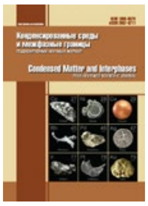

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Semi-polar GaN(11-22) on nano-structured Si(113): a structure for reducing thermal stresses

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Abstract

The article reports the growth of semi-polar GaN(11-22) layers using epitaxy from metal organic compounds on a nano-structured NP-Si(113) substrate. It was shown that upon the emergence of an island layer, elastic deformed structures of GaN(11-22)/NP-Si(113) form a nano-meter compliant silicon layer on a substrate while elastic stresses conditioned by the difference of temperature coefficients of GaN and Si in such a structure decrease.

Keywords: Semi-polar gallium nitride, Nano-structured silicon, Elastic and plastic structure deformation

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1. Introduction

Semiconductor materials of wide band III-nitrides (AlN, GaN) have become the most important materials that can be used in emitters and detectors in the visible and ultraviolet spectral range, as well as in powerful electronic devices. AlN and GaN layers are usually grown on sapphire, silicon carbide, or silicon substrates. Silicon substrates are preferable due to their low cost, high availability, and potential integration of gallium nitride and silicon optoelectronics. The main disadvantages of obtaining gallium nitride on a silicon substrate are a high percentage of mismatch of crystal lattices (17%) and differences in the thermal expansion coefficients, which causes tensile stress in a layer when cooled from growth to room temperature. Strong bending and cracking of the GaN layer occurs in flat layers in case their thickness exceeds 1 μm [1]. As far as we know, the thickest GaN layer on a Si substrate was grown without cracks using surface faceting with a thickness of 19 μm and dislocation density of $1.1\cdot10^{7}$ cm^{-2} [2].

Recently, it has been proposed to use structured surfaces of Si(100) substrates, mainly in the form of linear, rectangular, or triangular micron and nano-micron sized ridges, to grow semi-polar layers. When using this technology, the preliminarily masked surface is treated with a chemical etching agent. Due to the anisotropic etching rate for different crystallographic directions, the Si(111) face can be exposed and a GaN(10-11) layer can be grown on a structured Si(100) substrate [3], or a GaN(11-22) layer can be obtained on a structured Si(113) substrate [4]. The use of faces of a structured substrate for the synthesis of semi-polar structures was shown in a number of reviews, for example, in [5, 6].

To obtain a semi-polar orientation layer, the angle between the planes of the emergence face and the substrate surface must be equal to the angle between the GaN "*c*" plane and the target semi-polar plane. The Si(113) substrate is suitable for growing semi-polar GaN(11-22) because the angle between the Si(111) planes and the (113) silicon substrate surface is close to the inclination angles of the semi-polar (11-22) plane to the (0001) plane.

The main problem of epitaxy in case of GaN heteroepitaxy on a silicon substrate is the reduction of elastic energy caused by the mismatch of lattice parameters and differences in thermal expansion coefficients, while dislocation density in the layer must be kept at a low level.

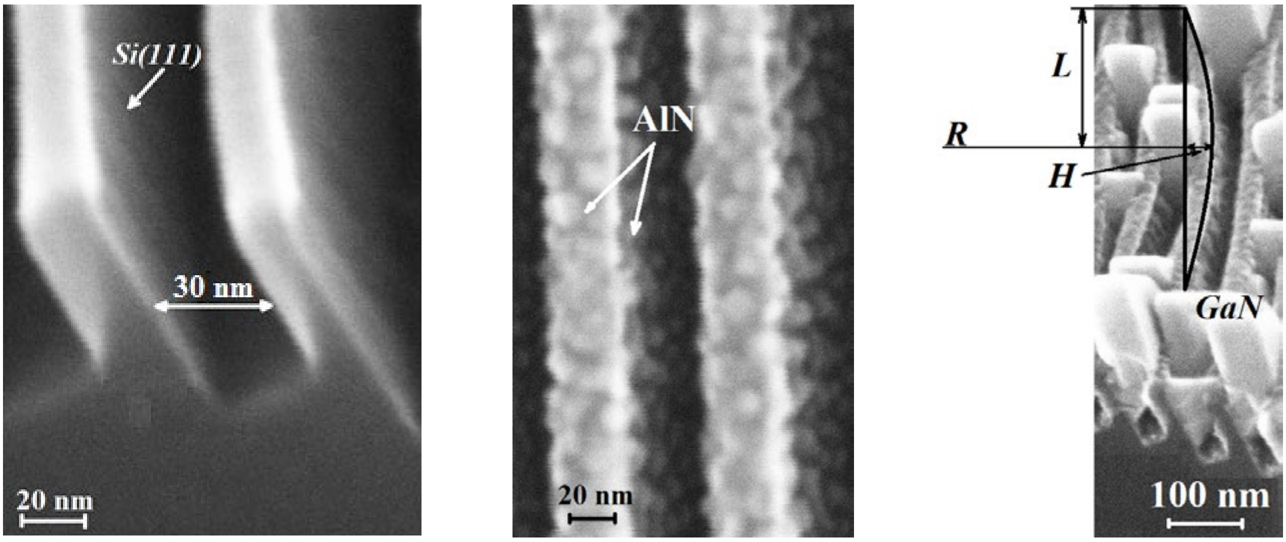
One of the promising technological methods allowing to reduce elastic stresses in the GaN(0001) layer is the use of a "compliant" Si(111) substrate due to the arrangement of pores in the near-surface layer [7].

