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Structural Properties of Free-Standing 50 mm Diameter GaN Wafers with (10 $\bar{1}$ 0) Orientation Grown on LiAlO $_2$

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ABSTRACT

(10 $\bar{1}$ 0) GaN wafers grown on (100) face of γ -LiAlO $_2$ were studied using transmission electron microscopy. Despite good lattice matching in this heteroepitaxial system, high densities of planar structural defects in the form of stacking faults on the basal plane and networks of boundaries located on prism planes inclined to the layer/substrate interface were present in these GaN layers. In addition, significant numbers of threading dislocations were observed. High-resolution electron microscopy indicates that stacking faults present on the basal plane in these layers are of low-energy intrinsic I $_1$ type. This is consistent with diffraction contrast experiments.

INTRODUCTION

The search for a suitable substrate for epitaxial growth of high quality III-nitride device structures is an extremely important issue. To date, almost all nitride films are grown on highly mismatched substrates, namely on α -Al $_2$ O $_3$ and 6H-SiC. Recently however, γ -LiAlO $_2$, which has a tetragonal crystal structure, attracted significant attention since its (100) face is very closely matched with the (10 $\bar{1}$ 0) face (M-plane) of wurtzite GaN. Lattice mismatch of -1.4% is expected along the c-axis ($[001]_{\text{LiAlO}_2} \parallel [1\bar{2}10]_{\text{GaN}}$) and of -0.1% only along the b-axis of γ -LiAlO $_2$ ($[010]_{\text{LiAlO}_2} \parallel [0001]_{\text{GaN}}$). Significantly, GaN devices grown with the M-plane orientation are expected to be free from spontaneous electrostatic fields along the growth direction. Growth of M-plane GaN(1 $\bar{1}$ 00) on γ -LiAlO $_2$ (100) substrate originally proposed by Hellman et al. [1] has been realized recently and indeed the lack of spontaneous electrostatic fields along the growth direction has been demonstrated [2,3]. For example, it was recently shown that the peak position of emission from C-plane GaN/AlGaIn multi-quantum well structures is strongly blue shifted with increasing excitation intensity, whereas the peak position for M-plane structures remains unchanged [4]. These first studies on M-plane GaN layers indicate however that despite the apparent good lattice match with the substrate, there occur high densities of structural defects in such GaN layers. Both the nature of these defects and their origin remain illusive and there is a need for more in-depth studies. In this paper we report results of such structural studies performed on free-standing 50 mm diameter GaN wafers obtained by growth on the (100)-face of γ -LiAlO $_2$ [5].

EXPERIMENTAL

Boules of LiAlO $_2$ were prepared from the melt by the Czochralski method, and sawed into wafers. After polishing, GaN layers about 350 microns thick were deposited on them by halide vapor phase epitaxy (HVPE) at 875°C. Subsequent to growth, the LiAlO $_2$ was removed by wet

chemical etching, leaving GaN wafers with the non-polar (10 $\bar{1}$ 0) orientation. The structural properties of these wafers before and after substrate removal were investigated by transmission electron microscopy (TEM).

RESULTS AND DISCUSSION

TEM images of the interface between GaN and LiAlO₂ indicate that approximately a 50 nm thick layer at the surface of the substrate has been modified and seems to be much more defective than the remaining part of the substrate, which has high structural quality (Figure 1a). Surprisingly, selected area electron diffraction shows that the orientation of the GaN film actually matches that of the original substrate, suggesting that the defective regions of the interfacial layer occur only as islands surrounded by regions where there is a full coherence (Figure 1b).

