Reduction of threading dislocations density in GaN on sapphire by *in−situ* Si_xN_y interlayer

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Introduction

The main problem in the epitaxy of GaN is lack of widely available GaN substrates. For that reason GaN epilayers must be grown on substrates made of different materials, most often sapphire or silicon carbide. Due to considerable lattice mismatch between GaN and the substrates, such layers are characterised by a high density of dislocations. It has been proofed [1] that while the density of dislocations is not crucial for the efficiency of emission from optoelectronic devices like lasers or LEDs, it imposes limitation on their lifetimes and lowers value of reverse bias voltage of the diodes. So the reducing of the density of dislocations seems to be especially important for the performance of photodetectors and transistors.

One method to reduce the density of dislocations in heteroepitaxial GaN layers is the Epitaxial Lateral Overgrowth (ELOG) [2]. Its main idea is to make lithographically *ex−situ* a SiO_2 mask in form of stripes on the surface of the primary GaN epilayer and then to continue the growth of GaN. The secondary layer, starting from the uncovered with stripes, overgrows them giving high quality layer, while dislocations are mainly limited to the area of spaces among stripes. This technique has allowed for serious advances in the technology of GaN lasers. However its drawbacks are cost and high degree of complication arising from the necessity of *ex−situ* lithography. For that reason it is important to investigate other methods, that lead to reducing density of the dislocations.

In this paper we report results of our investigation of the one of possible methods, which idea is similar to the ELOG technique, but can be fulfilled within a single growth process. The main point is to employ a Si_xN_y mask, which can be grown *in−situ*. The idea of *in−situ* Si_xN_y mask for the epitaxy of nitride compounds has been previously reported in literature [3] and [4], but the mask was deposited directly on the substrate, prior to the low temperature buffer, in order to reduce density of nucleation sites.

Experimental

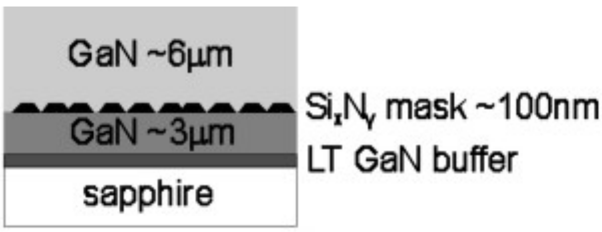

Fig.1. Drawing of the investigated structure with the embedded SiN mask.

The investigated structure is presented in Fig.1. The growth was performed in a horizontal, low pressure MOVPE reactor with standard precursors: trimethylgallium (TMG), ammonia (NH_3) and diluted silane (SiH_4) − 100ppm in H_2 and hydrogen as a carrier gas. In order to get insight into different stages of growth, we prepared a set of layers, which growth were interrupted at crucial stages. The main tool of characterisation was an Atomic Force Microscope (AFM). It allowed determining of densities of the dislocations by counting the pits observed on the surface. Dislocations with a screw component are associated with larger pits (~50nm), that give origin of atomic steps. Pure edge type dislocations correspond to smaller pits (~20nm), that are not related to atomic steps. Additionally the intermediate layers with rough morphology were observed with a Scanning Electron Microscope to check up if the AFM images were not strongly influenced by the geometry of the tip. The complete layers were also investigated with High Resolution X−ray Diffraction (HRXD).

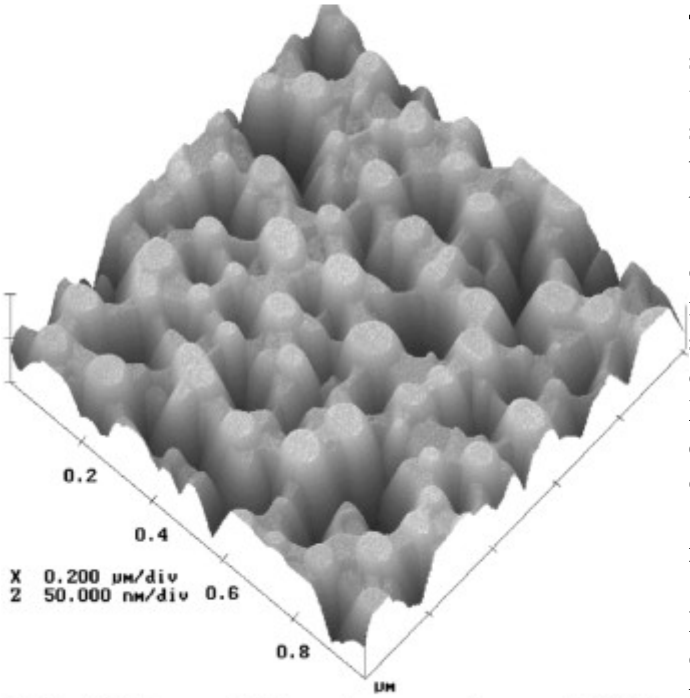

Fig.2. AFM image of SiN mask grown on the smooth GaN epilayer. Due to geometrical limitations of the AFM tip, it is not possible to determine the thickness (>80nm) or the density of uncovered openings.

