POLARITY DETERMINATION FOR MOCVD GROWTH OF GaN ON Si(111) BY CONVERGENT BEAM ELECTRON DIFFRACTION

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ABSTRACT

The polarity of laterally epitaxially overgrown (LEO) GaN on Si(111) with an AlN buffer layer grown by MOCVD has been studied by convergent beam electron diffraction (CBED). The LEO GaN was studied by cross-section and plan-view transmission electron microscopy (TEM). The threading dislocation density is less than 10^8 cm^{-2} and no inversion domains were observed. CBED patterns were obtained at 200 kV for the $\langle 1\bar{1}00 \rangle$ zone. Simulation was done by many-beam solution with 33 zero-order beams. The comparison of experimental CBED patterns and simulated patterns indicates that the polarity of GaN on Si(111) is Ga face.

INTRODUCTION

In recent years it has been demonstrated that GaN and related alloys grown by metalorganic vapor phase epitaxy exhibit superb properties for the design and production of light-emitting diodes and lasers operating in the short wavelength of the visible spectrum. LEO GaN on sapphire and silicon carbide substrates has been shown to result in a significant reduction of the extended defect density (3-4 orders of magnitude) which, in turn, has led to improvements in device performance for blue lasers, light-emitting diodes, p-n junctions, and field-effect transistors. For a review of relevant topics, see ref. [1]. The success of LEO growth has revived interest in alternative substrates such as Si(111), which has potential advantages for device integration, thermal management, and cost issues. LEO GaN with low dislocation density on Si(111) substrates has recently been demonstrated [2].

The most common growth direction for GaN is normal to the {0001} basal plane. The basal plane has a polar configuration with two atomic sub-planes each consisting of either the cationic or the anionic element of the binary compound. Thus, in the case of GaN a basal plane surface should be either Ga or N terminated (See Fig.1). Note that the polarity is a bulk property. The identification of the polarity in GaN can be carried out by several techniques such as X-ray photoemission spectroscopy [3], convergent beam electron diffraction [4,5,6], and chemical etching [7]. For a review of GaN polarity determination, see ref. [8]. In this paper we report on CBED studies of LEO GaN on Si(111) substrate and show that the polarity is Ga face.

EXPERIMENTAL

Two inch-diameter Si(111) wafers were etched in buffered HF for one minute before growth. After heating to the growth temperature of 900°C under hydrogen, the TMAl and NH_3 precursors were introduced in the MOCVD growth chamber and the AlN buffer layer was deposited at a total pressure of 76 Torr. The thickness of the AlN layer

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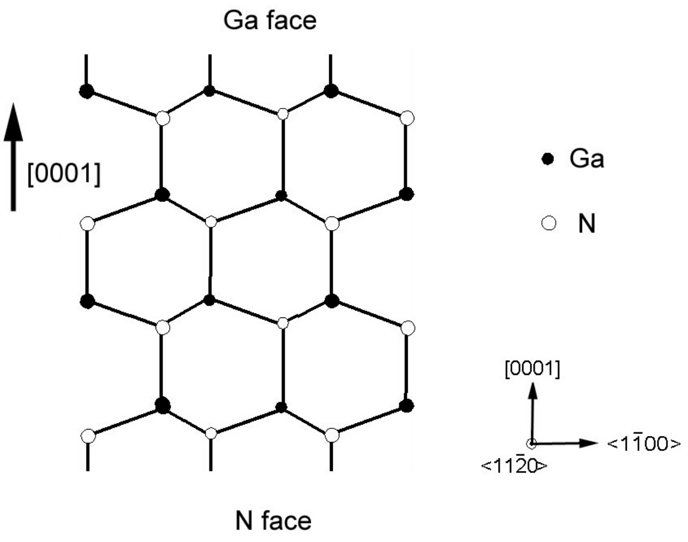

Figure 1. $<11\bar{2}0>$ projection of the GaN structure. [0001] is defined as the direction of Ga to N bond between Ga/N bilayers, as shown with the arrow in the figure.

was ~60 nm. The AlN layer was crack-free over the entire wafer, and the RMS roughness measured by AFM was on the order of 15 nm. The wafers were then coated with 200 nm-thick SiO_2 using plasma-enhanced chemical vapor deposition, and 5 µm-wide stripes oriented in the Si$<11\bar{2}>$ direction were patterned using standard UV photolithography and wet chemical etching. The width of the SiO_2 mask regions was 35 µm. The LEO GaN stripes were obtained by performing a regrowth at ~1060°C using TMGa and NH_3.

