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Optical properties of cubic AlGaN

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ABSTRACT

In this work we report optical characterization on several cubic c-AlGaN layers grown by MBE on SiC on Si pseudo-substrates, with different aluminum concentrations ranging from 0 to 70 %. Excitation power evolution of AlGaN photoluminescence (PL) spectra as well as reflectivity spectra allow to attribute PL peak to band gap recombination. PL energy dependence versus aluminum concentration is given. Reflectivity investigations are performed in the energy range between 1.5 eV and 4 eV on the samples. Theoretical calculations of multilayered structure reflectivity are fitted to experimental results, allowing an accurate determination of refractive index evolution versus Al concentration. From this analysis, qualitative information about interface roughness at AlGaN/SiC is also be derived.

INTRODUCTION

At present, most studies on GaN and AlGaN alloys are devoted to the wurtzite (hexagonal) phase as the growth of pure zinc-blende (cubic) phase is more difficult due to its metastable nature. However optimization of Molecular Beam Epitaxy (MBE) growth conditions has led to improve the quality of cubic materials grown on 3C-SiC pseudo-substrates [1]. The c-AlGaN/GaN material system has an expected maximum band offset of 1.6 eV : so intersubband absorption in GaN quantum wells could therefore reach the 1.55 µm wavelength for telecom applications. Such intersubband transitions have already been reported in the hexagonal phase [2] but not yet in the cubic phase. Cubic phase allows to get rid of the huge piezoelectric and spontaneous electric fields occurring in the hexagonal phase of nitrides [3,4] and which may be detrimental to optoelectronic device performance.

For the design of optoelectronic devices, optical constants for c-GaN and c-AlGaN need to be precisely known, but up to now, experimental determination of such constants for c-AlGaN ternary alloys still remain scarce in the literature. In this work we perform PL and reflectivity investigations on several layers with different aluminum concentration ranging from 0 to 70 %.

EXPERIMENTAL

The samples used in this study consist of cubic AlGaN layers grown by rf-plasma assisted Molecular Beam Epitaxy on SiC/Si pseudosubstrates. The growth was controlled by Reflection High Energy Electron Diffraction (RHEED). The samples are composed of a c-AlGaN layer deposited on a 20 Å AlN buffer grown on a SiC/Si pseudo-substrate. For A type samples the substrate consists of a thin (20 Å) carburated Si layer on bulk silicon. For B type samples a thick

(3 µm) c-SiC layer is deposited on top of the thin Si carburated layer. All c-AlGaN layers have a typical thickness of 0.5 µm. The layer thickness and the concentration of Al in alloys were measured by Rutherford Back Scattering (RBS).

PL measurements were carried out using the 244 nm line of an intra-cavity frequency doubled Argon ion laser as pump source at 8 K. For reflectivity measurements, a Xenon lamp dispersed through a monochromator was used as the test beam. The signal was collected by a silicon photo detector. Experimental spectra were fitted by calculation of the reflection coefficient of multilayered structures using the transfer matrix method based on Fresnel coefficients [5].

RESULTS AND DISCUSSION

Photoluminescence measurements

Normalized PL spectra recorded at 8K in samples with different Al concentrations are shown (inset figure 1-A), with the expected blue shift of PL energy as Al concentration increases. Some spectra exhibit several peaks. In order to check the nature of the PL peak (either intrinsic or defect recombination), reflectivity measurements were performed on the samples as well as PL investigations versus excitation power density. It is worth noting that a very low parasitic hexagonal phase content has been evidenced by Raman spectroscopy measurements in the c-AlGaN layers [6]. Therefore we do not expect any contribution of such parasitic phase to PL spectra.

In figure 1-A are plotted PL spectra recorded in a sample with 21 % Al content at different excitation power densities : a peak is arising at high energy 3.705 eV as excitation power increases. The high energy peak is therefore attributed to band gap luminescence, whereas PL peaks at lower energy originate most probably from Donor-Acceptor recombination, following previous studies made on cubic GaN layers [7].

In figure 1-B, PL and reflectivity measurements realized on the same sample at room temperature are presented. The high energy peak in PL spectra arises at the same position than the onset of absorption in reflectivity spectra. This confirms the fact that measured PL signal can be attributed to band gap luminescence. From such measurements PL band gap energy was plotted versus aluminum concentration at 8 K as shown in figure 2. We obtain a linear dependence (equation 1) of PL peak versus aluminum concentration in good agreement with previous work [8,9]. No bowing parameter is observed according with band gap calculation in c-AlGaN where a small bowing parameter is predicted [10].

$$E_{PL}= 3.286 +1.987*X \quad (1)$$

Reflectivity measurements

Typical reflectivity spectra exhibit intense interference oscillations as shown in figure 3. According to the sample structure - A or B type - two types of reflectivity spectra are observed. The first one with only one oscillation frequency corresponds to A type samples (grown on a thin carburated Si layer) and interference take place inside the AlGaN layer. The second one with two different frequencies are recorded in B type samples (grown on a thick SiC layer). In this case the lowest oscillation frequency is attributed again to interference inside the AlGaN layer whereas

the second system with high oscillation frequency corresponds to superimposed interference inside the thick SiC layer.