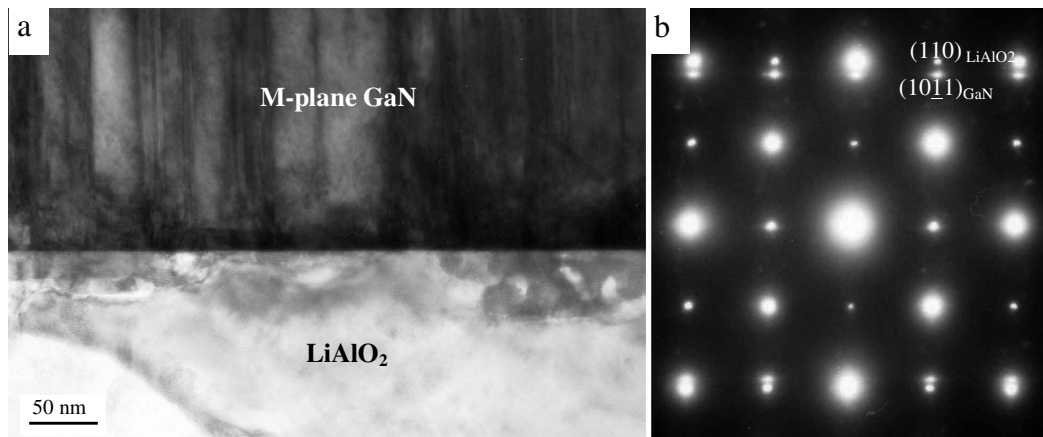


Figure 1. (a) TEM image of the interface between M-plane GaN(1 $\bar{1}$ 00) layer and γ -LiAlO₂(100) substrate. Notice ~50 nm thick defective layer at the surface of the substrate. (b) Selected area electron diffraction pattern of this interface area.

Several types of structural defects were observed inside M-plane (10 $\bar{1}$ 0) GaN wafers grown on LiAlO₂(100) substrates. Stacking faults (SFs) and the planar defects formed on the basal plane as well as boundaries located on prism planes and threading dislocations were the most dominant defects. All these defects will be discussed in the following.

Stacking faults on the basal plane

High densities of SFs located on the basal [*e.g.* (0001)] plane were observed inside GaN layers in both cross-sectional and plan-view specimens. The average separation between them was of the order of a few tens of nanometers. Many of such basal SFs are visible edge-on as thin dark lines in the dark-field TEM image obtained from the (0001) beam for the symmetrical [1 $\bar{2}$ 10] specimen orientation, shown in Figure 2a. They are revealing the characteristic bright-dark fringe contrast in weak-beam image, obtained also from a plan-view specimen inclined towards the *c*-axis (Figure 3a). Such a high density of these SFs located on basal planes affected also the selected area electron diffraction (SAED) patterns recorded from these layers. It can be seen in the [1 $\bar{2}$ 10] SAED pattern shown in Figure 2c, which reveals streaking of diffraction spots along [0001] direction caused by the presence of a high density of planar defects formed on the basal plane.

Diffraction contrast experiments showed that in cross-sectional samples SFs were in strong contrast for $\mathbf{g} = (10\bar{1}0)$ and in weak or no contrast for $\mathbf{g} = (11\bar{2}0)$ and $\mathbf{g} = (0002)$. Similarly, SFs were not visible when $\mathbf{g} = (0002)$ was selected and gave strong diffraction contrast when $\mathbf{g} = (1\bar{1}00)$ was used in plan-view samples.

In order to determine the actual nature of these SFs, a high-resolution electron microscopy (HREM) study was performed. A typical HREM image of a fault is shown in Figure 2d. Analysis of the HREM images indicates that these SFs have the following stacking sequence: ...ABABABABCBCBCBC..., where each capital letter represents a bi-atomic, Ga-N layer.

Three types of SFs can exist in the wurtzite structure [6]. There are two intrinsic (I_1 and I_2) and one extrinsic (E) stacking fault. They can be treated as thin layers of cubic stacking. I_1 , I_2 and E correspond to 3 (e.g. ABC), 4 (e.g. ABCA) and 5 (e.g. ABCAB) bi-atomic layers of cubic structure, respectively. Our experimental results indicate that basal SFs present in HVPE M-plane GaN($10\bar{1}0$) layers grown on $\text{LiAlO}_2(100)$ substrates are of the I_1 type. It is not very surprising since the I_1 sequence has the lowest stacking fault energy. This stacking fault is equivalent of the removal of a basal layer followed by the slip of one part of the crystal by $1/3[10\bar{1}0]$.

Not all planar defects formed on the basal were simple stacking faults. Some kind of thin domains were also observed. Several of them are shown by white arrows in Figure 2a. It is noticeable that contrast within such domains differs from that of neighboring material. However, the origin of these domains remains unclear.