TEM samples were prepared by wedge polishing followed by Ar^+ ion milling. Diffraction contrast images and CBED patterns were obtained on a JEOL 2000FX microscope operated at 200 kV. The surface topography was imaged using a Digital Instruments Dimension 3000 AFM operating in tapping mode. Simulations were done by software package “Desktop Microscopist 2.0” [9]. The simulated CBED patterns were calculated by solution of the many-beam equation with 33 zero-order reflections. It is well known that the polarity of GaN/Al_2O_3 grown by MOCVD is usually Ga face. We also checked the polarity of our MOCVD grown GaN on Al_2O_3 by CBED and confirmed that it is Ga face.

RESULTS AND DISCUSSION

Cross-section TEM micrographs are shown in Figure 2. The seed region has a threading dislocation density on the order of $\sim 10^{11}$ cm^{-2}, consisting predominantly of pure edge dislocations. In contrast, the LEO regions have a very low threading dislocation

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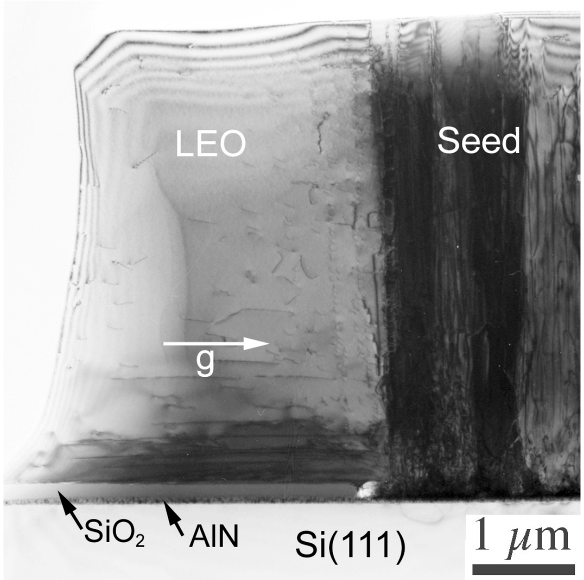

Figure 2. Cross-section bright-field TEM micrographs, g = $11\bar{2}0$. The irregular top and side surfaces are due to ion milling.

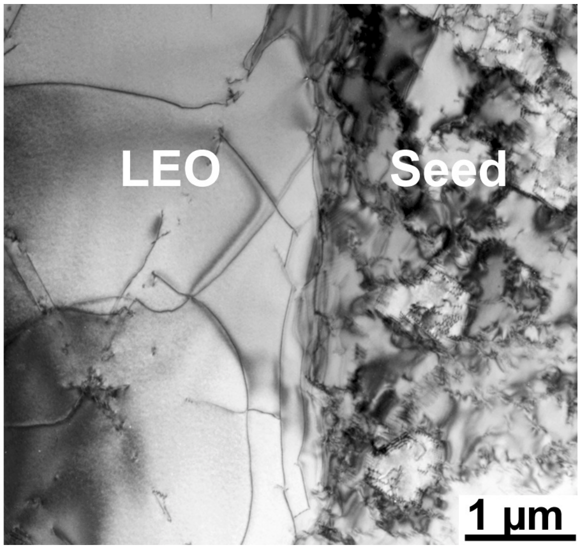

Figure 3. Plan-view bright field TEM image of LEO GaN/Si(111) clearly showing the seed (right) and overgrown region (left).

