AlGaN deep ultraviolet LEDs on bulk AlN substrates

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We report the growth of sub-300 nm ultraviolet light emitting diodes (UV LEDs) on bulk AlN substrates. Heteroepitaxial evolution study through interrupted growth experiments revealed that Al$_x$Ga$_{1-x}$N ($x > 0.5$) epilayers can be grown pseudomorphically with well-defined step-flow growth mode below a certain critical thickness. The build-up of compressive strain energy eventually induces a morphological roughening followed by the admission of misfit dislocations. LEDs grown on bulk AlN substrates exhibit noticeable improvement over those on sapphire in device impedance, efficiency and thermal characteristics under high-level injection, pointing to a promising substrate platform for high performance III-nitride ultraviolet optoelectronics.

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1 Introduction

Most of AlGaN-based deep ultraviolet ($\lambda < 300$ nm) light emitting diodes (UV LEDs) [1–4] are grown on mismatched sapphire substrates which severely limits the device performance due to a high density of dislocations ($10^9$–$10^{10}$ cm$^{-2}$) [4, 5]. Bulk AlN substrates have attracted much attention because of its close matching to AlGaN in lattice parameters and thermal expansion coefficients, in addition to a much higher thermal conductivity. Proof-of-concept demonstrations of III-nitride devices on AlN substrates have been reported [6, 7] though little is known about the heteroepitaxial process. In this paper, heteroepitaxial growth of AlGaN on bulk AlN is examined. A combination of structural and morphological studies indicates the compressive strain (~1.2% between AlN and Al$_{0.5}$Ga$_{0.5}$N) is not relaxed effectively by plastic dislocating due to a much lower density of dislocations in bulk AlN, resulting in elastic roughening that resembles previous reports in SiGe/Si and InGaAs/GaAs systems [8]. Good device performance for deep UV LED on AlN is reported including light output, device impedance and thermal characteristics under high-level injection, suggesting that AlN offers a promising new route to high performance UV optoelectronics.

2 Experiment details

The material growth was carried out by metalorganic chemical vapor deposition (MOCVD) in a horizontal-flow reactor (Aixtron 200/4 HT-S) using trimethylgallium (TMGa), trimethylaluminum (TMAI) and ammonia (NH$_3$). Silane and Meth-Cp$_2$Mg were used as n- and p-type dopants. Hydrogen (H$_2$) is the carrier gas throughout this study. Nominally c-plane AlN substrates ($\pm 0.5^\circ$) were solvent degreased followed by wet etching in HF before loading into the growth chamber. Prior to the homoepitaxial growth of AlN at 1150°C, the AlN substrates were annealed in-situ under a mixture of NH$_3$ and H$_2$ [3]. Three superlattices (SL 1, 2 and 3) with an average composition of 0.90,
0.73, and 0.57 were inserted between AlN and Al$_{0.50}$Ga$_{0.50}$N electron transport layer to study the strain evolution. Each superlattice includes 10 periods of alternating Al$_x$Ga$_{1-x}$N layers of 15 nm thick and paired compositions of $x = 1.0/0.8$, 0.8/0.65, and 0.65/0.50. Growth temperature of all the superlattices and Al$_{0.50}$Ga$_{0.50}$N layer was 1070°C. Deep UV AlGaN diodes with multiple-quantum wells (MQWs) active region [3] were grown on top of 1 µm n-type Al$_{0.50}$Ga$_{0.50}$N layer ([Si] $\sim$ 2×10$^{19}$ cm$^{-3}$). The Mg concentration on the p-side is maintained at a level of around 3×10$^{19}$ cm$^{-3}$ to ensure optimum conductivity before the generation of structural defects including inversion domain boundaries [9]. To characterize the surface morphology, atomic force microscopy (AFM) was conducted using a Digital Instruments Nanoprobe III model with tapping mode. The Al composition and structural quality of AlGaN were determined by X-ray diffraction (XRD, Bede D-1 diffractometer) using both symmetric and skewed symmetric scans. After the epitaxial material deposition, cylindrical mesa-etched LED devices with optical apertures of 100 µm and 50 µm diameters were fabricated and light was extracted with similar procedure to previous report [3]. None of these devices has any additional heat sinking or light extraction enhancement schemes applied.

3 Results and discussion  
AFM images after homoepitaxy of 0.3 µm AlN (not shown here) indicate an overall smooth background with parallel and straight atomic steps, suggesting a low density of screw- and mixed type dislocations. High-resolution X-ray diffraction is employed to examine microstructural quality. The 0.3-µm AlN homoepitaxy on AlN substrates typically exhibit a (0002) rocking curve linewidth around 0.01° (Fig. 1, dash-dotted line). Unlike previous reports [4] of MOCVD-grown AlN epilayers on sapphire, where a narrow symmetric scan is always accompanied by extremely wide asymmetric scans due to a high in-plane mosaicity, the (101$^2$) diffraction rocking curves yield values typically between 0.02° and 0.04° (Fig. 1, solid line). After AlN homoepitaxy, interrupted growth studies on compositionally graded AlGaN superlattices were carried out to reconstruct the hetero-nucleation process ex-situ. Dot-like surface undulation (0.1–0.2 µm in diameter, Figs. 2a and 2d) appears after the first superlattice (AlN/Al$_{0.80}$Ga$_{0.20}$N x10) deposition. At the end of the second superlattice (Al$_{0.80}$Ga$_{0.20}$N/Al$_{0.65}$Ga$_{0.35}$N x10), the surface remains atomically smooth (Fig. 2b). The appearance of straight atomic steps of one monolayer height (~2.5 Å) indicates a very low density of dislocations with a

![Fig. 1](image1.png)  
Fig. 1 (0002) and (101$^2$) rocking curves of 0.3 µm AlN homoepitaxy on bulk AlN. The shoulders on both sides of main peak are related to misorientation of AlN substrate.

