Structural and morphological characteristics of GaN-based hybrid heterostructures grown on por-Si

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Abstract. GaN/Si(111) heterostructures were grown by plasma-assisted molecular beam epitaxy on usual Si(111) substrates and compliant por-Si/Si(111) substrates without using AlN buffer layer. The positive influence of the high-temperature nitridation step, as well as the usage of a compliant substrate on crystalline quality, was confirmed. We got a crack-free 850-nm-thick GaN layer at room temperature by using the low-temperature GaN buffer layer with nanocolumnar morphology.

1. Introduction
A lot has recently been made to study various approaches to the integration of III-V optical functional elements and existing silicon signal processing technology. This integration is required for the development of the new generation of the electronic component base for datacom and computercom systems [1, 2] which require much higher throughput and lower power consumption than the currently existing optoelectronic elements. Last time, many approaches have been proposed to improve the crystalline perfection of heterostructures based on materials of the III-N system, but all of these approaches require a significant complication of the manufacturing technology leading to drastically increase in end-device cost. The solution to this problem can be the use of commercially available “compliant” Si substrates, which includes a thin nanoporous Si layer. In our previous works, it was shown that the usage of por-Si layer helps to decrease strain level and threading dislocation density in III-N layers grown directly on Si substrates [3–5]. In this paper, we present a new design of GaN/por-Si heterostructure with the original low-temperature GaN buffer layer, which is isotropically distributed an array of nanocolumns with the same diameters.

2. Experimental
The porous silicon layer in the process of obtaining a “compliant” por-Si substrate was formed on the single-crystalline plate of c-Si(111) by electrochemical etching in the alcohol solution of fluoric acid according to the standard technique [3–5]. The porous silicon layer was approximate of 30 nm thick, with a technologically defined average pore size of ~1–5 nm. All substrates were pre-treated using the Shiraki method [4]. After that all of the substrates were annealed at 820°C for 30 minutes in the growth chamber, followed by nitridation step at Ts=850°C for the same time and FN~0.1 μm/h. Low-temperature
(LT) GaN buffer layer with a thickness of 15 nm was formed at $F_{Ga}/F_{N}=1$ flux ratio and $T_c=650^\circ C$ then the main 820 nm thick high-temperature (HT)-GaN layer was grown at $T_S = 730^\circ C$ with a flow ratio of $V/III \sim 6$. Reflection high-energy electron diffraction (RHEED) was used for \textit{in situ} control of the surface morphology of the layers. The surface morphology was also investigated \textit{ex-situ} by atomic force microscope (AFM), scanning electron microscopy (SEM) and with an optical microscope (OM). Crystalline quality was studied by XRD and pole figures analysis, mobility and carrier concentration was determined by analysis of the Hall measurements data.

3. Results

Survey diffractograms for the investigated GaN/c-Si and GaN/por-Si samples are presented in figure 1 and they were obtained in the standard Bragg-Brentano geometry. Indexing of the obtained results demonstrated that in the experimental diffractogram patterns, the most intensive lines are as follows: a reflection from the plane (111) of Si substrate and the diffraction reflections (0002) and (0004) from GaN layer.

The XRD analysis data are shown in table 2. It can be seen that in accordance with the obtained results in the case of the film growth on the “compliant” por-Si substrate a coherent epitaxial growth was observed. Moreover, a lower concentration of threading dislocations for the sample grown on por-Si substrate was observed.

| Table 1. Results of the X-ray diffraction analysis |
|-----------------------------------------------|
| Sample | Lattice parameters | Deformation components | Distortion | Density of dislocations |
|        | $c$, Å             | $a$, Å                  | $e_{xx}$   | $e_{zz}$   | $\rho_{\text{crew}}$, cm$^{-2}$ | $\rho_{\text{edge}}$, cm$^{-2}$ |
| GaN/c-Si(111) | 5.1934               | 3.1141                  | -0.02      | 0.0015     | -0.07                         | 4.51·10$^{10}$ | 4.51·10$^{9}$ |
| GaN/por-Si(111) | 5.1951               | 3.1909                  | 0.0005     | 0.002      | 4                              | 4.3·10$^{10}$ | 4.3·10$^{9}$ |

Detailed analysis of the cross-section images of GaN/c-Si(111) and GaN/por-Si(111) (figure. 2 b and e) demonstrates that GaN/por-Si sample has more planar GaN-Si interface and considerably fewer extended local defects penetrating through the film thickness.
Regarding the surface of the epitaxial layer, the GaN/por-Si(111) (figure 2,f) has a pronounced relief caused by the coalescence of GaN 3D nucleation islands. These findings agree with the results of the study of the surface in the epitaxial GaN layers by atomic force microscopy (AFM) shown in figure 3;

In addition, figure 3 showed that due to the film growth on the compliant substrate when GaN 3D nucleation islands undergo coalescence, a characteristic ordered microrelief is formed on the surface of the film (see the distribution function of relief on the surface in Fig 3,d), which is not observed for the sample grown on c-Si(111) (figure. 3,c)

