# Crystal Quality Improvement of Semipolar $(20\bar{2}1)$ GaN on Patterned Sapphire Substrates by In-Situ Deposited SiN Mask

Tobias Meisch

*We present our results of* $(20\bar{2}1)$ *GaN growth on* $(22\bar{4}3)$ *patterned sapphire substrates. The substrates are patterned by etching trenches with c-plane-like side-facets. On these facets, the metalorganic vapor phase epitaxy (MOVPE) GaN growth starts in c-direction and forms triangularly shaped stripes eventually coalescing to a* $(20\bar{2}1)$ *oriented layer. X-ray rocking curves measured parallel to the stripes of the symmetric* $(20\bar{2}1)$ *reflection show a full width at half maximum of 675 arcsec. Well known from epitaxy of c-plane GaN, an in-situ-deposited SiN mask could help to reduce the defect density further. Systematic investigations of the deposition time and position of the SiN interlayer resulted in a significant improvement of crystal quality confirmed by X-ray and low temperature photoluminescence measurements. Additionally, MOVPE GaN templates with and without SiN mask were overgrown by hydride vapor phase epitaxy. Also now, the SiN interlayer improves the crystal and especially the surface quality of the HVPE layer.*

## 1. Introduction

Most of the common optoelectronic devices based on group III nitrides emitting in the visible and ultraviolet range are grown in the well-known c-direction. Lots of techniques are investigated already to achieve excellent crystal quality and smooth surfaces. Nevertheless, the crystal symmetry of the group III nitrides causes strong piezoelectric fields in heterostructures like InGaN/GaN, leading to a bending of the valence and conduction band. The wave functions of electrons and holes get spatially separated and the recombination probability is significantly reduced [1]. Furthermore, the effective band gap decreases resulting in a redshift of the emission spectrum. This behavior is known as Quantum Confined Stark Effect (QCSE). To reduce or even avoid these internal piezoelectric fields, the growth in non-c-directions has been proposed. The epitaxy of nonpolar GaN (perpendicular to the c-axis) is typically dominated by a poor crystal quality. Choosing semipolar directions like $(11\bar{2}2)$, $(10\bar{1}1)$ or $(20\bar{2}1)$ seems to be a good compromise between a reasonable crystal quality and a reduced QCSE. For these particular directions, the amount of the piezoelectric field is reduced to a quarter as compared to c-plane and additionally, the field direction is inverted. Therefore, an externally applied voltage counteracts the internal field and hence reduces the band bending. In particular, the $(20\bar{2}1)$ orientation has been found to be most appropriate for such optoelectronic devices [2]. However, the epitaxy of $(20\bar{2}1)$ GaN seems to be a big challenge. Typically, $(20\bar{2}1)$ GaN templates are produced by cutting thick c-plane wafers grown by HVPE, which results in wafers limited in size to just a few square mm [3]. This limitation can be overcome by growing such GaN layers on foreign substrates like sapphire or silicon with uncommon orientations. Similar as reported by Okada et al. [4], we are able to grow $(20\bar{2}1)$ GaN layers on $(22\bar{4}3)$ patterned sapphire substrates with a reasonable crystal quality. By etching trenches into these wafers, c-plane-like sidewalls are formed on which the growth of GaN starts developing triangular shaped stripes. After a suitable growth time, these stripes hopefully coalesce and form a planar $(20\bar{2}1)$ oriented surface (Fig. 1). By this procedure, we make use of the well-established growth in c-direction, eventually resulting in a semipolar surface. This approach offers some essential advantages: First, the growth of a full LED or laser diode structure in a single epitaxy run is possible. Moreover, the diameter of the template is just limited by the reactor size. In our studies, 2" diameter sapphire wafers were used. Well-known from the growth of c-plane GaN, a SiN mask can

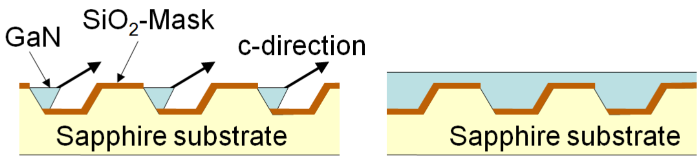


**Fig. 1:** Patterned sapphire substrate, schematically. All non-c-plane facets are covered with $SiO_2$ (brown) avoiding parasitic growth. The GaN nucleates on the c-plane sidewall, forms triangular-shaped stripes (left) and coalesces after a suitable growth time to a closed semipolar surface (right).

