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## Dislocation and morphology control during molecular-beam epitaxy of AlGaIn/GaN heterostructures directly on sapphire substrates

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We report on the growth and transport characteristics of high-density ( $\sim 10^{13} \text{ cm}^{-2}$ ) two-dimensional electron gases confined at the AlGaIn/GaN interface grown by plasma-assisted molecular-beam epitaxy on sapphire substrates. For structures consisting of a 25 nm  $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}$  barrier deposited on a 2  $\mu\text{m}$  insulating GaN buffer, room-temperature mobilities averaging  $1400 \text{ cm}^2/\text{V s}$  at a sheet charge density of  $1.0 \times 10^{13} \text{ cm}^{-2}$  are consistently achieved. Central to our approach is a sequence of two Ga/N ratios during the growth of the insulating GaN buffer layer. The two-step buffer layer allows us to simultaneously optimize the reduction of threading dislocations and surface morphology. Our measured sheet resistivities as low as  $350 \Omega/\square$  compare favorably with those achieved on sapphire or SiC by any growth method. Representative current-voltage characteristics of high-electron-mobility transistors fabricated from this material are presented. © 2002 American Institute of Physics. [DOI: 10.1063/1.1498867]

Molecular beam epitaxy (MBE) has proven to be a powerful technique for the growth of high mobility AlGaIn/GaN heterostructures on thick GaN templates. The combination of low impurity incorporation and sharp interface control inherent to the MBE process has been crucial to the ongoing efforts to improve the maximum low temperature mobility.<sup>1-5</sup> Despite the success of MBE growth on thick GaN templates, the direct growth of GaN films on sapphire substrates via plasma-assisted MBE has remained difficult. Only a few reports have indicated that high quality 2DEGs can be produced by plasma MBE growth directly on sapphire.<sup>6,7</sup> The difficulty can be traced to the simultaneous requirement of achieving a low threading dislocation density in the GaN buffer and smooth AlGaIn/GaN heterointerfaces, both of which are necessary for low density 2DEGs with very high mobility. On the other hand, for high carrier density ( $\sim 10^{13} \text{ cm}^{-2}$ )  $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{GaN}$  heterostructures fabricated into transistors operating at room temperature, the low temperature mobility is not the most important metric of film quality. Rather, the room temperature sheet conductivity, which is proportional to the product of mobility and carrier density, is the more important material parameter for high power operation. Recently, advances have been made in the growth of AlGaIn/GaN heterostructures via MBE on semi-insulating SiC substrates.<sup>8</sup> However, sapphire remains the most economical insulating substrate upon which growth processes and device fabrication techniques can be developed before they are transferred to more costly substrates. For these reasons, understanding the growth mechanisms that lead to high quality AlGaIn/GaN heterostructures on sapphire remains an important topic for the MBE community.

In this study, we report on the MBE growth of high quality  $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{GaN}$  heterostructures by plasma-

assisted MBE directly on sapphire [0001] substrates. For structures consisting of a 25 nm  $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}$  barrier deposited on a 2  $\mu\text{m}$  insulating GaN buffer, room temperature mobilities averaging  $1400 \text{ cm}^2/\text{V s}$  at a sheet charge density of  $\sim 1.0 \times 10^{13} \text{ cm}^{-2}$  are consistently achieved. Our results indicate that the growth of high quality GaN buffer layers is governed by the careful balance of two competing processes—threading defect reduction during the early stages of growth and maintenance of smooth surface morphology at the heterointerface.

In order to accommodate the  $\sim 13\%$  lattice mismatch between GaN and sapphire and to ensure Ga-face polarity, a thin AlN nucleation layer is first deposited. In our studies, the efficacy of the AlN nucleation layer is most sensitive to the Al/N ratio during deposition. Our best films utilize a nucleation layer with an Al/N ratio greater than unity. Such an aluminum rich nucleation layer is characterized in reflection high-energy electron diffraction (RHEED) by a dim and streaky  $1 \times 1$  pattern indicating an ad layer of metal on the growing surface. Given the low surface mobility of active nitrogen at the growth front, we speculate that the excess Al enhances the surface mobility of nitrogen, which promotes the formation of larger grains. AlN nucleation layers grown under less metal rich conditions are characterized by very bright and spotty RHEED patterns. Mobilities of the 2DEGs are always limited to less than  $1000 \text{ cm}^2/\text{V s}$  without the use of an Al rich nucleation layer. Furthermore, the quality of the nucleation layer does not appear to be very sensitive to the substrate temperature over the range of  $680\text{--}840^\circ\text{C}$ . We have grown samples with high room temperature mobilities ( $\sim 1200 \text{ cm}^2/\text{V s}$ ) over this entire temperature range. We use  $745^\circ\text{C}$ , as it is most convenient since the complete epilayer can be grown at a single substrate temperature. We also varied the nucleation layer thickness from 15 to 60 nm and have found only a minor influence on the quality of the resulting epitaxy, as measured by room temperature mobility. Rela-

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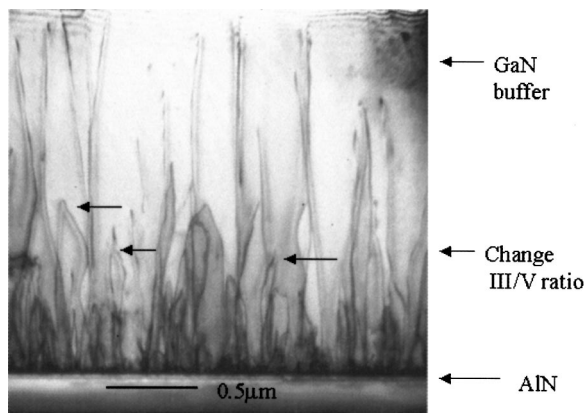


FIG. 1. Bright field cross-sectional TEM image of the GaN buffer region. Several of the dislocation reducing interactions are pointed to by the arrows.

tively small,  $\sim 10\%$ , variations are found. Our typical nucleation layer is 20 nm.

