Dislocation reduction in GaN grown on stripe patterned r-plane sapphire substrates

Hou-Guang Chen
Department of Materials Science and Engineering, I-Shou University, Kaohsiung 840, Taiwan

Tsung-Shine Ko, Shih-Chun Ling, Tien-Chang Lu, Hao-Chung Kuo, and Shing-Chung Wang
Department of Photonics, National Chiao Tung University, Hsinchu 300, Taiwan and
Institute of Electro-Optical Engineering, National Chiao Tung University, Hsinchu 300, Taiwan

Yue-Han Wu and Li Chang
Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu 300, Taiwan

(Received 4 December 2006; accepted 10 June 2007; published online 13 July 2007)

Extended defect reduction in GaN can be achieved via direct growth on stripe patterned (1 1 0 2) r-plane sapphire substrates by metal organic chemical vapor deposition. The striped mesa is along [1 1 2 0] with two etched sides in {0001} and {1 1 0 1} faces. GaN grown on both etched facets in epitaxy exhibit different crystallographic relationships with sapphire substrate which are (1 1 0 2)_{sapphire}||[1 1 2 0]_{GaN} and [1 1 2 0]_{sapphire}||[1 1 0 0]_{GaN}, and (0 0 0 1)_{sapphire}||(0 0 0 1)_{GaN} and [1 1 2 0]_{sapphire}||[1 1 0 0]_{GaN}, respectively. The dislocation densities can be significantly reduced through epitaxial growth on the inclined lateral faces of mesas. Dislocation density in the order of \( \sim 10^7 \) cm\(^{-2} \) can be achieved in the tilted GaN. © 2007 American Institute of Physics.

DOI: 10.1063/1.2754643

GaN and other related III-nitride based semiconductors are promising materials for applications in light-emitting devices covering the ultraviolet and full visible ranges of the electromagnetic spectrum. However, the intrinsic spontaneous and extrinsic piezoelectric polarizations which are always present in GaN-based heterostructures grown with the orientation of basal plane of wurzite structure can degrade electronic and optical properties. Thus, epitaxial growth of nonpolar III-nitride to prevent the polarization effect has attracted intensive attention in recent years and is regarded as one of the important solutions for high efficiency and high performance of nitride-based device applications.

Due to large lattice mismatch between GaN and sapphire substrates, highly defective GaN films are always formed by conventional metal organic chemical vapor deposition process. In order to reduce defects as demanded for device applications, epitaxial lateral overgrown (ELOG) and Pendeo epitaxy (PE) approaches have been widely proposed to reduce the defect density. Although the ELOG and PE processes can dramatically eliminate most of dislocations, the two-step growth and regrowth process is too complicated and time consuming. In addition to ELOG and PE, one-step GaN growth on maskless patterned sapphire substrates (PSSs) is a simplified method to enhance device performance and efficiency. Although PSSs may not reduce the dislocation density to the order of magnitude that ELOG can achieve, the geometrical effect of patterned substrate can effectively enhance light extraction. In this letter, we demonstrate that GaN grown on patterned r-plane sapphire substrates with asymmetric inclined facets can have a very low defect density in GaN epilayers without regrowth process.

In our study, fabrication of pattern of sapphire substrates was illustrated as follows. A SiO\(_2\) mask was deposited on (1 1 0 2) r-plane sapphire by plasma-enhanced chemical vapor deposition. The mask pattern consisted of 1 \( \mu \)m wide stripe oriented along the [1 1 2 0] direction and 6 \( \mu \)m wide opening that were defined by a standard photolithography process. The sapphire substrates were then wet etched using H\(_3\)PO\(_4\)-based solution at 300 °C for 5 min. Afterward, the sample was dipped into buffered oxide etch solution (NH\(_4\)F:HF=6:1) to remove the SiO\(_2\) mask for the following epitaxial growth. Figure 1(a) shows a scanning electron mi-

