Effect of SiC buffer layer on GaN growth on Si via PA-MBE

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Abstract. The study is devoted to comparison of GaN thin films grown on SiC/Si substrates made by the method of atoms substitution with the films grown directly on Si substrates. The growth was performed in a single process via plasma assisted molecular beam epitaxy. The samples were studied via optical microscopy, Raman spectroscopy, ellipsometry, and a comparison of their characteristics was made. Using chemical etching in KOH, the polarity of GaN films grown on SiC/Si and Si substrates was determined.

1. Introduction
Today, the development of electronics is skyrocketing, since it is increasingly being implemented in our life. This is the reason why one of the main goals of thin film technology is to develop new and prospective methods to grow cheaper semiconductor thin films of higher quality. One of the most promising material is gallium nitride (GaN) [1-3], which can be successfully used in power electronics, light emitting diodes and many other devices. However, there are still some limitations on the quality of growing GaN films caused by the absence of suitable substrates [4], since the common substrates, such as sapphire, silicon, etc., are not well-suited to GaN lattice and its thermal expansion coefficient. More suitable materials like silicon carbide [5] are still too expensive. Thereby, researchers are trying to find new approaches, for instance, deposition of different buffer layers [6] or even multi-layered buffers in efforts to grow high-quality GaN. To solve this problem and to produce cheap suitable substrates for GaN, we suggest to use the method of atoms substitution proposed in [7,8], which allows one to grow a thin SiC buffer layer of high quality directly on Si substrate. In the current work, we compared the crystalline properties of GaN films grown on SiC/Si substrate and directly on Si substrate via plasma assisted molecular beam epitaxy (PA MBE) [9]. This method has a series of advantages. Firstly, it allows one to grow films without using hydrogen and at low substrate temperatures. Secondly, depending on growth conditions and substrate type it allows producing GaN films of different polarity [10] which is important in view of further GaN use in various devices. The grown samples were studied via optical microscopy, ellipsometry, Raman spectroscopy and SEM. After growth, the samples were etched in KOH to determine their polarity: Ga-polar or N-polar.

2. Experiments
We used semi-insulating Si(111) substrates and SiC/Si(111) substrates made by the method of atoms substitution [7]. For the growth of the latter, we used p-type silicon. The growth parameters were as follows: total pressure (CO+SiH₄) 1.8 Torr, temperature 1250°C, content of SiH₄ in a gas mixture 16%.
The growth time was 15 min. Thickness of the resulting SiC buffer layer was 72 nm, according to ellipsometry. Epitaxial GaN layers were grown using Veeco Gen 200 facility, which allows one to use multiple substrates in one PA MBE growth process. Before the growth, silicon samples were cleaned via Shiraki [11] method. For nitrogen activation, a high-frequency plasma source RFN 50/63 (Riber) was used. The growth was performed in two stages: firstly, 200 nm thick LT-GaN layer has been grown at low temperature (T=650°C) and after that HT-GaN layer has been grown at higher temperature (T=730°C).

3. Results

The ellipsometric data of the samples is presented in Figure 1. According to ellipsometry, the thickness of the GaN film on Si(111) was ~800 nm, whereas the GaN film on SiC/Si(111) was ~780 nm in thickness. Ellipsometry also demonstrates that the GaN/Si(111) sample is slightly more transparent than the GaN/SiC/Si(111) sample. We also measured Raman spectra of the samples. Absolute position of the band of GaN $E_2$(high) $\approx68$ cm$^{-1}$[12], which is dependent on the mechanical stress in the film, was different for both samples. The estimation of residual mechanical stresses, based on the position of the band, gave 150 MPa tensile stress for GaN/Si sample and 190 MPa compressive stress for GaN/SiC/Si sample.

The samples were also subjected to X-ray diffraction, which has shown that FWHM of the rocking curve for GaN/SiC/Si sample was 36 arcmin, whereas for the sample GaN/Si it was 53 arcmin, and thus GaN grown on SiC/Si substrate has a higher crystalline quality.

