Optical transmission of strained GaN/sapphire structures

S Yu Kurin¹, M V Puzyk²,³, I A Ermakov², A A Antipov¹, I. S. Barash¹, A D Roenkova, V V Ratnikov⁴, A S Usikov²,⁵, B P Papchenko², H Helava³, Yu N Makarov¹,⁵ and A E Chernyakov⁶

¹Nitride Crystals Group Ltd., pr. Engel’sa 27, St. Petersburg 194156, Russia
²University ITMO, Kronverkskiy pr. 49, St. Petersburg 197101, Russia
³Herzen University, Nab. r. Moyki 48, St. Petersburg 194186, Russia
⁴Ioffe Physical Technical Institute, Polytekhnicheskaya 26, St. Petersburg 194021, Russia
⁵Nitride Crystals Inc., 181 E Industry Court, Suite B, Deer Park, NY 11729, USA,
⁶Submicron Heterostructures for Microelectronics Research & Engineering Center, RAS, 26 Polytekhnicheskaya Str., St. Petersburg 194021, Russia

Abstract. In this work we correlated transmission spectra of GaN layers grown on sapphire substrates by hydride vapour phase epitaxy with biaxial stress measured in the layers. It was observed that the sign of stress in the GaN layer is changed by Si doping and growth conditions. Transmission curves are shifted relative to each other depending on the stress in the layer. The cut-off wavelength of the transmission curves has a tendency to shift near parallel to a shorter wavelength range when the GaN layer is under the compression biaxial stress. When the GaN layer is under the tensile biaxial stress the cut off wavelength has a tendency to shift near parallel to a longer wavelength range.

1. Introduction

One of the challenges remaining in the epitaxial growth of III-N materials is the absence of affordable lattice-matched bulk GaN substrate. Sapphire and SiC substrates that are widely used in nitride-based technology are lattice mismatched substrates resulting in threading defects and biaxial strain lowering performance and shortening lifetime of the device structure. A possibility to control the strain at the heteroepitaxial growth of GaN-based structures on foreign substrates is critically important for optimization of the growth conditions to grow strain-less and defect-less layers and structures for understanding the electrical and optical properties of grown structures and, therefore, is of great practical interest. Optical characterizations provide a convenient way to examine the different properties of semiconductors. In particular, measuring the transmittance coefficient of GaN layers grown on sapphire substrates may give information about the strain in the material connected with a specific of the growth process.

In this work we studied transmission spectra of GaN layers grown by hydride vapour phase epitaxy (HVPE) on c-plane sapphire substrates in a horizontal quartz reactor [1]. Typically, HVPE has high growth rate in a range of 0.3-1.2 µm/min. Because of that, HVPE is commonly used for fabricating of GaN quasi-bulk material and GaN templates to use as substrates for III-N device structure growth. The wide range of the growth rate influences on the impurities incorporation that can affect the strain in the
grown layers [2]. We correlated transmission spectra of GaN layers grown on sapphire substrates with the biaxial stress measured in the layers. The AlGaN layers (tens of nanometers) were used as thin intermediate layers prior to the GaN layer growth.

2. Experimental details

Several 5-7 µm thick GaN layers were grown by hydride vapour phase epitaxy (HVPE) on 2-inch c-plane sapphire substrates in a horizontal quartz reactor [1]. The growth process was performed at 1040°C and atmospheric pressure with argon as a carrier gas. Ammonia (NH3) and hydrogen chloride (HCl) were used as precursors. For GaN growth, HCl was passed over Ga source. To grow the AlGaN alloy, HCl was passed separately over the Ga and Al sources. Si doping was realized by injection of free HCl gas through a separate quartz tube into a growth zone. Reaction of the HCl gas with the quartz walls of the injection tube and the reactor resulted in the n-type doping by Si. The growth procedure included in-situ sapphire substrate treatment followed by a composite AlGaN buffer layer and GaN layer growth. The growth conditions the AlGaN buffer and the GaN layer were change at the undoped and Si-doped GaN layers growth. Capacitance-voltage (C-V) mercury probe measurements at 1 MHz revealed Nd-Na concentration of (1-4) \(10^{16}\) cm\(^{-3}\) and (1-3) \(10^{18}\) cm\(^{-3}\) for undoped and Si-doped GaN layers, respectively, depending on growth conditions. All layers were crack free. The biaxial stress in the layers grown at different initial conditions was evaluated based on XRD measurements using Stoney’s formula [3].

For transmission spectroscopy we used a commercial spectrophotometer that was capable of recording spectra in the visible range as well as in the near infrared and UV. To compensate for the complicated intensity distribution of the light source the spectrometer did not measure absolute values but compared the signal from the sample to a reference beam. Additionally, a baseline was recorded prior to the actual measurements to calibrate the instrument.

3. Results and discussion

Figure 1 shows X-ray ω-scan rocking curve width (full width at half maximum, FWHM) for symmetric ((00.2) GaN) and asymmetric ((10.2) GaN) reflections with the GaN layers thickness. The FWHM is a figure of merit for crystal quality and usually decreases with the layer thickness (in a wider range of thickness) due to the threading dislocations annihilation for GaN layers grown on c-plane sapphire [4]. No clear dependency of the FWHM values with thickness can be observed in figure 1 and we may consider that difference in layer thickness of GaN samples studies is too small to have an effect on the total stress in the layer. Note also that the (00.2)FWHM and the (10.2)FWHM values for undoped GaN layers are closer to each other than that of Si-doped GaN layers. This is indicative that Si doping disturbs the GaN crystalline cell. Indeed, undoped GaN layers have larger c- and lower a- parameters that Si-doped GaN layers [5].