![Fig. 2](image2.png)  
Fig. 2 AFM images of high-Al content AlGaN superlattices on bulk AlN. The scan area is 10 µm × 10 µm for (a), (b) and (c), and 1 µm × 1 µm for (d), (e) and (f). (a) and (d) are SL 1; (b) and (e) are SL 2 and 1; (c) and (f) are SL 3, 2 and 1. AFM rms values and z scales (in brackets) are labelled.

screw component; the alternating saw-tooth feature (Fig. 2e) is related to difference in growth rate due to the atomic arrangement along [1100] and [0110] directions [10]. During the growth of the third superlat-
tice (Al\(_{0.65}\)Ga\(_{0.35}\)N/Al\(_{0.50}\)Ga\(_{0.50}\)N \times 10), surface morphology underwent a substantial change with the appearance of large (2-5 \(\mu\)m) plateaus or platelets separated by deep trenches or cliff-like edges with a height of 100 nm (Fig. 2c) and curved atomic steps (Fig. 2f). The deterioration of morphology at this stage is also correlated with decay in the intensity of specular optical reflectance recorded \textit{in situ}, suggesting that surface roughening on the scale of optical wavelength has occurred.

In a moderately mismatched (1–2\%) system, strain relaxation normally proceeds through a combination of elastic, morphological roughening and plastic, misfit dislocating \[8\]. For AlGaN grown on sapphire, the compressive strain is effectively relaxed through the inclination of pre-existing dislocations (mid \(10^5–10^6\) cm\(^{-2}\)) \[5\]. However, for AlGaN grown on bulk AlN, the compressive strain cannot be relaxed effectively by the same mechanism as AlGaN on sapphire due to a very low density of dislocations. Figure 3 shows the relations between surface morphology roughness, structural quality and strain relaxation \[11\] of 1-\(\mu\)m Al\(_{0.50}\)Ga\(_{0.50}\)N on AlN characterized by AFM and X-ray diffractions. An inverse relation between surface roughness (triangles) and degree of relaxation is demonstrated; Meanwhile, linewidths of (101\(_2\)) rocking curves (open squares) increase with the strain relaxation while the linewidths of (0002) rocking curves (solid squares) remains essentially constant. This result suggests that elastic roughening provides the initial route of relaxation followed by local admission of misfit dislocations due to stress concentration. The driving force for surface roughing is mitigated after plastic strain relaxation, and surface smoothness improves subsequently, resembling the observation in high Ge-content SiGe/Si system \[8\]. The different trends between linewidths of (0002) and (101\(_2\)) scans indicate the misfit dislocations generated are almost edge-type dislocations. Understanding and control of the compressive strain relaxation during AlGaN/AlN heteroepitaxy for device applications are currently in progress. For 1-\(\mu\)m Al\(_{0.50}\)Ga\(_{0.50}\)N on AlN, X-ray rocking curves as narrow as 122\(^\circ\) and 173\(^\circ\) have been observed along (0002) and (101\(_2\)) diffractions, respectively when the epilayer is fractionally relaxed, demonstrating a much improved structural quality than AlGaN with similar Al-content on sapphire \[1\].

![Fig. 3 Relations between surface roughness (triangles), linewidths of (0002) (solid squares), (101\(_2\)) (open squares) rocking curves and degree of relaxation of 1-\(\mu\)m Al\(_{0.50}\)Ga\(_{0.50}\)N on AlN](image)

![Fig. 4 L-I-V characteristics of deep UV LEDs with 50 \(\mu\)m diameter on sapphire (dashed line) and AlN (solid line). Inset is EL spectra with different currents (from 40 mA to 65 mA, 100 \(\mu\)m diameter).](image)
0.14%, approximately 4-5 times larger than the maximum power from an identical device on sapphire (in order to reduce the absorption from AlN substrates, backside output powers reported here were measured with the AlN substrates lapped to 150 µm after device processing). A series of electroluminescence (EL) spectra at increasing current injections (inset) for a 100 µm diameter device, illustrate a peak emission wavelength of 300 nm and a relatively small long-wavelength contribution. Furthermore, the light output power shows no thermal rollover. This is attributed to a ten-fold increase in thermal conductivity of AlN (~ 3.2 W/cm K [6]) over sapphire. While the absolute performance of UV LEDs on AlN at present is still below the state-of-the-art devices on sapphire [1] due to less-than-optimum junction and quantum well designs, the comparative study reported in this work for LEDs on different substrates indeed highlight the importance of dislocation reduction and point to the potentiality of native (AlN) substrates in UV optoelectronics.

4 Conclusions In summary, on bulk AlN substrates, AlN and Al$_x$Ga$_{1-x}$N (x > 0.5) with much improved structural quality, as well as good performance of AlGaN deep UV LEDs including efficiency, electrical and thermal characteristics, are achieved, indicating low dislocation density bulk AlN substrate is promising in supporting closely-matched epitaxy of AlGaN alloys for ultraviolet optoelectronics, although the evolution study suggests that the relaxation of compressive strain between AlGaN and AlN by surface islanding emerges as a dominant source of surface roughness and structural imperfection.

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