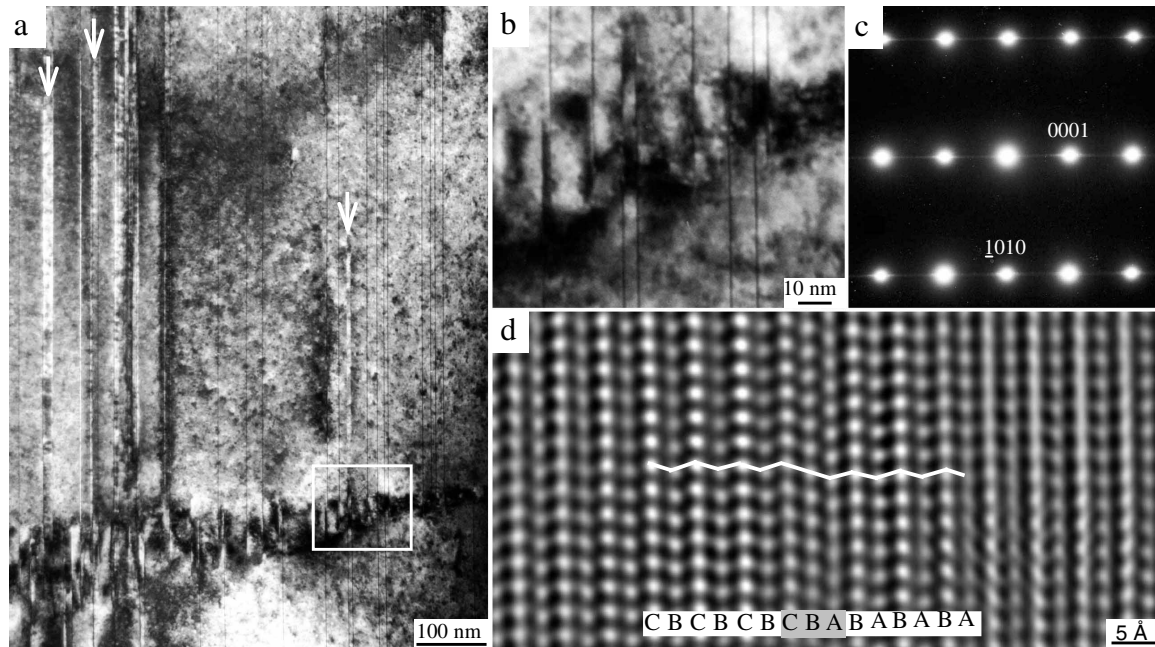


Figure 2. (a) Dark-field image ($\mathbf{g} = 0001$) of cross-sectional sample. Several domains are indicated by arrows. (b) Enlargement of the area marked by the rectangular frame in (a). Notice several basal stacking faults represented by narrow dark lines. Some of them terminate and some nucleate at the inclined boundary. (c) Selected area electron diffraction pattern obtained from cross-sectional sample. Notice spot streaking in the $[0001]$ direction due to large number of basal planar defects. (d) High resolution image of a basal stacking fault. Stacking sequence indicates that this is I_1 stacking fault.