![Figure 1](image1.png)

Figure 1. Thickness dependence of X-ray rocking curve width in Si doped GaN layers (a) and undoped GaN layers (b).

Figure 2 shows the radius of curvature evaluated in the same Si-doped undoped GaN layers grown on 2-inch sapphire substrates. All studied undoped GaN samples had concave shape (negative radius of
curvature) although growth conditions of the composite AlGaN buffer layer and the GaN layer were different between the samples. The concave shape is attributed to compressive biaxial stress in the sample.

On the other hand, Si-doped samples that were grown in the similar conditions of the AlGaN buffer layer growth had both concave shape (positive radius of curvature) and convex shape (negative radius of curvature). The convex shape is attributed to tensile stress in the sample. Thus, depending on the growth conditions Si-doped GaN layers can be grown on 2-inch sapphire substrates by HVPE having different shape.

Figure 3 shows biaxial stress in Si-doped and undoped GaN samples evaluated based on XRD measurements. It was observed that the stress can reverse sign from $\sigma^+$ (concave shape of the sample, tensile stress) to $\sigma^-$ (convex shape of the wafer, compressed stress) in Si-doped GaN layers depending on the growth conditions of the AlGaN buffer layer mainly. All undoped GaN layers were under compressive stress ($\sigma^-$) and have convex shape. The sign of stress in the undoped GaN layers did not change. Variation of the layer thicknesses did not influence the X-ray rocking curve width that indicates that the stress changing can be associated with the doping and the growth conditions only.

The transmission curves of undoped and Si-doped GaN/sapphire samples having different biaxial stress are given in figure 4. The sapphire substrate did not absorb light itself in the visible, near IR and UV spectral ranges. The transmission curves show that for high energies there is no transmission because all the light is absorbed. However, for low energies there are no appropriate electronic transitions so transmission is very high in this range. There is a relatively sharp delimitation (cut-off wavelength) between the areas of high and low absorption. A position of the cut-off wavelength corresponds to the band gap of GaN and strain in the layers grown.

The cut-off wavelength has a tendency to shift near parallel to a shorter wavelength range when the GaN layer is under compression biaxial stress ($\sigma^-$). The shorter cut-off wavelength means lager
When the GaN layer is under tensile biaxial stress ($\sigma^+$) the cut off wavelength has a tendency to shift near parallel to a longer wavelength range. Note that the parallel shifting of the cut-off wavelength in the transmission spectra was usually observed at a fine turning of the growth conditions when the only or a few parameters change a little. If growth conditions disturb crystalline quality (high dislocation density, high background impurity concentration) than the shift of the cut-off wavelength will not be parallel without sharp delimitation between the areas of high and low absorption and no direct correlation with the stress is observed.

**Figure 4.** Transmission curves of GaN/sapphire samples. The legend shows values of the biaxial stress measured in the particular sample.

**4. Conclusions**

Thus, it was observed that shape (convex, concave), radius of curvature and stress (sign of the stress) the sign of stress of the GaN layers grown by HVPE on 2-inch sapphire substrates are changed by Si doping and growth conditions. Transmission curves are shifted relative to each other depending on the stress in the layer. The cut-off wavelength has a tendency to shift near parallel to a shorter wavelength range when the GaN layer is under compression biaxial stress ($\sigma^-$). When the GaN layer is under tensile biaxial stress ($\sigma^+$) the cut off wavelength has a tendency to shift near parallel to a longer wavelength range. If growth conditions disturb crystalline quality (high dislocation density, high background impurity concentration) than the shift of the cut-off wavelength will not be parallel without sharp delimitation between the areas of high and low absorption and no direct correlation with the stress is observed.

**Acknowledgements**

Work at University ITMO was supported by the Ministry of Education and Science of Russian Federation (grant agreement 14.575.21.0054, unique identifier of research activities is RFMEFI57514X0054).

**References**

[1] Kurin S, Antipov A, Barash I, Roenkova O, Usikov A, Helava H, Ratnikov V, Shmidt N, Sakharov A, Tarasov S, Menkovich E, Lamkin I, Papchenko B and Makarov Yu 2014 *Phys. Status Solidi C* **11** 813-816.

[2] A. Usikov, 1, O. Kovalenkov, V. Soukhoveev, V. Ivantsov, A. Syrkin, V. Dmitriev, A. Yu. Nikiforov, S. G. Sundaresan, S. J. Jeliazkov, and A. V. Davydov. phys. stat. sol. (c) 5, No. 6, 1829–1831 (2008).

[3] Stoney G G 1909 *Proc. of Royal Society of London* **A82** 172-175

[4] Wagner V, Parillaud A, Buhlmann H J, Illegems M, Gradecak S, Stadelmann P, Riemann T and Christen J 2002 *J. Appl. Phys.* **92** 1307.

[5] Usikov A, Kovalenkov O V, Mastro M M, Tsvetkov D V, Pechenkov A I, Soukhoveev V A, Shapovalova Y V and Gainer G H 2002 *Mat. Res. Soc. Symp. Proc.* **743** L3.41.