Synthesis of semi-polar GaN(11-22)
on a nano-patterned Si(113) substrate

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Abstract. A method for synthesising hexagonal GaN on a Si(113) substrate with a nanostructure of about 75 nm on its surface (NP-Si(113) substrate) is proposed. It has been established that the method of metal-organic chemical vapor deposition on such a substrate makes it possible to form a semi-polar layer of GaN(11-22) with half-widths of the X-ray diffraction curve $\omega_\theta \approx 30$ arcmin.

It is shown that during epitaxy from organometallic compounds in hydrogen atmosphere at the initial stages of growth the layer orientation is given by the direction of Si(111) plane of nanocanals in NP-Si(113) and the growth rate of GaN layer in (11-22) and (0001) planes direction is comparable.

Keywords: semi-polar GaN(11-22), nano-patterned Si(113) substrate, epitaxy from the metal-organic chemical vapor deposition

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**Introduction**

Optoelectronic devices using the polar plane of GaN have a strong internal polarization field, which leads to dimensional separation of electrons and holes in quantum wells and a decrease in their radiative recombination. One of the possible ways to increase the luminescence efficiency of quantum-dimensional structures is to grow the III-nitride emitters along semi-polar orientations [1].

Growing of semi-polar GaN on a Si substrate that will be fully compatible with inexpensive modern Si-based integrated circuit technology is considered a promising direction [2, 3].

The biggest problems in the synthesis of semi-polar GaN-on-Si are, firstly, the lack of epitaxial coupling between the semi-polar GaN on any oriented Si substrate. For this reason, it is impractical to grow semi-polar GaN directly on a flat Si(100) substrate and therefore a structured Si(100) substrate with (1-11) and (-11-1) faces was used for the growing of GaN-on-Si [4, 5]. Secondly, the presence of a reaction between Ga and Si at the initial stage of the synthesis of the layer leads to a disorder of the planarity of the structure and to the defect formation [6]. Usually, to reduce such a reaction, an AlN buffer layer is initially grown. However, for the growth of GaN(11-22) on micro-structured silicon substrates, due to the large number of voids formed in the grooves during nucleation, the GaN layer has a high chance of reacting with Si facets [7].

Recently, to destroy the reaction of Ga and Si, it was proposed a method for the synthesis of GaN(11-22) on a microstructured Si (113) substrate with a special design in the form of additional grooves for ammonia access, and in this way the authors managed to reduce the parasitic reaction of Ga with silicon in the overgrown grooves [7].

This work is dedicated to the epitaxy of GaN(11-22) on a Si(113) substrate, on the surface of which it were formed the nanostructures with element sizes smaller than the free path of the Al adatom over the surface of the buffer layer. In order to achieve this goal, a U-shaped NP-Si(113) nanostructure with a period of 75 nm and a height of inclined narrow rectangular nanochrebs of 75 nm was formed using the technology [8] (Fig. 1).

The structural characteristics of the GaN layers were determined by X-ray diffraction analysis, scanning electron microscopy and atomic force microscopy.

![Fig.1. SEM image of NP-Si(113) substrate](image-url)
Materials and Methods

Initially, a buffer layer of AlN with a thickness of 20 nm was grown on all structures in a hydrogen atmosphere. Then an insular layer of GaN(11-22) with a size of ~ 0.05–0.1 µm and solid layers of GaN(11-22) with a thickness of 0.5–1 µm were grown.

X-ray diffraction analysis of the layers showed that the GaN(11-22) layers have a half-width of the X-ray diffraction curve \( \omega \approx 30 \) arcmin.

To clarify the pattern of the origin of the GaN layer on AlN, an island layer was first deposited (Fig. 2). The results are as follows:

A nanocrystalline layer of AlN with a thickness of about 20 nm completely covers the surface of nanoelements of the NP-Si(113) structure (Fig. 3, a). The geometry of nanocrystallites clearly indicates that islands with the GaN(11-22) plane are formed on the surface (Fig. 3, a, b). It can be seen that the GaN island layer tends to form a continuous one with the surface (11-22) (Fig. 3, b).

Results and Discussion

In our experiments, the edge length Si(111) is 75 nm, that is, the condition is fulfilled when the diffusion length of the Al atom on the surface \( L_{Al} \) of 40 nm [9] is commensurate with the edge length of the groove face and the atoms have a high probability of embedding in the crystal lattice on the surface. The origin and growth of the AlN layer occurs under conditions of ‘quasi-two-dimensional’ growth even at epitaxy temperature no higher than 1030° C for AlN. As it is known, the values of the surface energy for GaN(0001) of 0.185 eV/A² and for GaN(11-22) of 0.194 eV/A² [10] are close, so the growth rates of GaN layers on these planes should be almost the same.

The origin of the GaN layer occurs on the surface of the AlN/Si(111) face at higher growth rates than for AlN (Fig. 3, b) and after the coalescence stage, a continuous layer with a semi-polar GaN(11-22) surfaces formed. The fact of selective nucleation of nanocrystallites of semi-polar GaN(11-22) in the region of inclined nanochannels of the NP-Si(113) structure has been established.

![Fig.2. AFM image of GaN(11-22)/NP-Si(113) surface](image)

![Fig.3. SEM images of GaN of the insular layer (a) and crystal faces (b)](image)
The shape of the insular nuclei (Fig. 3,b) shows the presence of the ‘c-GaN’, ‘m-GaN’ planes and partially GaN(11-22). The orientation of the nanocrystallites in the array is set by the direction of the plane Si(111) of the nanochannels in NP-Si(113). The thickness of the layer in the direction of growth [0001] was about 50 nm, and it corresponded to the thickness of the layer from the surface of NP-Si(113) to the surface of GaN(11-22).

AFM measurements of the surface of the semi-polar GaN(11-22) layer with an area of 50 × 50 microns shows the presence of rectangular blocks with a size of 2 × 6 µm between which dips of up to 1.3 microns are observed. The distance between the grooves in the GaN(11-22) layer according to AFM data was about 10 microns (Fig. 2). From the AFM data (Fig. 2), it can be assumed that the sizes of the blocks formed on the surface of NP-Si(113) indicate the diffusion length of Ga atoms at the epitaxy of the GaN layer equal to 3-4 microns, which is less than the authors observed [11].

Conclusion

It is shown that during GaN(11-22) synthesis by MOCVD method in hydrogen atmosphere at the initial growth stages the layer orientation e is set by the plane direction of Si(111) nanochannels in NP-Si(113) and layer growth rates in (11-22) and (0001) plane directions are comparable. The proposed approach to growing semi-polar GaN(11-22) on a nano-patterned silicon substrate is promising for the integration of gallium nitride and silicon optoelectronics.

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