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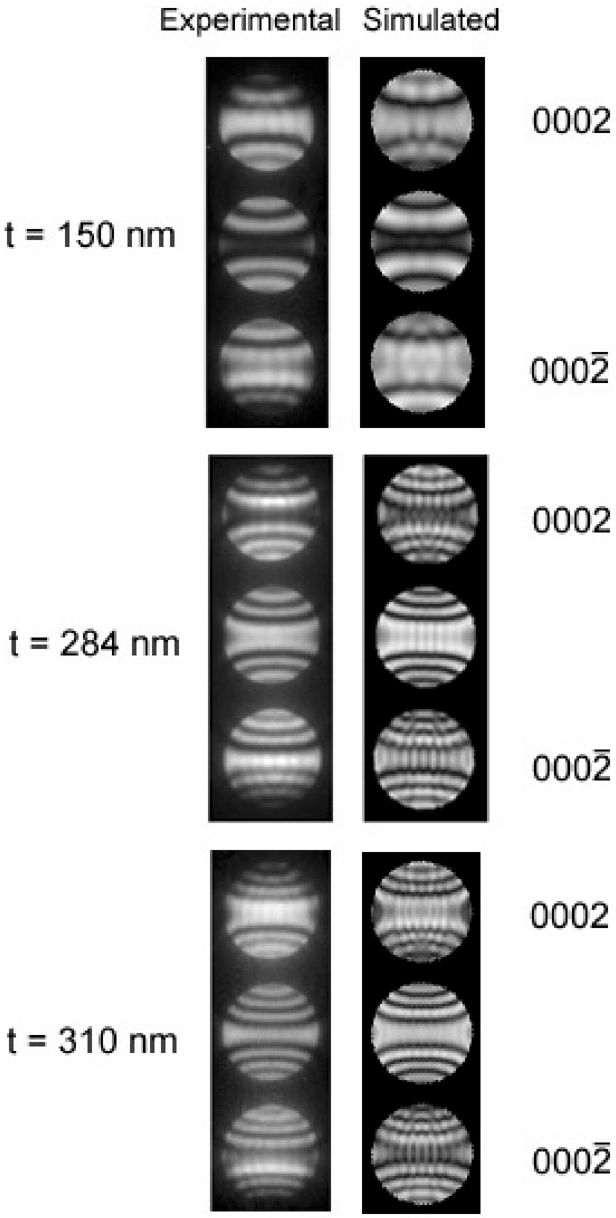

Figure 4. Experimental and simulated CBED patterns at different thickness. All patterns correspond to $[1\,\bar{1}\,00]$ zone axis.

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density and show an essentially single-crystalline microstructure. The plan-view TEM image (Figure 3) further confirmed that the threading dislocation density was reduced several orders of magnitude in the LEO region. No inversion domain boundaries were observed under both cross-section and plan-view TEM. We reasonably assume that the GaN/Si(111) grown by MOCVD has one unique polarity.

Figure 4 shows the comparison of experimental and simulated CBED patterns. The experimental CBED patterns were taken under $<1\bar{1}00>$ zone-axis at 200 kV from different thickness region of the cross section sample. One should pay attention when indexing the diffraction pattern. For some models of transmission electron microscopes, there is a 180° inversion between image and diffraction pattern. This can be checked by underfocusing the diffraction lens to image a plane above the diffraction pattern. The image will not be inverted with respect to the diffraction pattern [10]. The simulations were calculated with 33 zero-order reflections and mean absorption coefficient 0.05. A series of CBED patterns were calculated with different thicknesses from 100 nm to 400