Heteroepitaxy of a GaN layer on a Si substrate can result in the growth of elastically stressed thick epitaxial layers if the thickness of the substrate is less than the value at which its plastic deformation occurs [8]. Several experiments were conducted related to this area, including the growth of GaN on preliminarily prepared silicon nano-membranes [9] and on Si substrates etched on the reverse side to a thickness of 10 μm. However, due to the difficulties of handling nano-membranes and thin films this approach remains rather complicated for obtaining an effective "compliant" substrate. In our experiments we used a nano-sized structured layer that formed a semi-polar GaN(11-22) layer as an analogue of a "compliant" substrate.

This work is dedicated to the reduction of thermal stresses in semi-polar GaN(11-22) layers upon epitaxy on nano-structured NP-Si(113) substrates.

2. Experimental

Epitaxy of a semi-polar layer occurred on a nano-structured Si(113) substrate which had a formed U-shape (Fig. 1A) structure with a period of 30 nm and height of inclined nano-ridges of 75 nm. The nanomask was formed as a result of a two-stage process described in [11]. AlN and GaN layers on NP-Si(113) substrates were grown by metal organic chemical vapor deposition (MOCVD) on a modified EpiQuip unit with a horizontal reactor similar to [12]. Hydrogen was used as the carrier gas, while ammonia, trimethylgallium, and trimethylaluminum were used as precursors. There were structures of two types that consisted of an AlN buffer layer with a thickness of about 10 nm (Fig. 1b) and, first of all, a GaN island layer (Fig. 1c) and, second, a continuous GaN layer with a thickness of ~1 μm. X-ray diffraction analysis showed that continuous GaN(11-22)/NP-Si(113) structures



a b c

Fig. 1. SEM image of a NP-Si(113) cleavage of substrate (a), substrate covered with a thin layer of AlN (b), and an insular layer of GaN (c)

had the half-width of an X-ray diffraction curve ω_Θ ~ 30 arcmin.

Scanning electron microscopy (SEM) showed that after the growth of the AlN buffer layer, there were no distortions of the surface pattern of the structure (Fig. 1b), and after the synthesis of the island layer, deformations on the surface Si ridges were observed.

To evaluate the elastic stresses of structures with a continuous layer, Raman spectra were measured in the region of the E_2(high) phonon mode. As for GaN(11-22), line E_2(high) = 565.2 cm^{-1}, while, as we know, for an unstrained structure position E_2(high) = 568 cm^{-1}, which indicates the presence of GaN compression deformation. For GaN(11-22) layers, according to $\Delta\omega = K \cdot \sigma$, where K = 4.2 cm^{-1}/GPa we estimated the value of longitudinal elastic stressed which was −0.67 GPa, while the same value for the GaN layer grown on a Si(111) flat substrate was −1.19 GPa [12].

3. Results and discussion

Upon GaN heteroepitaxy on Si(111), the values of elastic stresses that occur due to the mismatch of lattice parameters are significantly greater as compared to the values of thermal stresses. We assumed that there was no plastic deformation in the island layer and, therefore, the behavior of the structured surface, which was determined using an electron microscope, would be identified mainly by the difference in the layer lattice and the substrate constants. Plastic deformation would occur in a continuous 1 µm thick GaN(11-22) layer at the epitaxy temperature, and the elastic stresses measured by Raman scattering would be determined by thermal stresses.

The bending of the ridges on the NP-Si(113) surface in a structure with an island layer clearly indicates the “compliance” of the structured substrate. The arcuate bending of the “ridge” (Fig. 1c) allowed us to evaluate the bending radius of a “compliant” Si layer parallel to the plane of the Si(111) face based on the values H, the height of arc, and L, half-length of the arc horde (Fig. 1c). For this we used the formula $R = \frac{L^2 + H^2}{2H}$. The bend radius of the ridge was about R = 510 nm.

In case of epitaxy of hexagonal GaN on cubic silicon with a thickness of about 400 µm, the critical layer thickness that results in plastic deformation would be small, as even in case of GaN epitaxy on a standard sapphire substrate with a thin AlN buffer layer it is about 29 Å [13]. We assume that this thickness slightly increases for islands, but they have no plastic deformations (Fig. 2a). Elastic stresses in the GaN layer cause a bending moment on the face of the Si(111) substrate, which leads to a curvature in the ridge. Assuming isotropic elastic behavior and spatially