FIG. 1. (a) SEM image of patterned sapphire substrate showing the etched facets on both sides of the striped mesa which are exhibited in different inclined angles. [(b) and (c)] Various magnified top-view SEM images of striped GaN grown on patterned sapphire. Based on the variation of image contrast, the striped GaN can be divided into five different regions. (d) Cross-sectional SEM image taken in tilt-view showing that each GaN stripe consists of two crystallites (as indexed by GaN I and GaN II) with facets in different orientations.
croscope (SEM) image of a patterned sapphire substrate with both etched sides of the striped mesa which exhibit facets in different inclined angles due to the low crystallographic symmetry characteristic on r-face sapphire oriented along the [1 1 2 0] direction. The patterned substrate was loaded into a low-pressure metal organic chemical vapor deposition system. A 30 nm thick AlN buffer layer was grown at 600 °C, followed by bulk GaN growth at 1120 °C with low V/III ratio of ~900–1200 and a pressure of 100 Torr. The morphology observation of GaN was carried out in a SEM (JEOL-7000F). Cross-sectional thin sample was prepared for transmission electron microscopy (TEM) observation using conventional mechanical polishing and Ar+ ion milling at 3.5–4 kV. TEM was performed on a Philips Tecnai 20 microscope.

The top-view SEM images of GaN grown on patterned sapphire are presented in Figs. 1(b) and 1(c). GaN stripes grown on the striped pattern of sapphire can be observed in Fig. 1(b). In the high-magnification image of Fig. 1(c), the GaN stripes exhibit periodical image contrast along the direction normal to the stripes. Within each period, the contrast varies from one to another region. According to SEM image contrast, the GaN stripe can be divided into five regions, as designated in Fig. 1(c). Also, it can be seen that the density of pits is varied on these five regions. Particularly in region 2, we can see a much larger quantity of pits than in the rest of the regions. In order to investigate the cross-sectional profile of GaN stripes from which one can realize the three dimensional morphology of GaN stripe, a cross-sectional sample was prepared by cleaving along the sapphire [1 1 0 1] direction. A tilt-view SEM image [Fig. 1(d)] shows that each period of GaN stripe consists of two differently oriented crystallites (as indexed by GaN I and GaN II) terminating with facets. Each terminated facet has the corresponding image contrast and feature shown from the regions in Fig. 1(c).

The microstructure of the GaN stripe was studied by TEM. A typical low-magnification bright-field (BF) TEM image shown in Fig. 2(a) demonstrates the periodicity of GaN crystallites (GaN I and GaN II) which have already been seen in SEM. Figure 2(b) in high magnification shows one complete GaN stripe with the corresponding selected-area electron diffraction pattern in Fig. 2(c). The diffraction pattern shows that there are two sets of [1 1 0 0] zone axis GaN reflections from GaN I and GaN II with a rotation angle of ~57.4°. The crystallographic orientation relationships between GaN stripes and sapphire substrate are then determined to be \((1 1 0 2)_{\text{sapphire}} \parallel (1 1 2 0)_{\text{GaN}}\) and \((1 1 2 0)_{\text{sapphire}} \parallel [1 1 1 0]_{\text{GaN}}\) for GaN I, and \((0001)_{\text{sapphire}} \parallel (0001)_{\text{GaN}}\) and \([1 1 2 0]_{\text{sapphire}} \parallel [1 1 1 0]_{\text{GaN}}\) for GaN II, respectively. Clearly, GaN I has \((1 1 2 0)\) a plane on the top surface with \((0001)\) c plane at the lateral one. The region (region 2) above the sapphire striped mesa contains a very high density of defects, such as threading dislocations (TDs) and stacking faults (SFs) which are usually observed in epitaxial a-plane GaN grown on r-plane sapphire. However, the defect density in GaN I is much reduced with the distance away from the mesa in the lateral direction. Examination of the neighboring crystallite GaN II shows that the top surface parallel to the r plane of sapphire is \((1 1 2 0)\) facet with a narrow width, while the remaining two inclined facets are \((1 1 2 0)\) and \((0001)\) planes. Referring to SEM, we can see in Fig. 2 that regions 3–5 in GaN II contain lower densities of defects. Therefore, the defect density of each region has a close correlation with the number of pits observed in SEM. As previously mentioned, the low symmetry of r-face sapphire along \([1 1 2 0]\) causes the emergence of asymmetrically etched facets between both sides of the striped mesa. Figure 2(d) shows an enlarged image of the sapphire striped mesa, and each etched facet near \((0001)\) and \([1 1 0 1]\) planes, respectively, deviated from nominal faces by several degrees, based on the measurement of the adjacent angle among the facets. Notably, the GaN II which has an extremely low defect density directly grows on the \((0001)\) etched facets of the mesa. The measured defect densities (including TDs and SFs) corresponding to each GaN facet region are summarized in Table I.

