

The growth of the GaN and InGaN films of different thickness (Table 1) was performed in a standard MBE system

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Table 1

Assignments of strongest modes in the first-order Raman spectra of hexagonal GaN and $\text{In}_{0.14}\text{Ga}_{0.86}\text{N}$ samples grown on (0 0 0 1) Al_2O_3 substrate

Sample	Thickness (μm)	E_2 (low) (cm^{-1})	$A_1\text{g}/\text{Al}_2\text{O}_3$ (cm^{-1})	E_1 (TO) (cm^{-1})	E_2 (high) (cm^{-1})	A_1 (LO) (cm^{-1})
MBE-GaN [20]	1	144		558	567	734
MBE-GaN [21]	1.2				569	730
MBE-GaN [21] doped with In	1.2				568.3	
MBE-GaN	1		418.10		569.72	738.24
MBE-GaN/MOVPE-GaN	0.13/2.1	139.01	417.50		568.63	733.35
MOVPE-GaN	2		418.21		568.01	
MOVPE-GaN with defects	0.03		416.40		576.62	
MBE-InGaN	0.6		416.51		559.5	748.46
MBE-InGaN/MOVPE-GaN	0.6/2	140.74	418.21		568.50	733.13

equipped with a radio frequency nitrogen plasma source from EPI [15]. They were either grown directly on sapphire without any nitridation or on $2\ \mu\text{m}$ thick MOVPE-GaN/sapphire template layers. Prior to the growth of the InGaN layers on the MOVPE templates no oxide removal process or another type of surface treatment was performed.

2.2. Characterization of the layers

The surface roughness and the *surface morphology* was analyzed by AFM method.

The *optical properties* of the layers were determined by SE and PL methods.

SE measurements were made with a Woollam apparatus. A Woollam software together with a parametric semiconductor model was used to simulate the measured SE spectra. Multilayer-model calculations were performed to compute the effective dielectric functions, the energy band gap and the microstructure of the system. The surface roughness (determined by AFM) was included in the model with the aid of the Bruggeman effective medium approximation (BEMA) [17].

The vibrational properties relationship [16] have been studied by Raman spectroscopy. Raman spectra were recorded in a Renishaw Raman Microscope, in backscattering configuration, equipped with an Ar laser for excitation ($\lambda = 514\ \text{nm}$ line, $10\ \mu\text{m}$ spot, spectral resolution of about $1\ \text{cm}^{-1}$). For calibration an undoped Si wafer was used.

3. Results and discussions

The hexagonal MBE- $\text{In}_x\text{Ga}_{1-x}\text{N}$ ($0 < x \leq 0.14$) films, $600\ \text{nm}$ thickness, were grown on sapphire and MOVPE GaN-template layer/sapphire. A comparative characterization of them is given in what follows.

3.1. Morphological properties

The AFM micrographs (of $20\ \mu\text{m}$) presented in Fig. 1 show well-formed crystal-like grains stacking on the surface of $\text{In}_{0.14}\text{Ga}_{0.86}\text{N}$ samples grown directly on sapphire (Fig. 1a) and on the MOVPE template layer (Fig. 1b). The micrograph from Fig. 1b indicates an improvement of the quality of the InGaN film, the grains are more uniformly distributed and of a better crystallinity. It has clear and regular grains with the average size estimated to be approximately $0.5\ \mu\text{m}$. The surface roughness of this film, $\text{RMS} = 16.857\ \text{nm}$, is lower in comparison with film from (Fig. 1a), $\text{RMS} = 34.857\ \text{nm}$ (both estimated from the micrographs of $20\ \mu\text{m}$) due to the use of MOVPE GaN-template layer [14]. The films grown directly on sapphire exfoliate easier.

3.2. Vibrational properties

The purity and the stability of the crystalline phase of our samples and the vibrational properties were estimated by Raman spectroscopy.

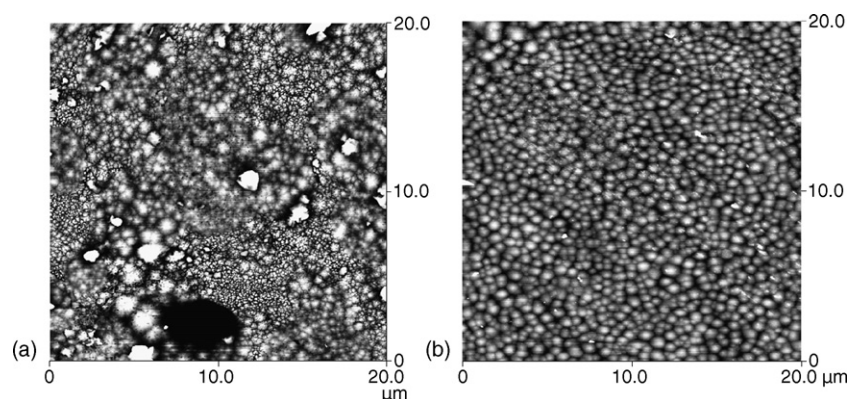


Fig. 1. Comparison between the AFM micrographs of $\text{In}_{0.14}\text{Ga}_{0.86}\text{N}$ layer grown: (a) directly on Al_2O_3 ; (b) on $\text{GaN}/\text{Al}_2\text{O}_3$.

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