help to stop defects penetrating to the surface and therefore reduce the defect density in the subsequent layers significantly. This SiN layer can be deposited in-situ in the MOVPE reactor. Silane ($SiH_4$) reacts with ammonia ($NH_3$) to a SiN layer, less than an atomic layer thick. As a result, the layer is not completely closed and thereby acts as a mask. As shown in Fig. 2, the top of a GaN layer gets covered with this SiN layer. Some defects are stopped by the mask itself. By pushing the GaN growth in c-direction (3D growth), the residual defects get bent to the side. The subsequent coalescence of the three-dimensional structures leads to a closed layer with a drastically reduced defect density. Based on the excellent results of this in-situ deposited interlayer during the growth of c-plane GaN [5], we transferred this technique to the epitaxy of semipolar $(20\bar{2}1)$ GaN. In order to achieve an optimal crystal quality, the position and deposition time of the SiN interlayer are varied systematically. Additionally, we studied the overgrowth of such layers by hydride vapor phase epitaxy (HVPE) to improve the layer quality further and to observe the influence of the SiN mask on these thick layers.

## 2. Experimental

### 2.1 Metal organic chemical vapor phase epitaxy

At the beginning of the structuring process, a nickel reflection layer for the subsequent photolithography steps is evaporated onto the sapphire wafer. A stripe mask with an

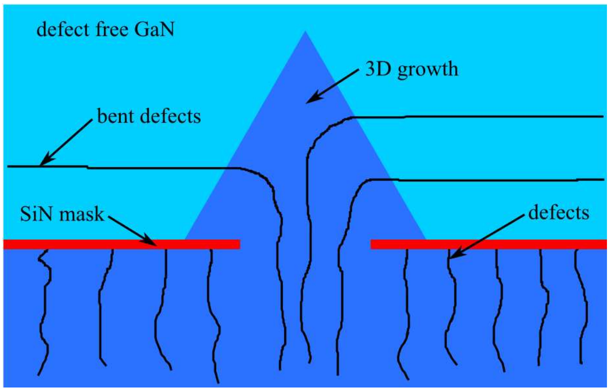


**Fig. 2:** Schematic illustration of the action of a SiN mask reducing the defect density in the subsequent GaN overgrowth.

opening of 3 µm and a period of 6 µm patterns the positive photoresist accordingly. By evaporation of an about 500 nm thick nickel layer and a subsequent lift-off process, a relatively stable etching mask is formed. Via reactive ion etching, the stripes get transferred into the sapphire substrate. Covering all non-c-plane-like facets with $SiO_2$ (Fig. 1) prevents parasitic growth.

The MOVPE growth was done in a commercial Aixtron-200/4 RF-S HT reactor using the standard precursors ammonia ($NH_3$), trimethylgallium (TMGa) and trimethylaluminum (TMAl). The growth starts with our about 20 nm thick standard AlN nucleation layer at relatively low temperatures. Choosing higher temperatures at the beginning of GaN growth improves the selectivity. A subsequent reduction of the reactor temperature pushes the growth in c-direction and the GaN stripes can grow out of the sapphire trenches.

The crystal quality of the GaN layers was investigated by high-resolution X-ray diffraction (HRXRD) with a Bruker D8 Discover diffractometer. From low temperature photoluminescence (PL) measurements in a helium cryostat, using a 1000 mm monochromator and a 1200 $mm^{-1}$ grid, we obtained more detailed information about defects close to the crystal surface.

First investigations [6] were done at growth conditions close to the ones suitable for c-plane growth. A poor selectivity of the AlN and the GaN layer on the patterned and masked sapphire wafer was observed. By increasing the growth temperature, the diffusion velocity of the molecules can lead to an enhanced selectivity. Indeed, by setting the temperature of the AlN layer to 1020 °C and the GaN growth temperature to about 1145 °C, we achieved well-formed GaN stripes without any islands (Fig. 3, left). The very top part of the GaN layer was grown at a lower temperature (about 1050 °C) to push the growth rate in c-direction leading to a more lateral growth in order to improve the coalescence. X-ray rocking curve (RC) measurements of the symmetric $(20\bar{2}1)$ reflection indicate a reasonable crystal quality. With the X-ray beam parallel to the stripes, the signal has a full width at half maximum (FWHM) of just 675 arcsec. Perpendicular to the stripes, the FWHM increases to 1470 arcsec. This may be due to a slight statistical tilt of each individual stripe. Surprisingly, the (0002) reflection measured in skew geometry with the X-ray beam parallel to the stripes gives a very narrow peak of just 70 arcsec. As shown in Fig.

