

MOVPE Growth of Semipolar GaN on Patterned Sapphire Wafers: Influence of Substrate Miscut

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*We describe epitaxial methods for two different semipolar GaN orientations on patterned sapphire substrates: With $(10\bar{1}2)$ (*r*-plane) sapphire substrates we achieve planar $(11\bar{2}2)$ GaN layers with smooth surfaces on a large scale. In the case of $(11\bar{2}3)$ (*n*-plane) patterned wafers the growth of $(10\bar{1}1)$ GaN is possible. We optimized the growth conditions for $(11\bar{2}2)$ GaN (especially the growth temperature) yielding a coalesced, planar semipolar surface. Thereafter we transferred the knowledge from $(11\bar{2}2)$ oriented growth to $(10\bar{1}1)$ oriented growth and investigated the general influence of substrate miscuts on surface and crystal qualities, respectively. Due to the fact that the angle between $(10\bar{1}1)$ and (0001) in the case of GaN and the angle between $(11\bar{2}3)$ and (0001) in the case of sapphire are slightly different, we detected an imperfect surface. Choosing the right substrate miscut angle the crystal and / or the surface quality of GaN could be improved. The third important point is the non-homogeneous defect density distribution in the crystal. The right miscut could help to push the growth of the areas with less defects over the areas with a high defect density to improve the total crystal quality.*

1. Introduction

At present, optoelectronic devices like LEDs or laser diodes based on GaInN - GaN heterostructures are usually grown in *c*-direction. Due to the crystal geometry of GaN, strong piezoelectric fields are present within such heterostructures. These internal electric fields bend the energy levels leading to a charge carrier separation in the quantum wells. The reduced overlap of the wavefunctions of electrons and holes leads to a reduced recombination probability - the efficiency of a LED (e.g.) decreases. In addition, a red shifted emission wavelength as a result of a reduced effective bandgap is observable, known as "Quantum Confined Stark Effect" (QCSE).

One promising way to reduce the negative effect of QCSE on the efficiency is to grow GaN in non-*c*-direction. A growth direction with a vanishing QCSE is called non-polar - in the case of a reduced QCSE semi-polar, respectively. The growth in non-polar directions is typically affected by a very high defect density [1, 2]. To avoid this problem, a balance between a reduced QCSE and an acceptable crystal quality needs to be found by growing on semipolar surfaces.

Okada et al. [3] presented a possible method to grow GaN in the well known *c* direction obtaining yet a semipolar surface: They patterned *r*-plane sapphire substrates by etching trenches with *c*-like side facets into the wafer. With the help of selective epitaxy, crystal

growth just on the c -facets is possible. At the beginning, GaN forms triangular shapes which coalesce to a planar semipolar surface (cf. Fig. 1) after a suitable growth time.

Our main ambition is to grow $(10\bar{1}1)$ GaN on n -plane sapphire substrates. The general influence of miscut in the crystal quality has to be investigated. A slight misorientation between $(11\bar{2}3)$ sapphire and $(10\bar{1}1)$ GaN can be observed. The different crystal structures of the two materials are responsible for the different angles between $(10\bar{1}1)$ and (0001) in the case of GaN (61.95°) and $(11\bar{2}3)$ and (0001) in the case of sapphire (61.22°), respectively [4]. Based on this fact, slightly tilted triangular shapes (around 0.7°) which build a rough surface are expected. On the other hand, previous investigations of Schwaiger et al. [5] showed that the $-c$ -wing exhibits a higher defect density than the $+c$ -wing. Therefore, one possibility to improve the total crystal quality is to overgrow the $-c$ - by the $+c$ -wing by choosing a vanishing miscut. So a compromise between crystal and surface quality has to be found, which means finding the most promising substrate miscut.