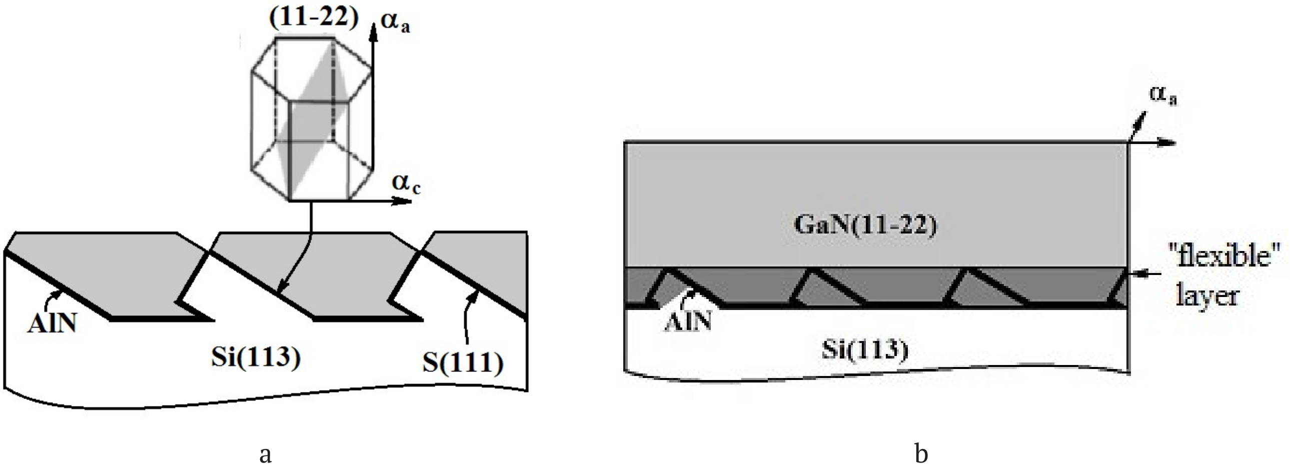


Fig. 2. A schematic representation of the growth of GaN(11-22) layers on a NP-Si(113) substrate: a) insular; b) solid

homogeneous biaxial misfit deformation between the GaN layer and the "compliant" substrate layer, the curvature κ = 1/*R* can be calculated using the expression [14,15]:

$$\frac{1}{R} = 6m\varepsilon_m\left(\frac{h}{h_S}\right)\left(\frac{1+h}{1+mh\left(4+6h+4h^2\right)+m^2h^4}\right), (1),$$

where $m = \frac{M_f}{M_S}, h = \frac{h_f}{h_S} = 1$.

While with ε = 0.17, E_{GaN} = 295 GPa and ν_{GaN} = 0.25, and E_{Si} = 165.5 GPa and ν_{Si} = 0.18, value *R* = about 290 nm, which is approximately twice less than the experimentally estimated value. The difference can be explained by the influence of the mechanical connections of the "compliant" layer with the rest of the substrate on the bending radius.

Upon heteroepitaxy of a continuous GaN layer, the value of the elastic stresses of GaN(11-22)/NP-Si(113) structures emerging during cooling depended on the difference in the thermal expansion coefficients of GaN and Si Δα = αGaN – αSi. The thermal expansion coefficient of an isotropic silicon substrate was $\alpha_{Si} = 3.6\cdot10^{-6}$ K^{-1} [16], while the thermal expansion coefficients for anisotropic semi-polar GaN differed in the direction of the axes: "*a*" – $\alpha^{l}_{GaN(a)}$ – $5.6\cdot10^{-6}$ K^{-1} и "*c*" – $\alpha^{l}_{GaN(c)} = 4.8\cdot10^{-6}$ K^{-1} [17]. Then, according to expression 2 [13], stresses along axes "*a*" and "*c*" would have values $\sigma_a = -0.78$ Gpa and $\sigma_c = -0.47$ GPa:

$$\sigma_f = \frac{E_{GaN}}{1-\nu_{GaN}}\frac{\Delta\alpha\Delta T}{1+\frac{E_{GaN}(1-\nu_{Si})h_{GaN}}{E_{Si}\left(1-\nu_{GaN}\right)H_{Si}}}, \quad (2)$$

where Δ*T* =1000 °C, *H* = 400 μm, *h* = 1 μm. When estimating stresses for a heterostructure with a continuous layer, a significant role is attributed to, first of all, the degree of correlation between the compliant layer with its bulk part and, second, the possible impact of the faceting of the crystallized layer surface on the value of thermal stresses, similar to [18]. The value of thermal stresses, estimated using expression (2), shows a satisfactorily correspondence to the value of stresses in the structure obtained by Raman spectra. Indeed, according to Raman data, the stress value in a 1 μm thick GaN layer was -0.67 GPa, which corresponded to the effective value of the thermal expansion coefficient for GaN(11-22).

During epitaxy of a semi-polar GaN(11-22) layer on a nano-structured NP-Si(113) substrate in the course of the formation of islands, the compliant near-surface layer was elastically deformed on the nano-structured Si(113) substrate, which formed a compliant layer and reduced the value of thermal deformation of the semi-polar layer (Fig. 2b).

4. Conclusions

Therefore, it was found that at the initial stage of GaN(11-22) epitaxy the nano-structured Si(113) substrate formed a "compliant" layer that can reduce thermal stresses. This approach can be useful for the technology of structure integration based on GaN-on-Si.

Contribution of the authors

The authors contributed equally to this article.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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