3 (right), low temperature PL measurements indicate a defect-dominated crystal surface. Just a very weak signal at 3.459 eV related to $D^0X$ [7] recombination is detectable.

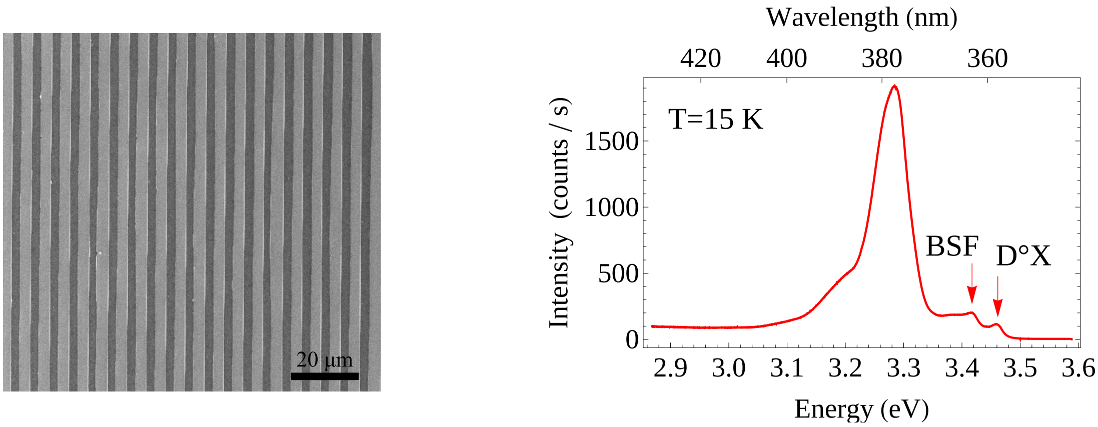


**Fig. 3:** Left: SEM micrograph of $(20\bar{2}1)$ GaN on $(22\bar{4}3)$ patterned sapphire substrate. High reactor temperature leads to a high selectivity of GaN and results in homogeneous GaN stripes, free of any island growth. Right: Low temperature PL measurements indicate a defect-dominated GaN stripes [8].

As described in the introduction, a SiN interlayer was deposited on top of an about 1 µm thick GaN layer (9:50 min growth, before coalescence of the stripes) to improve the crystal quality further. The deposition time of the SiN mask was systematically varied from 4:30 min to 6:00 min. Subsequently, an about 2 µm thick GaN layer was grown. As shown in Fig. 4 (left), a mask deposited for 4:30 min already seems to improve the crystal quality. X-ray RC measurements of the symmetric $(20\bar{2}1)$ reflection show a peak with a FWHM of 453 arcsec. Increasing the deposition time maskes the SiN mask less porous eventually blocking the nucleation in the pores, which may lead to enhanced polycrystalline nucleation on the SiN mask (Fig. 5). An optimal deposition time was found at 5:00 min. RC measurements of the $(20\bar{2}1)$ reflection give a fairly narrow peak with a FWHM of just 320 arcsec. Low temperature PL measurements confirm an improved crystal quality (Fig. 4, right). The ratio of the $D^0X$ (3.467 eV) and BSF ($I_1$) (3.405 eV) peak intensities is decreased, compared to the sample without SiN layer. Additionally, the defect related signal at 3.288 eV seem to be significantly suppressed.

The position of the SiN interlayer determines, where the defects running to the surface get stopped. By depositing it far away from the nucleation layer, the defects can already lead to a rough surface (e.g. V-pits). Choosing a position close to the start of the epitaxy, the GaN buffer layer could be strained, which causes new defects after the SiN interlayer again. Therefore, the position of the mask seems to be an important parameter. Consequently, we varied the growth time of the buffer layer systematically from 6:50 to 9:50 min. The deposition time of the SiN layer itself was fixed to 5:30 min. As shown in Fig. 6 (left), the reduction of the buffer layer thickness leads to an improved crystal quality, obviously saturating at about 7–8 min. PL investigations (Fig. 6, right) indicate a clear decrease of the BSF density. Both the intensity of the signal related to BSF ($I_1$) and the peak related to BSF (E) became weaker as compared to the $D^0X$ intensity.