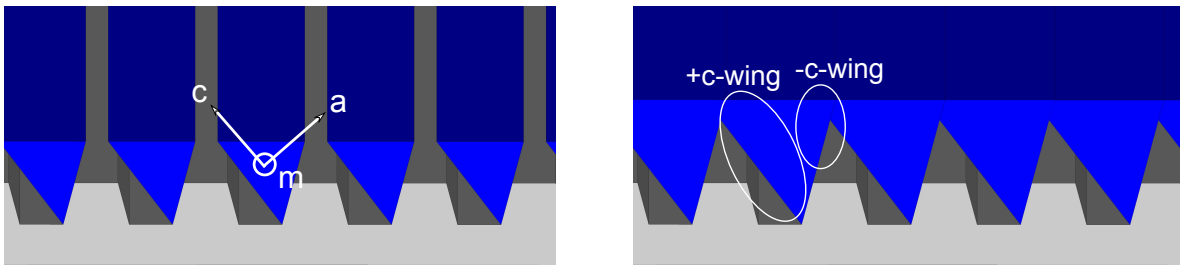


Fig. 1: Growth of GaN stripes (blue) with triangular shapes on a patterned substrate (grey). The triangular shapes (left) coalesce after a right growth time to a planar surface (right).

2. Experimental

The first step for obtaining semipolar GaN is to pattern the sapphire substrate with trenches having a c -plane-like side facet. At first a 200 nm thick layer of SiO_2 which later acts as a mask for selective area growth is deposited. It is followed by an about 500 nm thick nickel layer structured via lithography with a stripe mask ($3\ \mu\text{m}$ opening, $6\ \mu\text{m}$ period). With reactive ion etching (RIE), the pattern is transferred into the sapphire - the resulting grooves have a width at the bottom of about $1.5\ \mu\text{m}$, a depth of about $1.2\ \mu\text{m}$ and possess a c -plane-like facet.

All samples investigated in this study were grown in a low-pressure horizontal MOVPE reactor (Aixtron) with the precursors trimethylgallium (TMGa), trimethylaluminium (TMAI) and high purity ammonia.

The growth starts with an oxygen doped AlN nucleation layer at low temperature, followed by the GaN layer. The reactor pressure was set to 150 mbar and the V/III ratio was 650.

The crystal quality of the GaN layer was investigated by high resolution X-ray diffraction (HRXRD). With the help of a scanning electron microscope (SEM) we were able to determine the surface morphology. Surface roughness was measured via atomic force microscopy (AFM).

To investigate the influence of the substrate miscut on the growth of GaN it is important to know the crystal orientation angles as exactly as possible. A sample holder for the HRXRD machine was developed to measure the miscut angle with an accuracy of about 0.05° . Using a conventional laser pointer, the sample alignment in the X-ray machine is easy to perform: While rotating the sample, the laser beam reflected on the surface produces a rotating point on a screen. Two micrometer screws allow to tilt the sample until the reflected beam describes a nearly constant point. Now the sample is perfectly aligned in the X-ray machine and the misalignment of the crystal structure within the substrate is measurable.

3. $(11\bar{2}2)$ GaN on $(10\bar{1}2)$ Sapphire

As mentioned above, our main target is to grow semipolar $(10\bar{1}1)$ GaN on $(11\bar{2}3)$ sapphire. S. Schwaiger already started some investigations in $(10\bar{1}1)$ GaN growth during his PhD thesis. Due to the changing of growth conditions over a large time range a rough adaptation of the most important parameters (e.g. temperature) is necessary. An additional problem is the limited number of n-plane wafers available for our institute. Therefore, we started our experiments with $(11\bar{2}2)$ GaN on $(10\bar{1}2)$ (r-plane) sapphire. After optimization, we can transfer the obtained knowledge to $(10\bar{1}1)$ GaN on $(11\bar{2}3)$ sapphire.

