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# Study of interference effects on the photoluminescence of AlGaN/GaN quantum wells

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In this work we compared the optical properties of AlGaN(50 nm)/GaN(5 nm) quantum wells (QWs) grown by plasma-assisted molecular beam epitaxy (PAMBE) technique, on Si(111) substrates and sapphire substrates. Optical properties were acquired by photoluminescence (PL) and reflectance (R) spectroscopies. Reflectance spectra shows interference oscillations of the reflected beam at Air/AlGaN and the beam reflected at bottom interface with Si substrate. Such oscillations vanish at the band gap of GaN buffer layer (3.4 eV). The PL spectra of samples grown on Silicon substrate shows a photoluminescence modulation effect, attributed to interference of light emitted from the QWs that is reflected at different heterostructure interfaces. On sapphire substrate no modulation effect is present. This could be explained due to interfacial roughness and the smaller refractive index of sapphire in comparison to silicon. PL shows a strong emission around 3 eV, which is in agreement with recombination energy determined by self-consistent calculations, which consider a 4 MV/cm built-in electric field and low carrier densities.



**1 Introduction** Nitride semiconductor materials have enabled the design of nanostructures that can operate optically from the infrared to the ultraviolet of the electromagnetic spectrum, which are highly suitable for making devices like electroluminescent diodes, UV sensors and high efficiency solar cells of second and third generation [1]. Some of these devices are grown with microcavities to enhance optical characteristics like the output power [2]. Most common microcavities are based on super-lattices, however few years ago, some researchers propose simple microcavities designed to match with the wavelength of the incident light [3]. In this work we present the results of Fabry-Perot effects due to an inherent microcavity without the contribution of a top Bragg reflector. Our structure could be potentially employed for improvement of ultraviolet Light Emission Diodes with a GaN active layer using AlGaN barriers.

**2 Experimental** The structures were grown on a Riber C21 molecular beam epitaxy (MBE) system. Active Nitrogen (N) flux was provided by an rf-plasma source operated at 150 W with a $N_2$ flow of 0.25 sccm. We employed two types of substrates: silicon and sapphire. Ratio of III/N fluxes was higher than one to ensure a metallic rich growth condition that leads to a smoother surface, a decrease in defect density and higher electron mobility [4]. In the case of silicon substrates, they were previously chemically cleaned by employing the Ishizaka and Shiraki method [5]. Surface oxides on substrates were thermally desorbed at 900 ºC. Next, substrate temperature was decreased to 750 ºC, at this temperature a 7x7 surface reconstruction was observed by Reflection High-Energy Electron Diffraction (RHEED) indicating a successful oxide desorption. Then a metallization of the Si surface with an aluminum layer (~5 monolayers) was performed at 850 ºC during the onset of nitrogen plasma source. This was done to avoid nitrogen incorporation and the formation of SiN which involves amorphization of Si surface. After this process an AlN layer was grown at 850 ºC with a nominal thickness of 27 nm. After that, a 5 period superlattice of AlN/GaN was grown to get a smoother surface, followed by a GaN buffer layer with a thickness of 600 nm employing a substrate temperature of 800 ºC. Finally, a series of 5 quantum wells were grown with a GaN 5nm-thick active layer and 50 nm-thick AlGaN barriers with an aluminum composition of 30%. A growth stop of 80 s was applied after each of the five GaN active layers. For the growth on sapphire substrates, we performed a surface nitridation process at 900 ºC for 20 min. Then substrate temperature was decreased to 800 ºC to grow an AlN buffer layer, followed by the same growth procedure as for Si substrates.

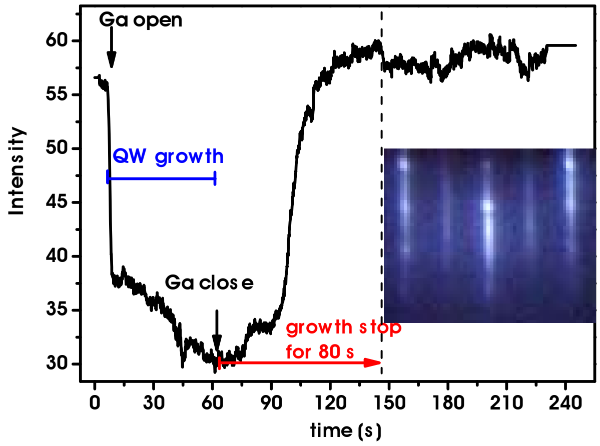


**Figure 1** RHEED intensity during growth of the GaN active layer of quantum wells.

**3 Results** Figure 1 shows the intensity behavior of RHEED specular spot during QWs growth. We can observe that the RHEED intensity decreases just after the Ga shutter is opened, which indicates an increase in surface roughness. When Ga shutter is closed, the RHEED intensity recovered during the 80 s growth stop, which suggests a smoothing of the surface. At the end of the growth we observed a (2x2) RHEED pattern (inset in Fig. 1), which confirms an atomically flat surface with Ga polarity [6].