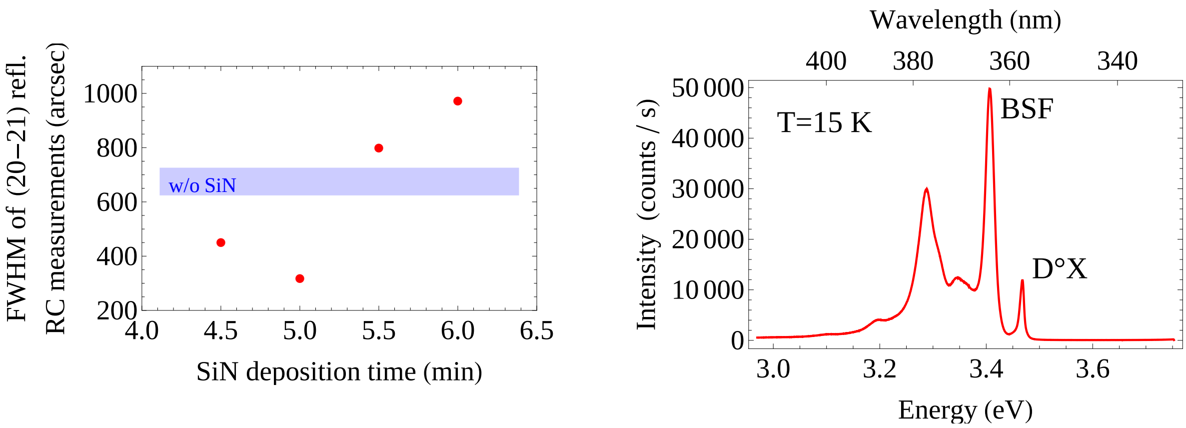


**Fig. 4:** FWHM of X-ray $(20\bar{2}1)$ reflection RC measurements as a function of SiN deposition time. Right: Low temperature PL spectrum of $(20\bar{2}1)$ GaN with a SiN deposition time of 5:00 min.

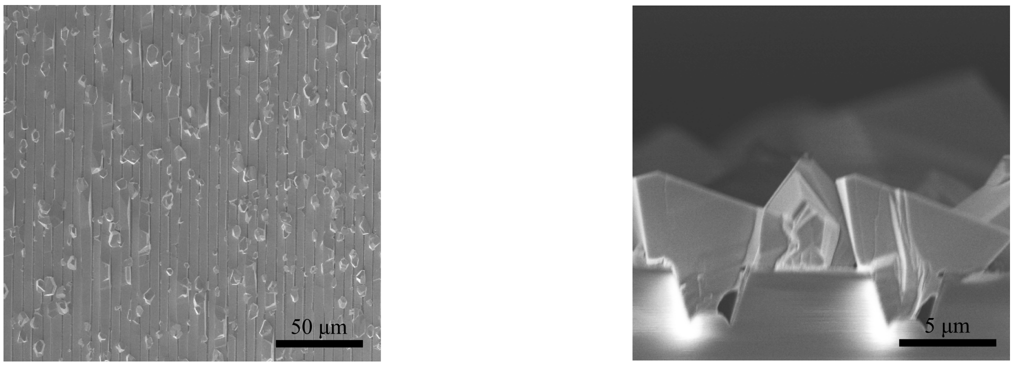


**Fig. 5:** SEM top-view (left) and cross-section (right) micrograph of $(20\bar{2}1)$ GaN with a SiN interlayer, deposited for 6 min showing parasitic polycrystals growing on the surface.

## 2.2 HVPE overgrowth

Next, we investigated the influence of the SiN interlayer on HVPE overgrowth. The temperature of the hot wall reactor was set to 1070 °C. The GaN HVPE layer was grown for 15 min with a V/III ratio of 77, similar to our c-plane growth conditions [9]. SEM investigations confirm the expected high growth rate of about 160 µm/h (Fig. 7, left) leading to a total layer thickness of about 40 µm. The GaN stripes, still separate after the MOVPE growth, seem to coalesce at the very beginning of the overgrowth process. The surface of the sample without SiN shows flaky structures with a height of about 2 µm (Fig. 7, right). Such structures could be caused by defects penetrating through the surface leading to strong step-bunching effects. The X-ray RC $(20\bar{2}1)$ reflection has a FWHM of about 700 arcsec, indicating similar crystal quality as in the MOVPE template. However, PL investigations show a significant decrease of the BSF related signal (Fig. 8, left). At 3.472 eV, an extremely intense and narrow donor-bound excitonic signal with a FWHM of just 5.9 meV is detectable.