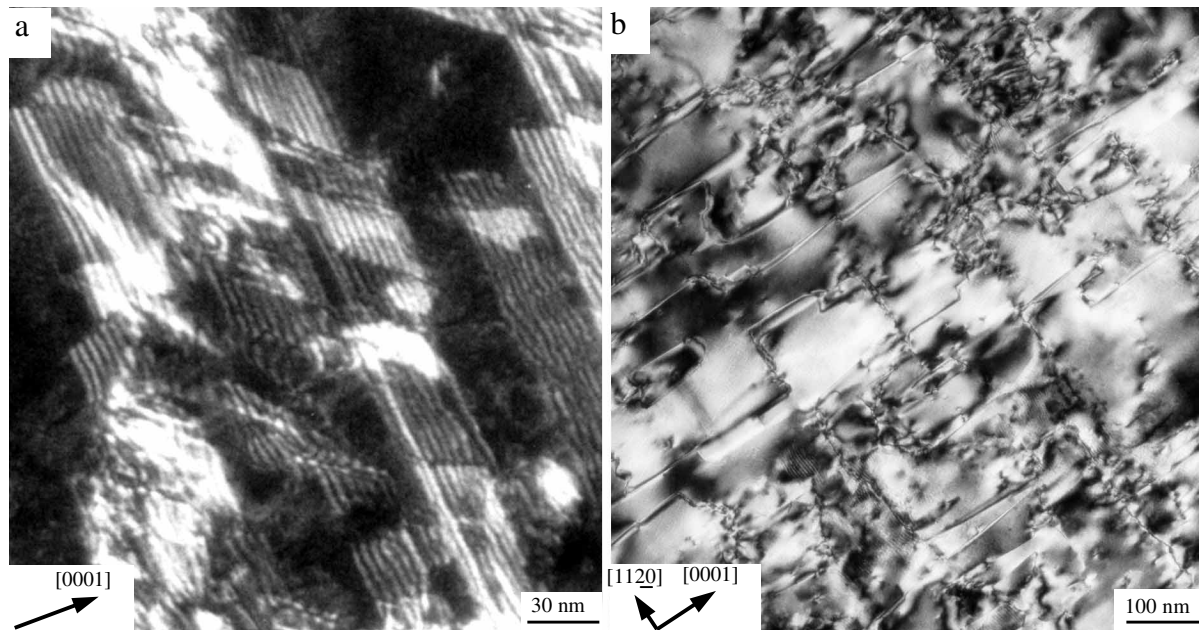


Figure 3. TEM images of plan-view specimens. (a) Weak-beam image [$\mathbf{g} = (1\bar{1}00)$] showing several basal stacking faults, inclined towards the c-axis, revealing characteristic fringe contrast. (b) Dark-field image [$\mathbf{g} = (0002)$] showing a dense network of inclined boundaries visible in cross-sectional images.

Boundaries

The second major type of defect present in HVPE M-plane GaN layers is a stacking mismatch boundary, which seemed to be located primarily on a prism plane inclined to the growth plane. Several such boundaries are shown in Figure 4 (indicated by arrows). It was noticed that they interact with SFs located on the basal plane and play a role of nucleation/termination sites for them (Figures 2b, 4a and 4c). Weak-beam dark field images recorded under $(\mathbf{g}, -3\mathbf{g})$ conditions with $\mathbf{g} = (0002)$ showed very clearly these boundaries (Figure 4d). In these conditions SFs on the basal plane are not visible whereas boundaries reveal characteristic bright-dark fringe contrast. Partial dislocations associated with nucleated/terminated basal SFs are also clearly visible in such images. It can be seen that each boundary is composed of segments lying between these partial dislocations. Bright-dark fringe contrast changes direction from segment to segment suggesting presence of steps along such boundaries.

Diffraction contrast experiments performed for cross-section specimens indicate that the displacement vector associated with these boundaries is parallel to the $[0001]$ direction. This is consistent with plan-view observations where boundaries are visible for $\mathbf{g} = (0001)$. In plan-view they are seen as a dense array which in part can be seen in Figure 3b.

It was noticed also that these boundaries provided sites for crack formations; a number of cracks were observed along these boundaries in both cross-section and plan-view specimens.

