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High-quality nonpolar 4H-AlN grown on 4H-SiC (11̅20) substrate by molecular-beam epitaxy

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Growth of very high-quality nonpolar (11̅20) α-plane face 4H-AlN on 4H-SiC (11̅20) substrate was investigated. Nonpolar 4H-AlN (11̅20) was isopolytically grown on 4H-SiC (11̅20) substrate by molecular-beam epitaxy. A reduction of defects such as stacking faults and threading dislocations was achieved by keeping the growing surface flat. To this end, the SiC substrate was HCl gas etched and the V/III ratio was optimized for AlN growth. A full width at half maximum of symmetrical x-ray diffraction ω scan of the 4H-AlN layer was 40 arc sec. Transmission electron microscopy revealed the stacking fault density to be $2 \times 10^5 \text{cm}^{-1}$, and the partial and perfect threading dislocation densities to be $7 \times 10^7$ and $1 \times 10^7 \text{cm}^{-2}$, respectively. © 2006 American Institute of Physics. [DOI: 10.1063/1.2352713]

Group-III nitride semiconductors such as gallium nitride (GaN) and aluminum nitride (AlN) with nonpolar growth direction, [11̅20] or [1̅100], have attracted much attention owing to their potential applications in high-efficiency light-emitting devices.1 Various substrates for growth of nonpolar III-N have been investigated. Naturally, a III-N (1120) or (1100) substrate would be the best option.2 However, obtaining large-size nonpolar wafers is rather difficult because of the plateletlike growth habit in bulk growth of III-N. Currently, sapphire (11̅20) r-plane, on which GaN (11̅20) is grown,3,4 is widely used owing to its availability (3 in. diameter is commercially available) as well as its thermal stability in the nitride growth environment. Various groups have reported the growth of nonpolar GaN on sapphire (11̅20) by molecular-beam epitaxy (MBE),5 metal-organic chemical vapor deposition (MOCVD),6 and hydride vapor phase epitaxy.1 However, due to the large mismatch wurtzite (11̅20) on corundum (11̅20) between nonpolar III-N and sapphire (11̅20), the quality of GaN grown on sapphire (11̅20) is inferior to that grown on sapphire (0001). For example, a stacking fault (SF) density of $4 \times 10^3 \text{cm}^{-1}$ and a threading dislocation (TD) density of $3 \times 10^{10} \text{cm}^{-2}$ were reported for MOCVD-grown GaN on sapphire (11̅20).5

To improve the crystallinity, the epitaxial lateral-overgrowth technique was developed for nonpolar GaN. Haskell et al. reported a SF density of $3 \times 10^8 \text{cm}^{-1}$ and a TD density of $5 \times 10^6 \text{cm}^{-2}$ for the wing region.8,9

We focused on SiC (11̅20) and (1̅100) substrates for nonpolar AlN growth because of the following reasons. (1) Layer-by-layer growth of AlN in the initial stage is possible on SiC (0001), indicating good wetting of AlN on SiC.8,9 (2) The lattice mismatch between AlN and SiC is much smaller than that between AlN and sapphire (11̅20). (3) Crystalline structure of SiC, 4H or 6H, resembles wurtzite more than it resembles sapphire (11̅20). To the author’s knowledge, the first growth of nonpolar AlN on nonpolar SiC was performed by MBE by Stemmer et al.11 They confirmed the epitaxial growth of 2H-AlN (11̅00) on 6H-SiC (11̅10). However, they did not report the crystal quality of AlN. We attempted to grow AlN on 6H-SiC (11̅20) and confirmed growth of 2H-AlN (11̅20).12 We investigated the quality of the AlN layer. Full width at half maximum (FWHM) of the x-ray diffraction (XRD) ω scan was 240–3000 arc sec, which is comparable to that of GaN/sapphire (11̅20). We also attempted to grow AlN on 4H-SiC (11̅20). The AlN layer grown in this case exhibited far superior crystalline quality; its FWHM was 90 arc sec. Furthermore, reflection high-energy electron diffraction (RHEED) revealed that the AlN layer did not have the 2H structure, but rather the 4H structure, i.e., the same structure as the SiC substrate. The crystalline structure of the substrate was replicated in the grown layer. We speculate that the formation of the isopolytic mismatch (no mismatch in crystalline structure between the AlN layer grown and the SiC substrate) may have resulted in such a high-quality AlN. Although XRD showed a very small FWHM value, high-resolution transmission electron microscopy (HRTEM) revealed that the 4H-AlN layer grown contained high-density SFs ($5 \times 10^6 \text{cm}^{-1}$) and TDs ($4 \times 10^{10} \text{cm}^{-2}$). Further reduction of SFs and TDs is necessary to use the 4H-AlN for device applications.