In the second run, the MOVPE template with 9:50 min GaN buffer layer growth and 5:00 min SiN deposition time was chosen. The growth conditions were unchanged. SEM

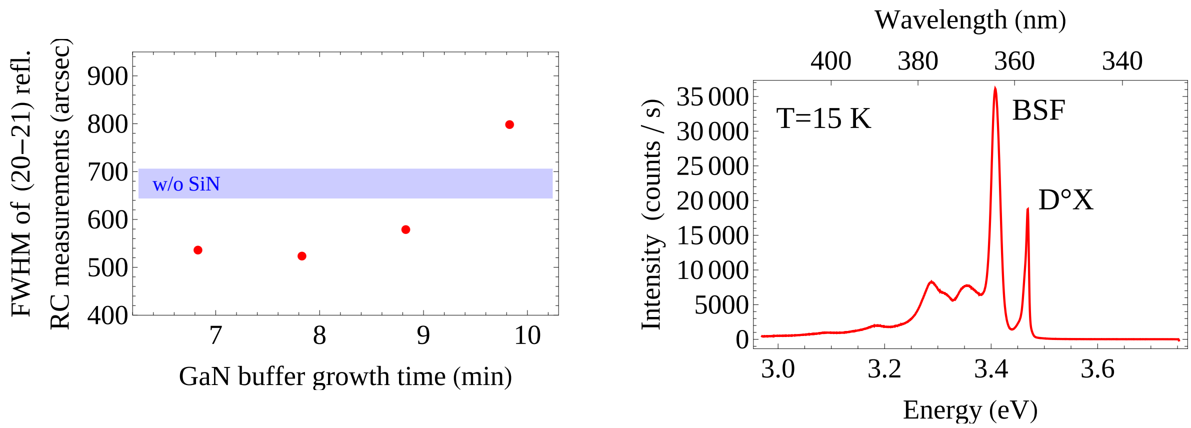


**Fig. 6:** Left: FWHM of X-ray $(20\bar{2}1)$ reflection RC measurements as a function of the GaN buffer layer growth time. Right: Low temperature PL spectrum of $(20\bar{2}1)$ GaN with 7:50 min buffer layer growth time and a SiN deposition time of 5:30 min.

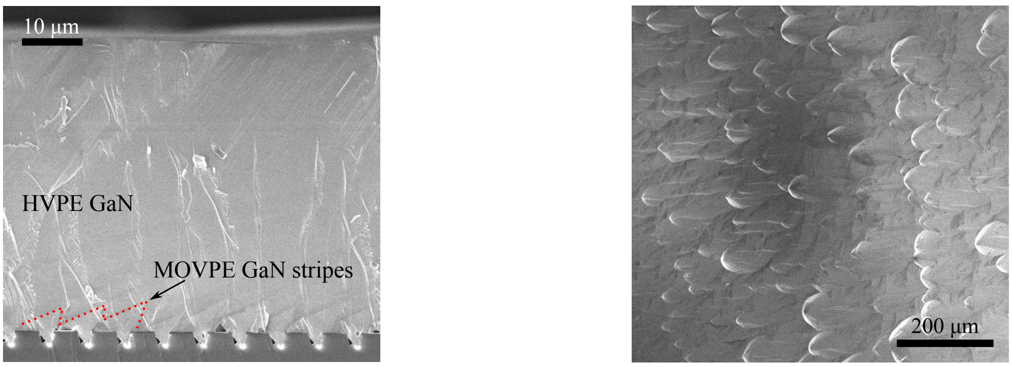


**Fig. 7:** Left: SEM cross section of $(20\bar{2}1)$ HVPE GaN on MOVPE template without SiN interlayer. The MOVPE GaN stripes are marked with a red dashed line (left). The surface shows flaky structures, with a height of about 2 µm (right).

investigations show a clear improvement of the surface quality (Fig. 9). The flakes mentioned above are much less developed. Moreover, the FWHM of the symmetric $(20\bar{2}1)$ reflection considerably decreased to 545 arcsec. Low temperature PL measurements confirm a further improvement of crystal quality as compared to the HVPE sample without SiN (Fig. 8, right). The signal at 3.429 eV, related to BSF ($I_1$), decreases as compared to the $D^0X$ related peak. Therefore, we conclude, that a SiN interlayer in the MOVPE template can help to improve the crystal quality and, in addition, the surface morphology of the HVPE overgrown layer, although the FWHM of the $D^0X$ related signal is slightly increased to 16 meV.