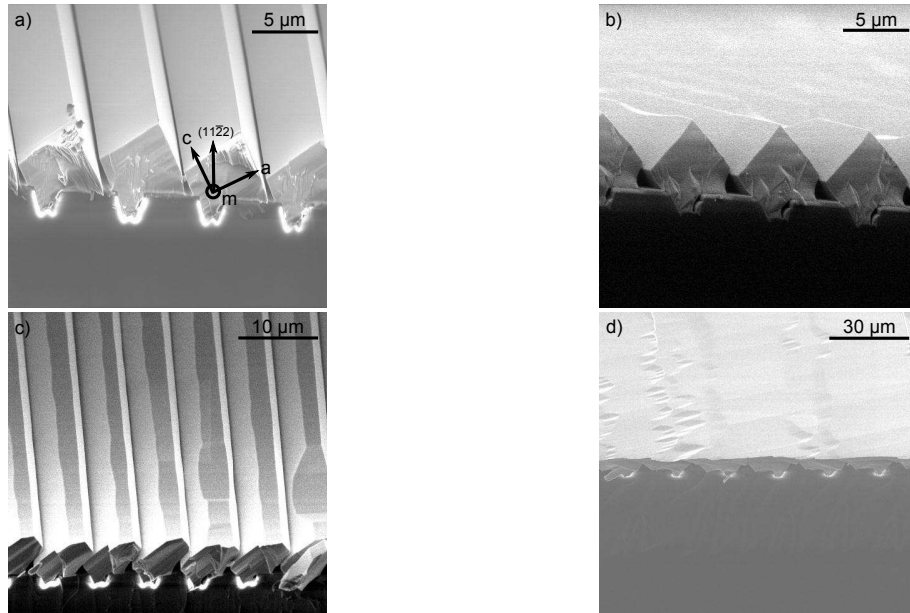


Fig. 2: Growth of $(11\bar{2}2)$ GaN on patterned $(10\bar{1}2)$ sapphire at different growth temperatures: a) 1130°C , b) 1110°C , c) 1070°C and d) 1040°C .

As shown in Fig. 2, at high growth temperatures (part a) (1130°C) and b) (1110°C)) the growth rate in a- is approximately the same as in c-direction. For closed layers, the growth rate in c-direction has to be increased by decreasing the temperature. In part c) (1070°C) one can see very first beginnings of coalesced stripes and a closed planar surface. By a further reduction of the growth temperature to 1040°C a coalesced and planar surface in $(11\bar{2}2)$ direction was obtained.

4. $(10\bar{1}1)$ GaN on $(11\bar{2}3)$ Sapphire

In the case of $(11\bar{2}2)$ GaN we were able to grow stripes with the right shape to form a coalesced semipolar layer with a reasonable surface. We just transferred the growth recipe to achieve $(10\bar{1}1)$ GaN.

As already explained, for this crystal orientation we want to investigate the influence of substrate miscut on crystal and surface quality. $(11\bar{2}3)$ sapphire substrates (20 mm x 20 mm) with miscuts of 0° , 0.5° , 1.0° , 1.5° and 2.0° towards c -direction were available. We systematically investigated the growth of GaN on these substrates with unaltered growth conditions for each growth run.