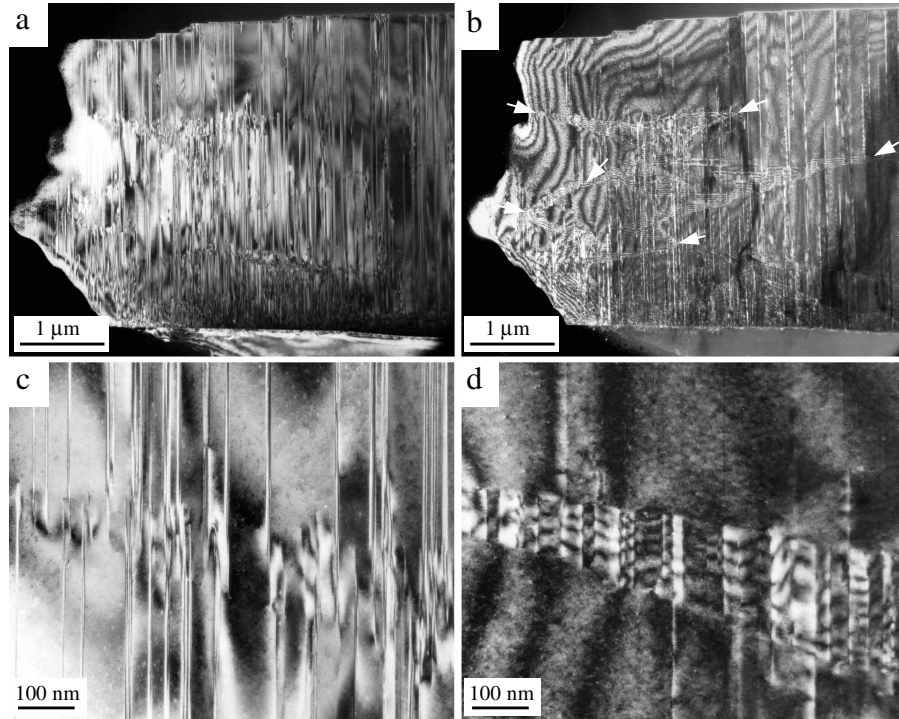


Figure 4. (a) and (c) Dark-field images [$g = (10\bar{1}0)$] and (b) and (d) weak-beam dark-field images [$g = (0001)$] of the GaN layer area adjacent to the LiAlO_2 substrate. Notice high density of basal SFs which are in strong contrast for $g = (10\bar{1}0)$. Numerous inclined boundaries are visible in (b). They reveal characteristic fringe contrast which direction changes from segment to segment (d).

Dislocations

Finally, HVPE M-plane GaN(10 $\bar{1}$ 0) layers grown on $\text{LiAlO}_2(100)$ substrates contained also substantial number of threading dislocations. These dislocations are inclined with respect to the film normal and were primarily located on the basal planes. Several of such dislocations with characteristic oscillating contrast are visible in addition to various basal SFs and one inclined boundary in dark-field images shown in Figure 5. The density of these dislocations decreased from the value of the order of 10^9 cm^{-2} close to the substrate to the value of the order of 10^8 cm^{-2} at the layer surface.

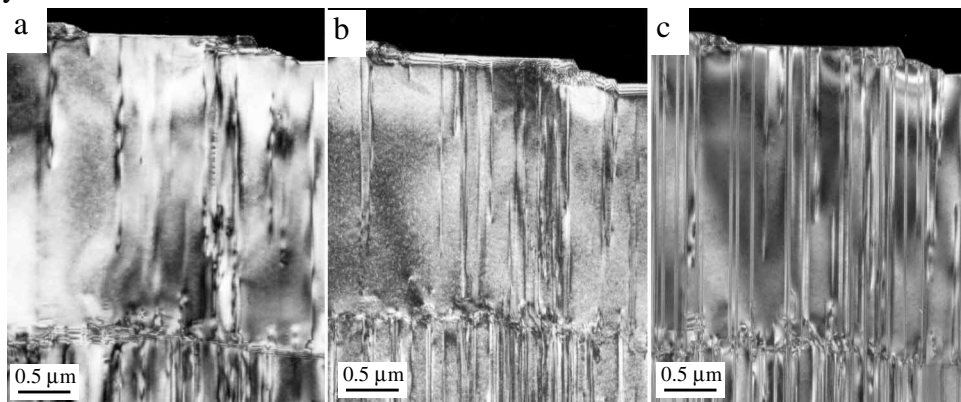


Figure 5. Dark-field TEM images of cross-sectional specimen recorded for (a) $g = (0002)$, (b) $g = (11\bar{2}0)$ and (c) $g = (10\bar{1}0)$.

SUMMARY

In summary, TEM studies showed a significant number of structural defects in HVPE-grown M-plane GaN layers despite their apparent good lattice matching to γ -LiAlO₂ (100) substrates. Several types of defects were observed. The most dominant ones were stacking faults formed on the basal c-plane. HREM indicates that these are low-energy, intrinsic I₁ faults. M-plane GaN layers contained also a network of boundaries located primarily on prism planes inclined to the substrate/layer interface. Significant number of threading dislocations was also observed.

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