## 3. Conclusion

Using $(22\bar{4}3)$ patterned sapphire substrates, we are able to grow semipolar $(20\bar{2}1)$ GaN stripes with a reasonable crystal quality. By inserting a SiN mask as a defect blocking layer, the BSF density in the subsequent GaN layer can be reduced significantly. We

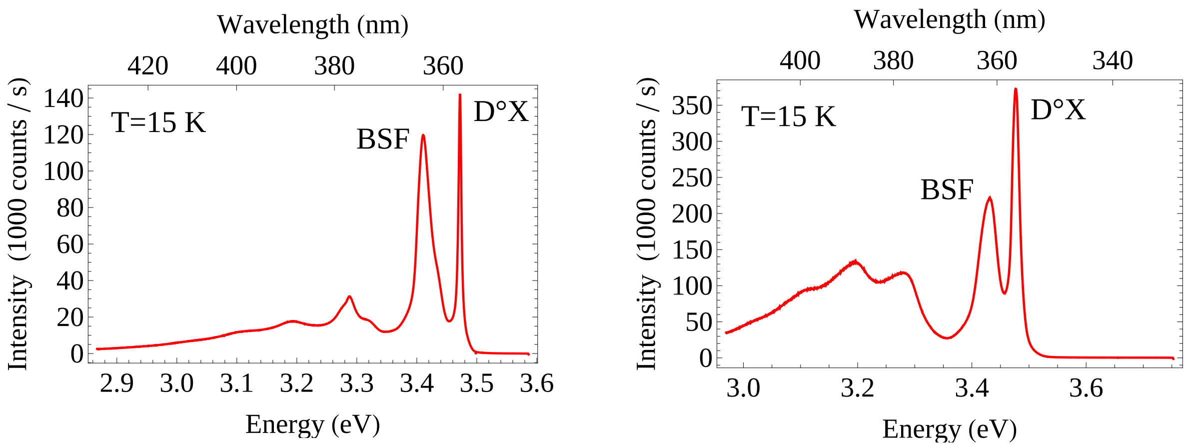


**Fig. 8:** Low temperature photoluminescence measurements of $(20\bar{2}1)$ HVPE GaN without (left) and with (left) SiN interlayer in the MOVPE template.

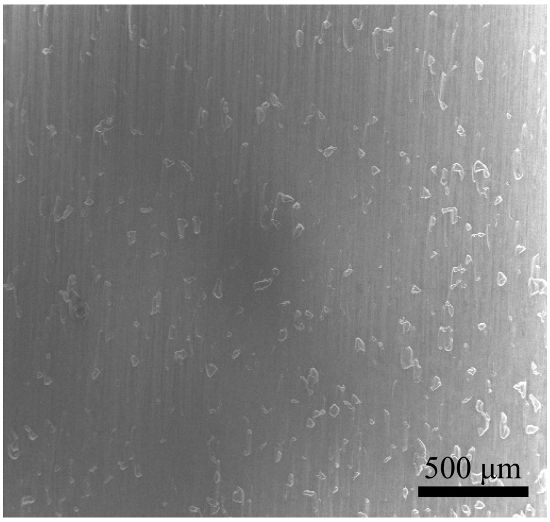


**Fig. 9:** SEM top-view of $(20\bar{2}1)$ HVPE GaN grown on a MOVPE template with SiN interlayer.

investigated the position and the deposition time of the SiN interlayer systematically and found an optimum achieving an excellent crystal quality. X-ray RC measurements of the symmetric $(20\bar{2}1)$ reflection show a narrow peak of just 320 arcsec. Low temperature PL measurements confirm the improvements using the SiN mask. By overgrowing the MOVPE sample with a 40 µm HVPE layer, the crystal quality could be further increased. A SiN layer in the corresponding MOVPE template helps to suppress the flaky surface structures of the subsequent HVPE overgrowth.

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