In the present study, we report growth of superior crystal quality 4H-AlN on 4H-SiC (11̅20). We have identified two critical factors that significantly improve the quality of 4H-AlN layers. The one is to prepare an atomically flat and damage-free 4H-SiC substrate surface, and the other is careful optimization of the V/III ratio. Since AlN tends to have the 2H structure, lateral growth along the [0001] direction may result in 2H inclusion, i.e., stacking faults. A very flat initial surface and optimized V/III ratio (slightly Al-rich conditions) ensure a very smooth grown surface, which prevents lateral growth and thereby leads to high phase purity.

The substrates used in this study were commercially available 4H-SiC (11̅20) wafers. Since the polishing process...
for 4H-SiC (11̅20) has not yet been established, many polishing scratches are observed on the wafer surface as shown in Fig. 1(a). The substrates were etched by a HCl–H₂ gas mixture at high temperature to remove the scratches. The etching conditions established for 6H-SiC (0001) substrates were used: temperature of 1300°C, H₂ including 0.3% HCl, etching time of 10 min. After gas etching, a very smooth SiC surface was obtained. Several line depressions were observed, whose density is approximately 5 × 10⁶ cm⁻¹ and could be dramatically reduced in the present study. Since the SF density almost agrees with the density of line depressions observed in the AFM image, the line depression may be a growth defect originating from a SF.

To evaluate the TD density, plan-view TEM observation was carried out. Figure 3(a) and 3(b) show the bright field images of a 4H-AlN epilayer with g = 11̅00 and g = 0004, respectively. The TD density was measured on the basis of which the SF density was estimated to be 2 × 10⁵ cm⁻¹. For reference, the image of 4H-AlN previously reported is shown in Fig. 2(b), where two bundles of SFs are observed. The SF density is approximately 5 × 10⁶ cm⁻¹ and could be dramatically reduced in the present study. Since the SF density almost agrees with the density of line depressions observed in the AFM image, the line depression may be a growth defect originating from a SF.
respectively. Dark lines running along [1100] correspond to stacking faults in the TEM image under the $g = 1100$ diffraction condition [Fig. 3(a)]. Since a partial TD exists at the end of the SF,\textsuperscript{15} the density of partial TDs having Burgers vectors $b = \frac{1}{2}(1100)$ is estimated at about $7 \times 10^7$ cm$^{-2}$ by examining a wider area of 22 $\mu$m$^2$. A perfect TD was observed in the TEM image under the $g = 0004$ diffraction condition [Fig. 3(b)]. Two perfect TDs were found in an area of 22 $\mu$m$^2$, indicating that the density of TDs having [0001] component is about $1 \times 10^7$ cm$^{-2}$. These TD densities are extremely small for heteroepitaxial AlN on any substrates. XRD shows a very sharp diffraction peak as mentioned above, supporting this result.

Table II shows the in-plane and out-of-plane (growth-direction) lattice constants of AlN epilayer and SiC substrate measured by XRD. The in-plane lattice constants of AlN are equal to those of SiC (to within an error of 0.1%), indicating that the AlN layer grows on the SiC substrate almost pseudomorphically. Pseudomorphic growth may contribute such a low dislocation density.

In conclusion, we have performed the growth of high crystal quality AlN on 4H-SiC (1120) substrates by using an atomically flat SiC surface and optimized V/III ratio. The AlN grown was found to be high-phase purity 4H-AlN. Symmetric and asymmetric XRD $\omega$ scans showed very sharp peaks with FWHM of less than 100 arc sec. Density of the basal plane SFs was estimated to be $2 \times 10^5$ cm$^{-2}$, and densities of partial and perfect TDs to be $7 \times 10^7$ and $1 \times 10^7$ cm$^{-2}$, respectively. The SF and TD densities of 4H-AlN were reduced by two orders of magnitude, compared to that of the 4H-AlN previously reported. High-quality 4H-AlN grown on 4H-SiC (1120) is a very promising template for future deep-UV high-Al-composition AlGaN optical devices.

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TABLE II. Lattice constants of AlN epilayer and SiC substrate measured by XRD.

<table>
<thead>
<tr>
<th></th>
<th>AlN (Å)</th>
<th>SiC (Å)</th>
<th>Difference (%)</th>
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</thead>
<tbody>
<tr>
<td>$d_{(0001)}$</td>
<td>10.032</td>
<td>10.042</td>
<td>−0.10</td>
</tr>
<tr>
<td>$(2/\sqrt{3})a_{(1100)}$</td>
<td>3.079</td>
<td>3.082</td>
<td>−0.10</td>
</tr>
<tr>
<td>$2d_{(1120)}$</td>
<td>3.105</td>
<td>3.081</td>
<td>+0.78</td>
</tr>
</tbody>
</table>


\textsuperscript{5}H. M. Ng, Appl. Phys. Lett. \textbf{80}, 4369 (2002).