Experimental spectra are modeled using a transfer matrix method based on Fresnel coefficients, taking into account the true multi-layer structure of the device, and keeping as a parameter the refractive index of the c-AlGaN layer. This calculation shows that the amplitude of oscillations directly depends on the roughness at the different interfaces [11] : in the present case SiC/Si and AlGaN/SiC interfaces. Qualitatively, the rougher the interface, the lower the reflexion coefficient and the lower the oscillation amplitude. In figure 3, the amplitude of the low frequency interference oscillations appears to be significantly higher in A type sample than in B type sample. Such interference being mainly sensitive to SiC/AlGaN interface roughness, we therefore deduce that B type substrates have a higher roughness than A type ones. This is in good agreement with a topological analysis performed by Atomic Force Microscopy (AFM) on the SiC/Si pseudo-substrates before the AlGaN growth : the round mean square roughness amplitude measured on a 20µm X 20µm surface was found to lie between 5nm and 8nm for B type substrates, whereas it was as low as 0.2nm for A type ones. Further investigations are planned to derive more quantitative information about interface roughness from the correlation between reflectivity measurements and AFM surface analysis.

We focus now our attention on the determination of the refractive index of the c-AlGaN alloy versus energy for several Al concentrations. In figure 4 are plotted the results derived from the modeling of experimental reflectivity spectra using the transfer matrix method. Experimental data are fitted using a Sellmeir relationship (equation 2).

$$n(\lambda) = \sqrt{1 + \frac{p1}{(p2^2 - \lambda^2)}} \qquad (2)$$

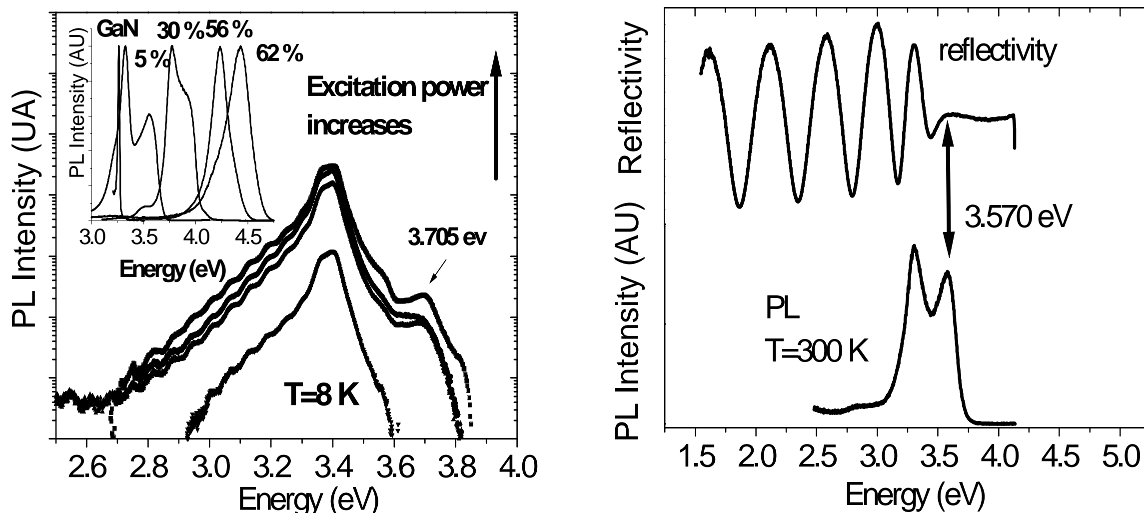

Figure 1. A). PL evolution versus excitation power for an AlGaN sample (21% Al) at 8K. Inset 1-A : Normalized PL spectra recorded at 8K on different AlGaN samples.
B) Reflectivity and photoluminescence recorded in an AlGaN sample (5% Al) at 300K.