In order to further investigate the defect distribution in the GaN stripe, the \(g \cdot b\) weak beam dark field technique was employed. Figures 3(a) and 3(b) show the dark field images of GaN I taken from \(g = 1 1 2 0\) and 0002, respectively. A very high density of dislocations and stacking faults can be observed in region 2 where GaN grows directly on part of the top \((1 1 0 2)\) face and the side \((1 1 0 1)\) face of the mesa. However, the lateral region (region 1) contains a relatively lower dislocation density than region 2. Based on the \(g \cdot b\)

---

**TABLE I. Defect densities in different regions with corresponding terminated facets.**

<table>
<thead>
<tr>
<th>Terminated facet</th>
<th>Region 1</th>
<th>Region 2</th>
<th>Region 3</th>
<th>Region 4</th>
<th>Region 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Defect density</td>
<td>((1 1 2 0))</td>
<td>((1 1 2 0))</td>
<td>((1 1 2 0))</td>
<td>((1 1 2 2))</td>
<td>((0001))</td>
</tr>
<tr>
<td>((\text{cm}^{-2}))</td>
<td>(~4 \times 10^8)</td>
<td>(&gt;1 \times 10^{10})</td>
<td>((5 \times 10^7)) – (10^8)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
rule, where \( \mathbf{b} \) is the Burgers vector of dislocation, the majority of dislocations in region 1 are in contrast in dark field image with \( g=0002 \) [Fig. 3(b)], indicating that a large fraction of dislocations may be edge and mixed types. The GaN II was also characterized individually by the weak beam dark field imaging technique. It is remarkable that the dislocation density can be found to be extremely low in the dark field image taken from \( g=11 \overline{2} 0 \) and 0002 conditions, respectively, as shown in Figs. 3(c) and 3(d). It is noticed that threading dislocations from both sapphire \( r \)-plane and \( c \)-plane to the GaN II surfaces are hardly found. From the dark field image in Fig. 3(c), dislocation bending toward the \( [11 \overline{2} 0] \) direction can be observed, as indicated by the short white arrow. These bending dislocations terminate finally at the boundary between GaN I and GaN II; therefore, very few dislocations extend to terminated facets (regions 3–5) so that very few pits can be found in the SEM images [Figs. 1(c) and 1(d)].

The unique asymmetric sidewall structure leads to two distinct crystallites with different orientations grown on both sides of stripes. From TEM observations of the initial growth stage (5 min) of GaN I, as shown in Fig. 3(e), it is noticeable that the GaN nuclei with smaller sizes were grown in region 1 where sapphire surfaces have various degrees of tilted angles toward the sapphire \([1 \overline{1} 0 1]\) direction. Therefore, the off-angle surface might result in the difference between the GaN growth rates of the two regions. Hence, the growth of GaN would originate from the top face of the mesa (region 2), and then the growth front would laterally extend to region 1, due to faster growth rate along the \([0001]\) direction. Thus, the lateral growth mechanism for ELOG and PE growth methods may be applied for the GaN I growth of reduced defect region (region 1). On the other hand, the growth directions of GaN II are likely constrained by GaN I and sapphire substrate. The competing growth mode of the two crystallites (GaN I and GaN II) can be evidenced by the zigzag interface, as shown in Fig. 3(c). The growth directions of GaN II are toward parallel and perpendicular to the inclined (0001) face of sapphire mesa. In addition, the inclined (0001) face with a finite area might lead to a special stress gradient field that induces the dislocation bending just above the inclined side face of the mesa.

In conclusion, a low dislocation density \((\sim 10^7 \text{ cm}^{-2})\) in GaN grown on stripe patterned \( r \)-plane sapphire can be achieved through epitaxial growth on inclined step facets without regrowth process. Thus, the development of the appropriate mesa structure and growth condition, in particular, growth rate ratio of (0001) face to \([11 \overline{2} 0]\) face is critical for obtaining epitaxial nonpolar GaN of low dislocation density with an applicable size. Clearly, understanding the mechanism for dislocation reduction may open a new window for growing high-quality nonpolar crystals of wurtzite structure (GaN, AlN, ZnO, etc.) in epitaxy.

This work was supported by the MOE ATU program and in part by the National Science Council of the Republic of China (R.O.C.) in Taiwan under Contract Nos. NSC 95-2120-M-009-008, NSC 95-2752-E-009-007-PAE, and NSC 95-2218-E-214-003.