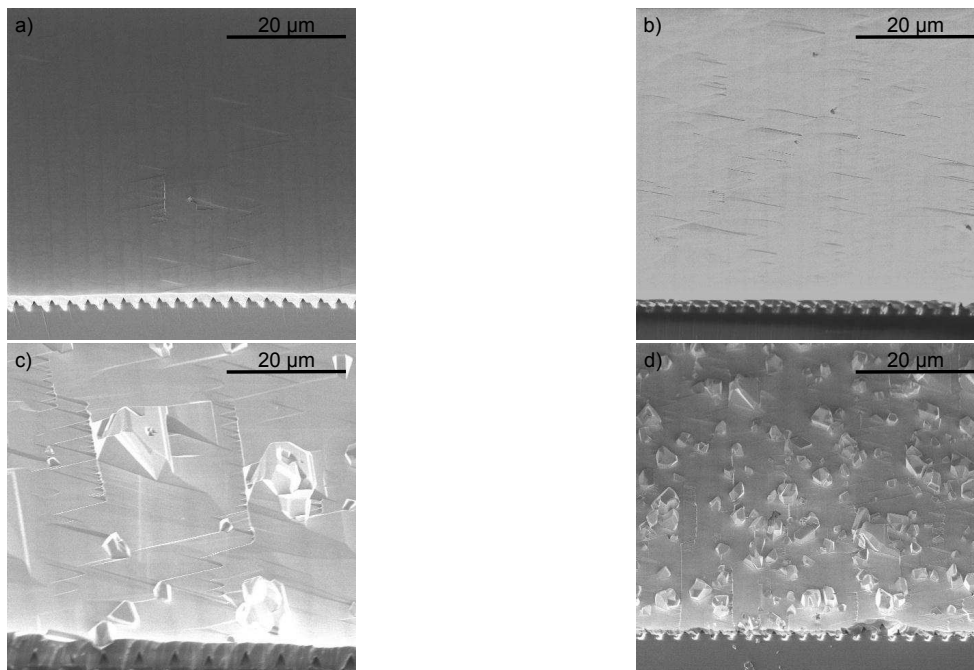


Fig. 3: SEM picture of semipolar $(10\bar{1}1)$ GaN on $(11\bar{2}3)$ sapphire with different miscut angles to c -direction: a) 0° , b) 0.5° , c) 1.0° and d) 1.5° . A higher miscut angle shows a lower surface quality. In the case of 2° miscut, growth of an approximately planar surface was not possible.

As shown in Fig. 3, the higher the miscut, the lower the surface quality. In the case of 0° , we achieved a very smooth surface over a large area with a RMS roughness of 2.5 nm in an area of $10\ \mu\text{m} \times 10\ \mu\text{m}$ (cf. Fig. 5). One possible reason for the decreasing surface quality at higher miscuts could be the decreasing width of the trenches. SEM measurements show clearly the trend to small but deep grooves in the sapphire (cf. Fig. 4). In the case of substrates with a 2° miscut, the trenches were just 530 nm wide (instead of about $1.5\ \mu\text{m}$ in the case of no miscut) - growth of a planar surface was not possible at these conditions.