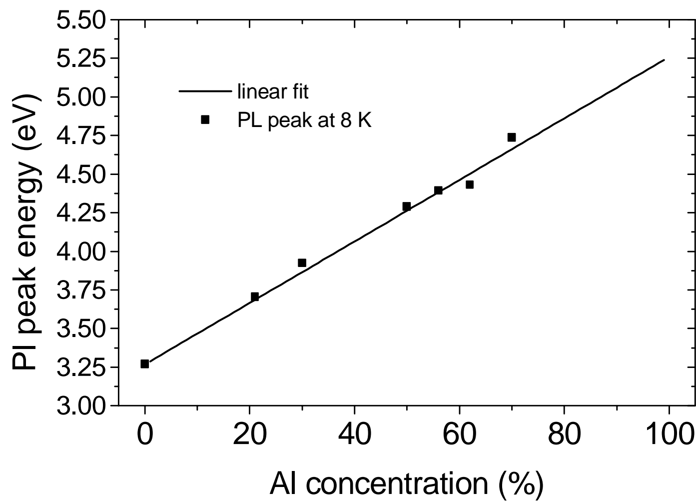

Figure 2. PL peak energy evolution versus Al concentration at 8 K

Parameters p1, p2 and sample types are reported in table I for each Aluminum concentration. As can be seen in figure 4 the refractive index decreases as Aluminum content increases in good agreement with the empirical observation that refractive index decreases when direct band gap increases. For comparison we have reported in figure 4 the unique data previously reported in the literature of refractive index in cubic AlGaN for 5, 30, 50, 52 and 62 % Al at 3.1 eV [12]. Our results are significantly higher than these data which have been measured by spectroscopic ellipsometry and fitted using a large number of parameters. We would like to emphasize here that in our measurements, we keep only the AlGaN refractive index as a parameter, as we have an independent determination of layer thickness and composition by RBS. Moreover the reflectivity method takes into account a large number of interference oscillations from 1.5eV up to 4eV.

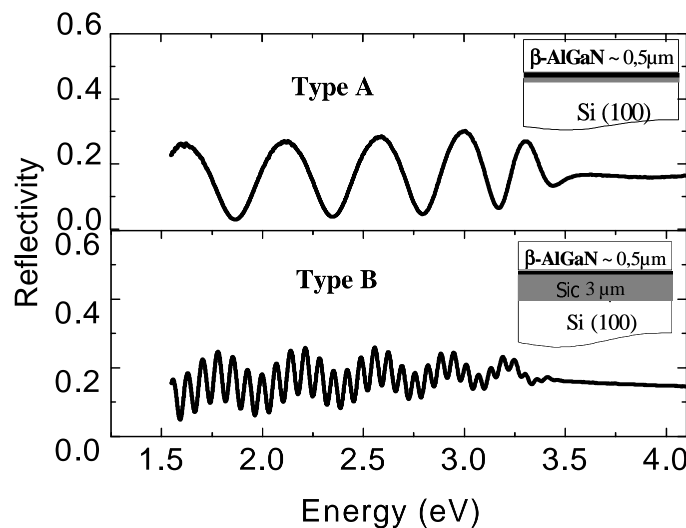

Figure 3. Experimental reflectivity spectra recorded at 300K for A and B type samples.

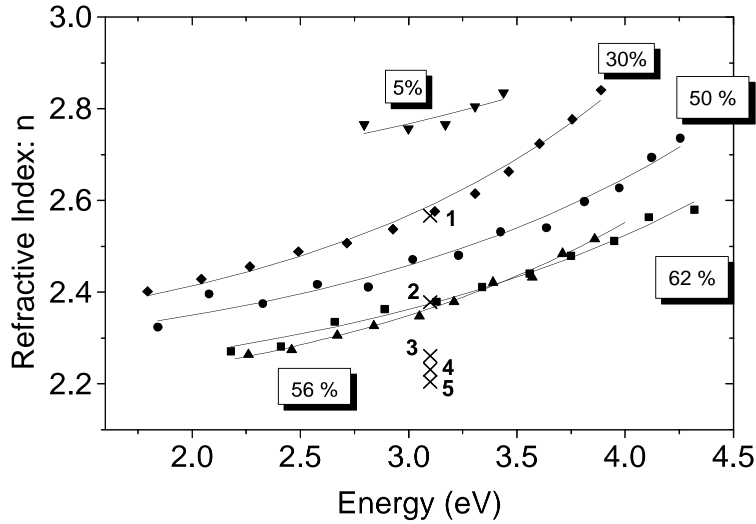

Figure 4. : Refractive index dispersion for several AlGaN samples, solid lines are fits to a Sellmeir-type relationship. Cross points 1, 2, 3, 4, 5 are refractive index values reported from literature [11], for 5, 30 , 50, 56 and 62% Aluminum concentration at 3.1 eV.

Table I. Sellmeir parameters for different Al contents.

% Aluminum (Type)	P1	P2
5 (A)	446	8.7
30 (A)	176	6.4
50 (B)	218	7.2
56 (B)	171	6.8
62 (B)	173	6.9

CONCLUSIONS

From the comparison between PL and reflectivity spectra of several c-AlGaN layers deposited on pseudo-substrates SiC/Si, we attributed the high energy PL peak to band gap recombination. A linear dependence of band gap luminescence versus Aluminum content is reported. The determination of refractive index of cubic AlGaN layers was achieved for the first time by reflectivity measurements in the spectral range 1.5eV-4eV, for Aluminum concentrations ranging between 0% to 70%. As layer composition and thickness were independently determined by RBS, the c-AlGaN refractive index was the only parameter allowed to vary when fitting reflectivity spectra. Qualitative information about SiC/AlGaN interface roughness has been deduced from the analysis of reflectivity spectra in agreement with AFM.

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