The primary GaN layer was grown in a standard way starting with a LT (500ºC) GaN buffer, followed by a 3 μm layer grown at 1100ºC and 400mbar. The layer had smooth morphology. After completing the primary layer the TMG was switched off and without changing the temperature, the SiH_4 switched on. The deposition of Si_xN_y mask was continued until the GaN surface was covered with coalescing hill−like objects (Fig.2). The next step was switching back from SiH_4 to TMG. The secondary GaN layer started from distinctly separated crystallites (Fig.3). At that stage the temperature was lowered to 1025ºC which stimulated vertical growth and delayed coalescing of the crystallites. After developing of the grains, the temperature was again increased to 1100ºC to restore lateral growth. For comparison a 9μm reference layer that differed only with the lack of the Si_xN_y insert was also grown. Quality of the obtained layer was dependent on the thickness (deposition time) of inserted Si_xN_y mask. Too thin interlayer did not lead to noticeable improvement of the morphology. On the contrary too thick mask gave opposite effect and caused polycrystalline growth. In our case the best results were obtained for a mask grown for 300s. Comparison of the optmised (Fig.5) and reference (Fig.4) layers showed noticeable reduction in the number of dislocations.

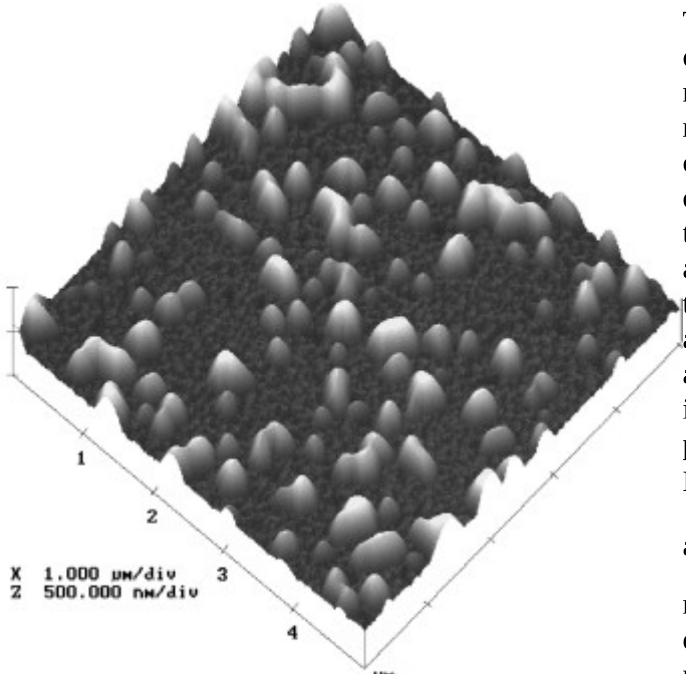

Fig.3. AFM image separated GaN after 50 seconds deposition on the top of SiN mask. The crystallites are nucleated on the spots where the SiN mask leaves uncovered primary GaN layer and hence preserve the crystalline ordering.

The total density of dislocations determined onthe basis of a few AFM scans for the epilayers with and without mask was equal to $2x10^{8}cm^{-2}$ and $1.2x10^{9}cm^{-2}$ respectively. The change in the density of dislocations concerned mainly the edge dislocations. Their density dropped by one order of magnitude, while the change in the number of screw type dislocations was decreased by a factor of 2. Another characteristic feature visible from the AFM images were highly parallel ordering of the atomic steps in the case of the layer with the mask. Such a ordering was preserved on areas of the order 50x50µm i.e. much larger than presented in Fig.5. The structural properties of the layers were determined on the basis of HRXD including symmetrical ω and $2\theta / \omega$ scans and asymmetrical radial Φ scans. The quality of a mosaic structure can be described by correlation lengths determining size of columnar domains − in the direction normal L_v and parallel to the substrate surface: L_c along <110> and L_d along <210> basal directions according to Miller indices). Other significant parameters are the twist angle of GaN columns α_{ϕ} and the out−of−plane misorientation angle of coherent domains α_{Ω}.