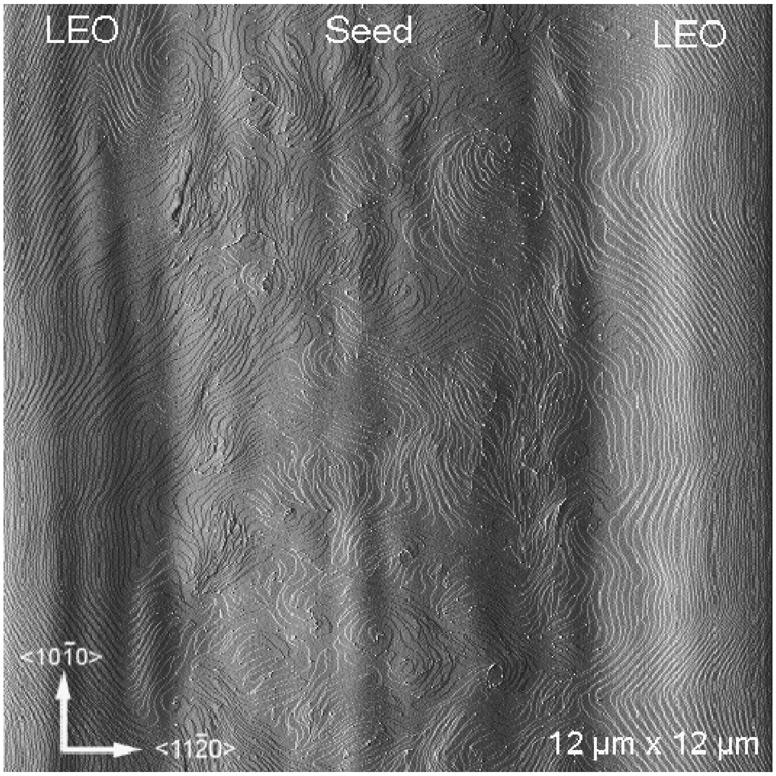

Figure 5. Surface topography measured by AFM. The contrast is related to the amplitude of the tip vibration during tapping-mode imaging.

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nm in 10 nm steps. The pattern which best matched the experimental data was selected. From central disks comparison, the sample thickness was obtained. From diffraction disks comparison, the polarity was obtained. From the matching of experimental and calculated patterns, it is clear that the polarity of the LEO GaN on Si(111) is Ga face.

Figure 5 shows the surface topography of LEO GaN grown on Si(111) over 144 μm^2 area. Although the surface is undulated and shows spiral growth, the topography clearly consists of c/2-high atomic steps. In the seed region the pure screw and mixed-character threading dislocations (~$2x10^9$ cm^{-2}) are visible as surface depressions (~20 nm in diameter) that terminate atomic steps. The lack of such step terminations in the LEO GaN regions clearly shows that the threading dislocation density is reduced significantly. Overall the surface is quite smooth. Our results are consistent with the framework summarized by E. S. Hellman [8]: "smooth films grown by MOCVD are usually Ga face".

CONCLUSION

The polarity of MOCVD growth GaN/Si(111) with AlN buffer has been studied by convergent beam electron diffraction. Comparing the experimental patterns and simulated patterns, it is shown that the polarity of GaN film is Ga face.

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REFERENCES

[1] J. S. Speck and S. J. Rosner, Physica B, in press.
[2] H. Marchand, N. Zhang, L. Zhao, Y. Golan, S. J. Rosner, G. Girolami, P. T. Fini, J. P. Ibbetson, S. Keller, S. DenBaars, J. S. Speck, U. K. Mishra, MRS Internet J. Nitride Semicond. Res., **4**, Article 2, 1999.
[3] T. Sasaki, T. Matsuoka , J. Appl. Phys. **64**, 4531 (1988).
[4] Z. Liliental-Weber , J. Washburn, K. Pakula, and J. Baranowski, Microsc. Microanal., **3**, 436 (1997).
[5] F.A. Ponce, D.P. Bour, W.T. Young, M. Saunders, J.W. Steeds, Appl. Phys. Lett. **69**, 337 (1996).
[6] P. Vermaut, P. Ruterana, G. Nouet, Phil. Mag. A **76**, 1215 (1997).
[7] J. L. Weyher, S. Müller, I. Grzegory, S. Porowski, J. Cryst. Growth **182**, 17 (1997).
[8] E. S. Hellman, MRS Internet J. Nitride Semicond. Res. **3**, Article 11, 1998.
[9] Available from Virtual Laboratories (Tel. 505 828 1640).
[10] M. H. Loretto and R. E. Smallman, *Defect Analysis in Electron Microscopy*, (John Wiley & Sons Inc., New York, 1975), chapter 1.3.

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