To determine the orientation of the GaN layer achieved by growth of nanocolumns following coalescence into the 2D layer, pole figures were obtained for the samples grown as on c-Si(111), as the compliant substrate of por-Si: pole figures for the reflection of (111) from Si, (0002) from GaN and
(1012) from GaN. Figure 4 a and b revealed differences between reflections from c-Si and por-Si surfaces. There were no other reflections in the pole figure obtained for the sample grown on por-Si substrate, but two low-intensive reflections Si(111) and Si(111) were observed in the pole figure of the structure grown on c-Si. The appearance of these reflections in the pole figure is probably due to the disorientation of crystallites in the silicon substrate within the interface. Thus, the electrochemical etching of the original single-crystalline substrate of c-Si during the production of the compliant por-Si has a positive effect on the quality of the interface, as was evidenced in the pole figure (111) from Si for por-Si due to the absence of additional reflections in that figure. It should be noted that the presence of Si reflections in addition to those ones of GaN in the pole figure (1012) is caused by the proximity of the interplanar spacing for these phases. Basing on the intensity distribution of the X-ray reflections in the pole figure of (1012), it follows that the real space direction (110) in silicon is parallel to the (100) direction in GaN. In other words, for both samples, the Si substrate defines the orientation of the growing nanocolumn structure that further undergoes coalescence into the 2D layer.

![Figure 4. Experimental pole figures: (a,b) - (111) reflection of Si; (c,d) – (0002) reflection of GaN; (e,f) – (1012) reflection of GaN. (a,c,e) – GaN/c-Si(111) sample; (b,d,f) – GaN/por-Si(111) sample.](image)

Measurements of the conductivity type, charge carrier concentration and mobility by van der Pau technique were performed at room temperature. The results are shown in Table 2.

| Sample                  | Charge carrier concentration, $\text{cm}^3$ | Mobility, $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ |
|-------------------------|--------------------------------------------|--------------------------------------------------|
| GaN/c-Si(111)           | $7 \cdot 10^{19}$                          | 8.4                                              |
| GaN/por-Si(111)         | $2 \cdot 10^{18}$                          | 52.1                                             |
4. Discussion

A more detailed analysis of the diffractograms indicated that for the GaN films grown on a single-crystalline substrate, there were low-intensive asymmetric reflections from the epitaxial GaN were present. The appearance of these diffraction peaks indicates that GaN nanocolumns subjected to coalescence in the process of 2D layer growth were disoriented relative to the direction of growth. As for the film grown on the compliant por-Si substrate, there were no any additional reflections in the diffractogram pattern, assuming that the film grows in a single-crystalline state.

The crystal cell of the epitaxial GaN layer is almost matched by its lattice parameter with the porous sublayer in the plane of growth, while in the direction of growth; the unit cell undergoes a considerable distortion (D~4) due to the Poisson effect. The growth of the GaN layer on the crystalline c-Si substrate results in a partial relaxation of the lattice as in the plane, as in the direction of growth. Moreover, nanocolumns of GaN formed during the initial stage of synthesis on the standard c-Si substrate were characterized by a greater misorientation in the plane of growth (small-angle rotation relative to each other) and a slope relative to normal directed towards the sample surface than those grown on the “compliant” substrate. Furthermore, the growth of the layer on the compliant por-Si substrate made it possible to reduce the density of the edge and screw dislocations.

As it was discussed above the characteristic ordered microlrelief was observed on the cross-section of AFM data. This fact can be explained if we assume that the 3D nucleation layer in the case of growth on por-Si layer was formed as a homogeneously distributed array of nucleation nanocolumns with approximately the same diameters. It is well known that the most energy-efficient crystallographic plane of silicon for GaN nucleation was the \{111\} plane. We assume that selective etching of the \{111\} plane during formation of por-Si sublayer first results in the formation of a surface morphology described in [6], that represents isotropically distributed hillocks of Si; if the thickness of the porous layer is about \~10 nm, the hillocks are of approximately equal size and truncated, with their upper plane being the \{111\} crystallographic plane of silicon. Thus, the nucleation of GaN on the truncated planes of the etched hillocks is energy efficient, while high surface mobility of adsorbed atoms results in complete coverage of the corresponding \{111\} plane of each hillock with every single nucleating island. This concept can explain the abrupt increase of the distribution uniformity for the diameters of nanocolumns grown on the por-Si compared with those grown on the usual Si(111) substrate.

Hall measurements (see Table 2) showed that the GaN layer with nanocolumn structure grown on c-Si and por-Si is of p-type conductivity. Values of Hall’s charge carrier concentration and carrier mobility showed that for the film on the crystalline silicon, the charge carrier concentration is higher, while mobility is lower than for the layer grown on por-Si. The obtained results agree with the published data for bulk films of GaN [7, 8].

Thus, the usage of compliant Si substrates with the nano-porous Si layer helps to achieve thick GaN layers with better coherency and better crystalline quality on Si(111) substrates without using additional AlN buffer layers. In other words, the use of a “compliant” Si substrate is an appropriate approach for the formation of semiconductor instrumental heterostructures based on GaN by the MBE PA technique.

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