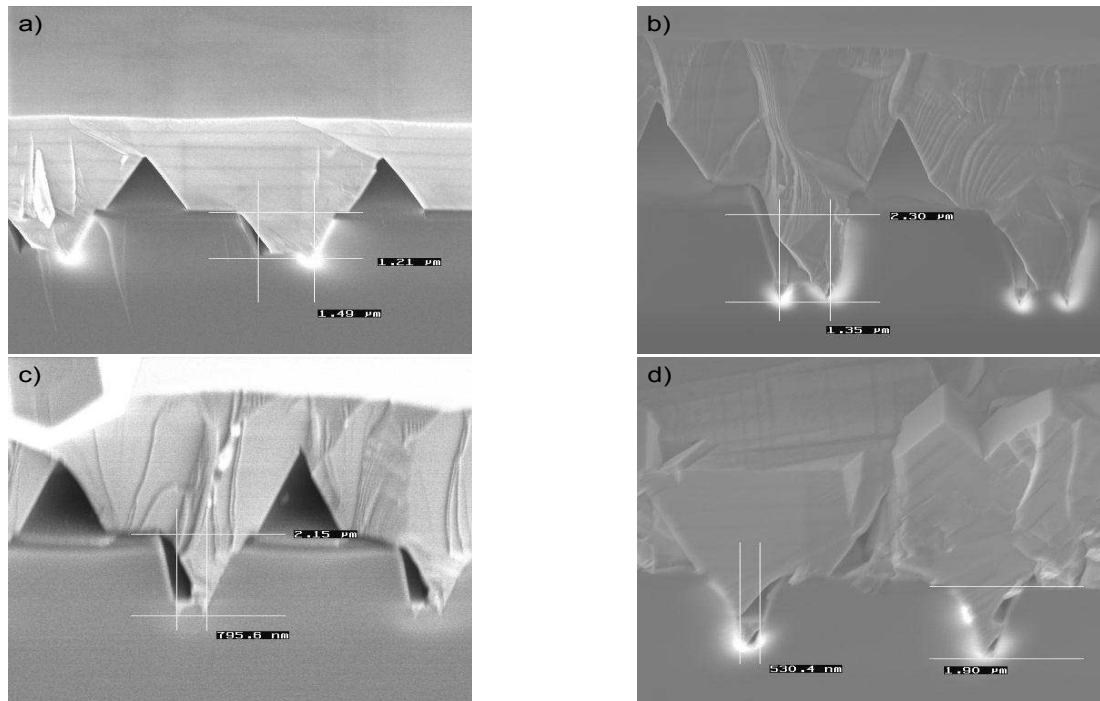


Fig. 4: SEM picture of semipolar $(10\bar{1}1)$ GaN on $(11\bar{2}3)$ sapphire with different miscut angles to c -direction: a) 0° , b) 0.5° , c) 1.5° and d) 2° . The higher the miscut, the smaller the trenches.

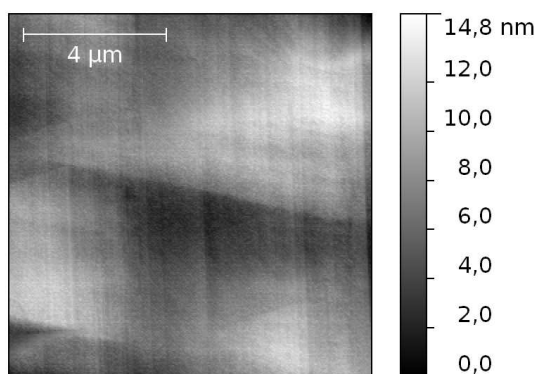


Fig. 5: AFM measurement on a planar $(10\bar{1}1)$ GaN surface on a sapphire substrate with 0° miscut with a RMS roughness of 2.5 nm.

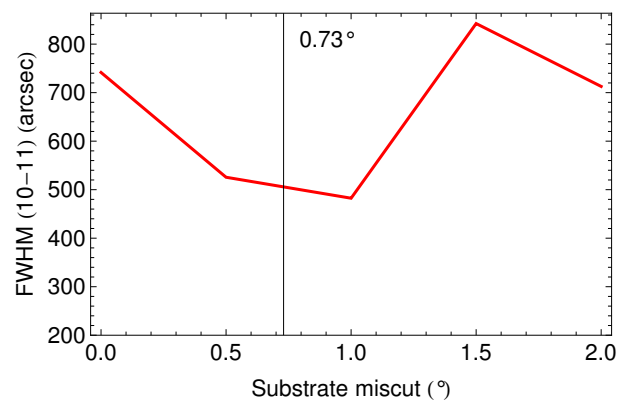


Fig. 6: FWHM of $(10\bar{1}1)$ rocking curve measurements over miscut angle. 0.73° is the misalignment between GaN layer and sapphire substrate.

Independently, we found (cf. Fig. 6) that the highest crystal quality with a FWHM of around 478 arcsec of $(10\bar{1}1)$ rocking curve is achieved with a substrate miscut of 1° . As already explained in the introduction, $(10\bar{1}1)$ GaN has a misorientation of about 0.73° to the $(11\bar{2}3)$ sapphire surface. Hence, we expected a maximum of crystal quality around this miscut angle. These investigations confirm our assumption.

5. Conclusion

With patterned $(10\bar{1}2)$ sapphire we developed a process to grow $(11\bar{2}2)$ oriented GaN with a smooth surface on large areas. The successful knowledge transfer to $(10\bar{1}1)$ GaN gives us the possibility to investigate the influence of substrate miscut in surface and crystal qualities, respectively. We could show that a misorientation of 1° to c-direction results in the best crystal quality. We reached a FWHM for $(10\bar{1}1)$ rocking curve measurements of around 478 arcsec. However, the disadvantage of the miscuts unequal zero is the decreasing surface quality. Obviously, the etching results depend on the substrate miscut. One possibility to solve this problem is to increase the trench dimension - which means using a larger mask for lithography.

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