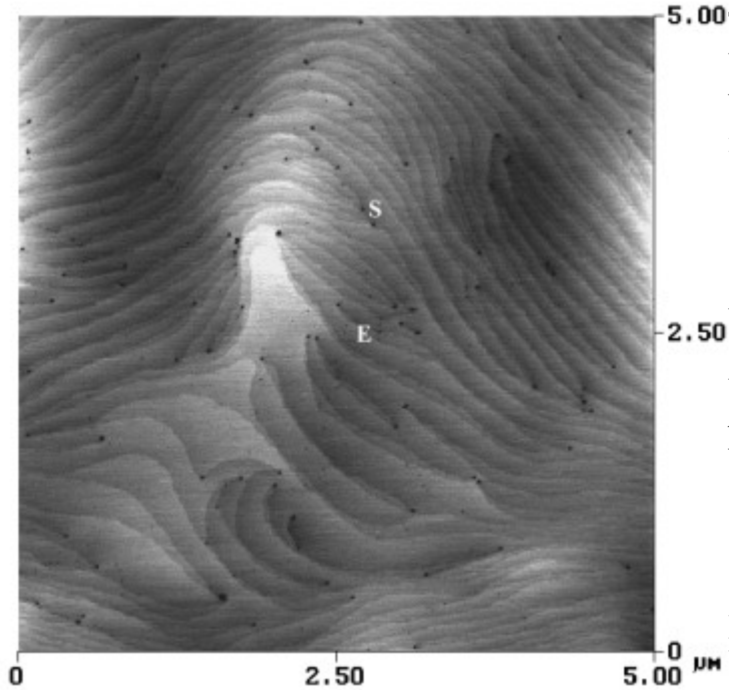

Fig.4. AFM image of the 9µm reference GaN layer grown without SiN mask. Pits related to pure edge and screw type dislocations are denoted by E and S respectively. Edge dislocations often appear themselves in a form strings (eg. right of E).

The lateral correlation lengths (L_c and L_d) and the tilt angle α_{Ω} can be determined from FWHM broadening for the symmetrical (00*l*) scans. The normal correlation length L_v is found from $2\theta / \omega$ scans [5]. Measurements were done for all crystallographic directions of type <110> and <210>. The obtained results unambiguously show, that Si_xN_y layer increases the size of coherent scattering areas. The lateral correlation lengths for the layer with the embedded mask were found to be L_c 360nm and L_d 320nm. For the reference layer without the mask the corresponding values were L_c 230nm and L_d 240nm. The values of vertical correlation length L_v were found to be 3.5µm and 2µm respectively. The twist angles α_{ϕ} were similar in both cases with values 3.8° and 3.7°. The Si_xN_y mask was the reason of the slightly increased tilt angle α_{Ω} 130 arcsec in comparison with 110 arcsec obtained for the reference layer without the mask. Summarising, the embedded Si_xN_y mask did not change the growth mode but significantly increased size of grains.

Discussion

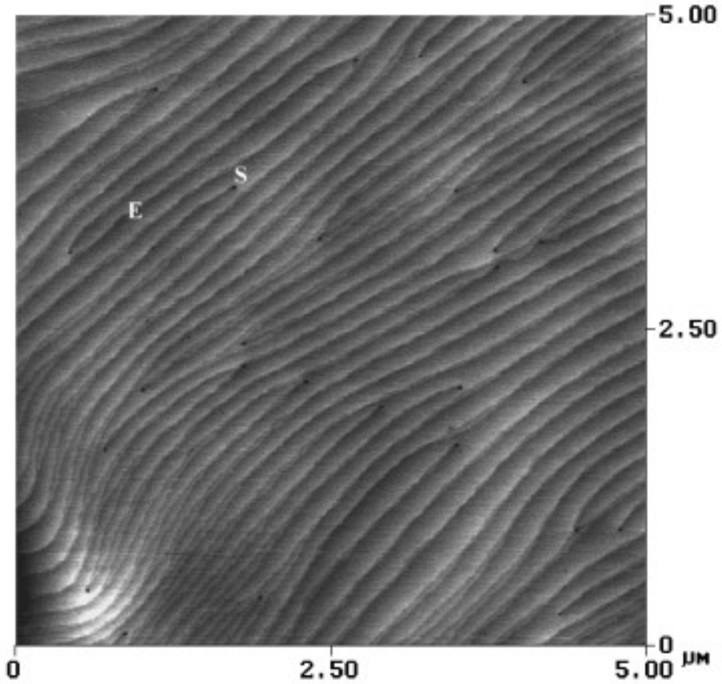

Fig.5 AFM image of an optimised GaN layer on sapphire with an embedded SiN mask. Parallel ordering of the atomic steps is kept in the areas up to 50×50μm.

Described observations can be explained as follows. It is known that the GaN heteroepitaxial layers grow in columnar mode. The individual grains have slightly different orientation, so the boundaries between them must contain dislocations. In simple model it may be assumed, that edge dislocations are responsible for relative twist and screw type ones for the tilt of the grains. The density of dislocations should be dependent on the number of the grains and degree of their misorientation − mosaicity of the epilayer. Growth of GaN on the Si_xN_y mask starts in separated openings. The resulting crystallites grow laterally and in the effect create a continuous layer. The process is very similar to growth of GaN on the LT GaN buffer. However in our case the resulting grains are better ordered because they preserve ordering of the primary GaN layer.

If the number of openings in the mask is too large (greater than the number of the columns in the primary layer) the number of grains in the secondary layer is not changed. On the contrary, if the number of openings in the mask is lower than the number of columns in the primary layer, the number of grains in the secondary layer is reduced. However too small number of openings in the mask prevents obtaining of the continuous. Concluding the improvement of the structural quality of GaN epilayers on sapphire by embedding of an in−situ Si_xN_y mask was achieved. Much work regarding optimisation of the mask is required to obtain better control over distance between the openings.

References

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