The samples were characterized structurally by high resolution X-ray diffraction (HRXRD) on a Panalytical MRD Xpert diffractometer. We employed $K_{\alpha}$ radiation of Cu and spectra were obtained with a two bounced monochromator and a three bounced analyzer in a triple axis arrangement. Diffraction patterns were obtained to verify the formation of wurtzite structure for GaN and AlGaN layers. Also we obtained rocking curves for the diffraction of {0002} planes of GaN, AlGaN and AlN. From the full width at half maximum (FWHM) of the rocking curves (Table 1) we found that crystalline quality is slightly better for growth over silicon substrates.

**Table 1** FWHM of HRXRD rocking curves of {0002} planes of GaN, AlGaN and AlN on Si and Sapphire substrates.

| Substrate | Si | Sapphire |
|---|---|---|
| GaN | 0.47 | 0.49 |
| AlN | 0.63 | 0.69 |
| AlGaN | 0.59 | 0.51 |

Photoluminescence (PL) signal was obtained by optical excitation of samples with a He-Cd laser and luminescence was analyzed employing a Horiba/Spex 1404 0.85m Double Spectrometer. Sample grown on Si(111) substrate presents a PL spectrum centered at 3 eV, which is modulated by oscillations that coincides with its reflectance spectrum (Fig. 2). For sapphire substrate, PL spectrum is centered at 3.1 eV without oscillations.

For both samples, we obtained a strong red shift in spectra due to combined effect of internal electric field and the carrier distribution. By using the mode spacing expression as in Ref. [2], we calculate a 700 nm thickness of the vertical cavity formed between the air/AlGaN and the GaN/AlN interfaces, considering the peaks located at 2.9 and 3.1 eV, respectively.

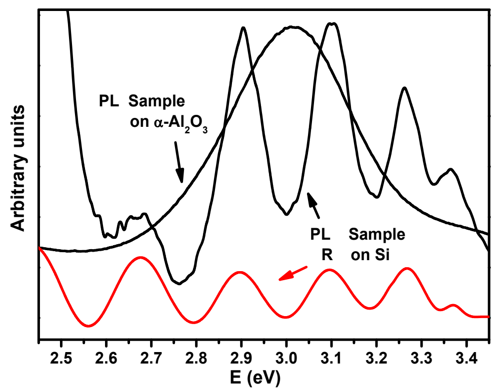


**Figure 2** PL of AlGaN/GaN QWs grown on Si (red) and sapphire (black). Reflectance of QWs grown on Si (blue).

For further investigation of the modulation effect on the photoluminescence spectrum, we measured PL and R spectra at different emission angles relative to sample normal and different incident angles as shown in Fig. 3. Maximum modulation peaks present a shift to higher energies as a function of incidence angle.

Equation (1) describes the energy position dependence of constructive interference as function of the measurement angle. From this equation, when the angle $\theta_m$ at which the spectrum is measured increases, energy of constructive interference increase, because $cos(\theta_m)$ decrease.

$$h\nu = \frac{(2m+1)hc}{d_{buffer}n(\lambda)}\frac{1}{cos(\theta_m)} , \quad (1)$$

where $d_{buffer}$ is the thickness of microcavity, $n$ the refraction index and $(2m+1)$ are integers which define maximal reflectivity points [7].

In order to determine the theoretical position of luminescence, we calculated a band diagram for a single quantum well obtained by self-consistent solution of Schrödinger and Poisson's equations by employing a variational method, which can be resumed in the following equations:

$$\sigma_{pol} = P_{tot,layer1} - P_{tot,layer2} , \quad (2)$$

$$\sigma_{pol} = (P_{SP} + P_{PE})_{GaN} - (P_{SP} + P_{PE})_{AlGaN} , \quad (3)$$

$$h\nu = E_g + E_e + E_{hh} + \delta_{E_e} + \delta_{E_{hh}} , \quad (4)$$

$$\delta E_i = \frac{2maeE}{\hbar^2} z^{22} , \quad (5)$$

where $E_g$ is the gap of the semiconductor QW, $E_{e(hh)}$ is the electron (hole) energy without electric field in the QW and $\delta_{E_{e(h)}} = H_{e(h)} - E_{e(h)}$ is the induced energy shift for electrons (holes) which depends on the carrier density and the built-in electric field [8].