![Figure 1](image1.png)

**Figure 1.** Ellipsometric data of GaN/Si(111) sample (a) and GaN/SiC/Si sample (b).

During our studies, we have noticed formation of untypical islets of triangular shape with a characteristic size of the order of a few tens of microns on the surface of both samples in the regions far away from the center. Since the islets were found on both substrates and were of a similar nature but had some differences in the formation (on GaN/Si substrate they were more clearly visible and of higher concentration than on GaN/SiC/Si substrate), we studied them via Raman spectroscopy to understand their origin. Optical image of the islets on GaN/Si sample is presented in Figure 2a.
Using a confocal micro-Raman setup Witec Alpha 300R equipped with a piezo-table, the area containing triangular islets was studied. Figures 2b and 2c show the Raman maps (20 * 20 points) constructed using the intensity of silicon band (521 cm\(^{-1}\)) (Fig. 2b) and GaN band (568 cm\(^{-1}\)) (Fig. 2c). The maps correspond to the rectangular region marked in Figure 2a. It is clearly seen that triangular islet has composition different from surrounding substrate. The substrate dominates on the Raman map of silicon band (see figure 3b), whereas the islets dominate on the Raman map of GaN. Consequently, it can be concluded that these triangular islets consist of gallium nitride. One should note that Raman spectra of the substrate far from the islets also contain low-intensity band of GaN (Fig. 3). Thus, it can be supposed that the substrate is covered by thin GaN film and by triangular GaN islets on it, like in Stranski-Krastanow growth mode, which takes place when mechanical stresses in the film are quite high. It should be noted that difference in GaN band intensity on such islets and on substrate is much greater on the GaN/Si sample than on GaN/SiC/Si sample, which confirms conclusions about elastic stresses in the GaN film grown on SiC/Si. The origin of dark round defects (Fig.2a) is not fully understood.

**Figure 2.** Optical image of the GaN/Si surface demonstrating triangular islets (a) and Raman maps constructed using intensity of silicon band (521 cm\(^{-1}\)) (b) and GaN band (568 cm\(^{-1}\)) (c).

**Figure 3.** Raman spectra of the sample on the substrate far from islet (red line) and on the islet (black line).
Since many optical and electrical properties of GaN thin films and devices are determined by the polarity [13] of these films, we conducted a series of experiments to determine the influence of the substrate on the polarity of the grown structures. For this, we etched samples in KOH via standard procedure [14] and after that studied surface morphology via scanning electron microscopy (see Figure 4). One of the samples (GaN/SiC/Si) demonstrated pyramidal structures on the surface, which are typical for N-polar GaN. The other sample (GaN/Si) surface was not affected by etching procedure, and therefore it is Ga-polar.

4. Conclusions

In this work, we considered the growth of GaN films on SiC/Si(111) substrate made by the method of atoms substitution and directly on Si(111) substrate in one process of plasma assisted molecular beam epitaxy. Resulting samples were studied via different diagnostic methods: optical microscopy, ellipsometry, Raman spectroscopy, SEM. The total thickness of the films was estimated, and it was shown that GaN/Si sample is slightly more transparent than GaN/SiC/Si sample. Also, by means of X-ray diffraction, it was demonstrated that crystalline quality of GaN film grown on SiC/Si substrate is higher than on Si(111) substrate. The estimation of mechanical stress gave the value of 150 MPa tensile stress in GaN/Si(111) sample and 190 MPa compressive stress in GaN/SiC/Si(111) sample. Formation of triangular-shaped islets on the surface of the samples has been revealed, corresponding Raman maps of the islets were constructed, and it was shown that the islets consist of GaN. The islets are forming more actively on GaN/Si substrate than on GaN/SiC/Si. The obtained results suggest that SiC buffer plays a positive role during GaN growth.

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