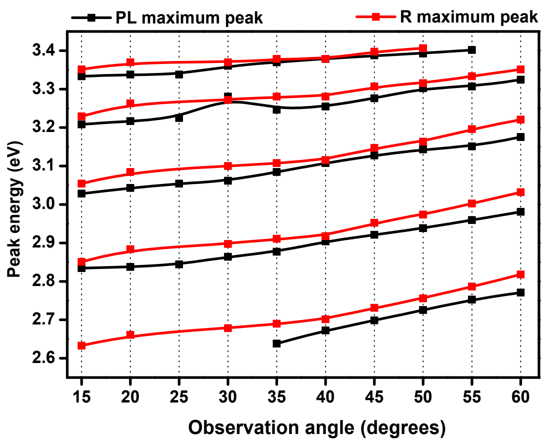


**Figure 3** Angle dependence of PL (black squares) and reflectance (red circles) maximum for sample grown on Si.

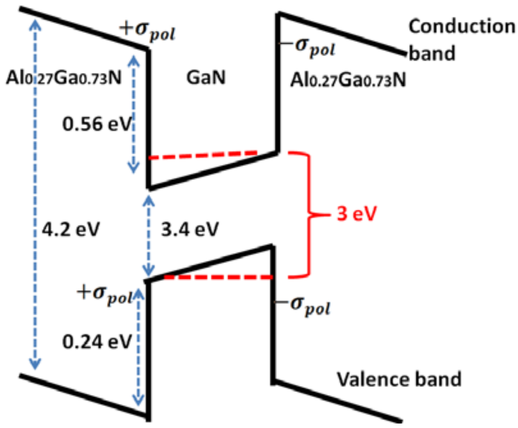


**Figure 4** Band diagram of a single quantum well using variational method.

In the construction of the band diagram we consider a band gap of 3.4 eV for GaN and 4.4 eV for AlGaN, and a low density of carriers regime ($\eta$<1010 $cm^{-2}$) at which, it is not possible to get screening of internal electrical fields. In addition to this, the AlGaN barriers must growth under biaxial tension, due to a shorter lattice parameter than GaN. The barrier will show spontaneous polarization ($P_{sp}$) and piezoelectric ($P_{pz}$), while QW only presents spontaneous polarization. ($P_{sp}$). The results of such calculation are summarized in Fig. 4. From this model we obtained a recombination energy $E_{PL}$=3 eV, which correspond to the transition energy between the highest hole level and the lowest electron level. This occurs when the band offset is 0.7 eV for the conduction band and an internal piezoelectric field is 3.3 MW/cm.

**4 Discussion** Fabry-Perot interferences effects have been reported previously in InGaN/GaN heterostructures [9]. In our case, we have proven to get a Fabry-Perot interference using a thinner structure based in a AlGaN/GaN layers. We think that the GaN/AlN superlattice at the very beginning of the whole structure could contribute to obtain a higher reflection of light generated at QWs during PL excitation. In order to theoretically verify this hypothesis, we calculated the reflectivity for such structure using an expression which do not depend on layer thickness but wavelength [10]. We found that reflectivity percentage of the rays originated at QWs for this superlattice structure is 60% at 325 nm wavelength. Another possible effect of the superlattice is to decrease the strain of GaN buffer layer, and also to smooth out the surface roughness of AlN layer. Here it is important to comment that we grew the same structure but without the GaN/AlN superlattice and found no modulation effects on luminescence.

We neither found PL modulation effects on set of samples grown over silicon substrates with similar conditions, but employing lower substrate temperatures of 780 ºC and 760 ºC. The interference effects are present in samples, grown with the highest substrate temperature. It is clear that with decrease of substrate temperature, we decrease the surface mobility of adatoms during the growth. For such reasons, we think that this effect is very sensitive to interface roughness

**5 Conclusion** We have found Fabry-Perot interferences effects in GaN/AlGaN QWs grown on Si substratres. The PL interference peaks have a shift to higher energies when the angle $\Theta_m$ at which the spectrum is measured increases, according to the interference condition. The photoluminescence modulation is due to the Fabry-Perot interference of the emitted light from the QWs when it is reflected at the AlN/GaN SL/Si(111) and AlGaN/air interfaces. We consider such effect is not present in sample grown on sapphire due to higher roughness of AlN/sapphire interface, which is more dispersive, and also because the effective transmission coefficient for sapphire substrate is higher than silicon.

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