Following the AlN nucleation layer, a 2  $\mu\text{m}$  thick insulating GaN buffer is grown. The entire structure is grown at a substrate temperature of 745  $^\circ\text{C}$ , and the growth rate is 0.5  $\mu\text{m}/\text{h}$ . In our experience the electrical properties of the 2DEG depend most critically upon growth conditions of this buffer region. The growth of the buffer layer is actually divided into two stages in which considerably different fluxes of gallium are used. The first 750 nm of the GaN buffer is growth under slightly *nitrogen stable* conditions. We define the transition from nitrogen stable to Ga stable growth as the point where a rough-to-smooth transition is observed in RHEED. During this stage of growth the RHEED pattern is bright and slightly spotty, and a weak chevron pattern is visible when the substrate is rotated away from the  $[11\bar{2}0]$  or the  $[1\bar{1}00]$  azimuths. The observed RHEED pattern is indicative of three-dimensional (3D) growth and a somewhat

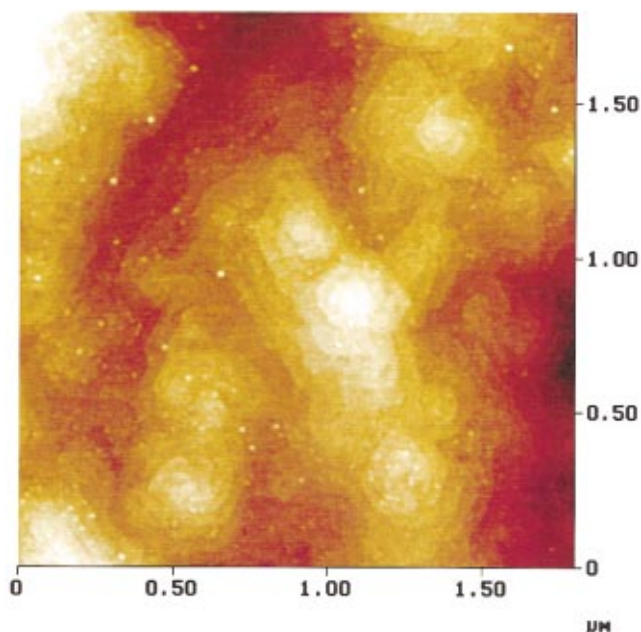


FIG. 2. (Color) AFM image of the surface of an  $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{GaN}$  heterostructure. The surface displays the spiral hillocks characteristic of MBE growth and monolayer steps are clearly visible. The density of spiral hillocks is  $\sim 5 \times 10^8 \text{ cm}^{-2}$ . The full height range of this image is 7 nm and the root mean square roughness is 1 nm.

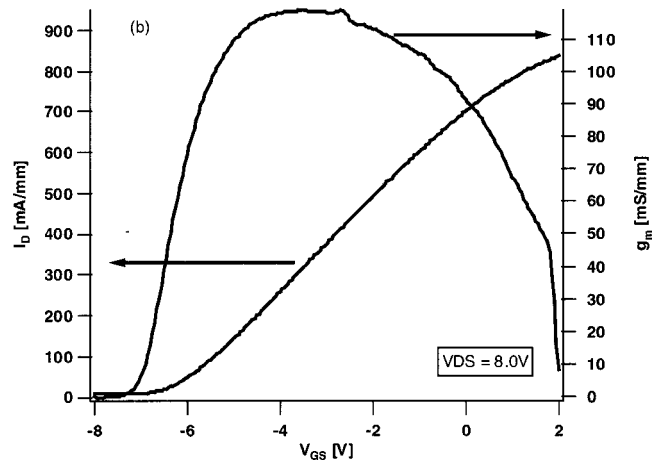
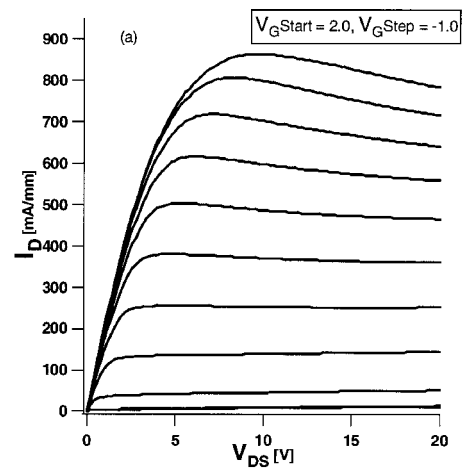


FIG. 3. (a) dc current–voltage characteristics of a typical device processed from run No. 4. The unprocessed wafer displayed a mobility of  $1430 \text{ cm}^2/\text{Vs}$  at a carrier density of  $1.1 \times 10^{13} \text{ cm}^{-2}$ . The sheet resistance of the processed material was  $405 \Omega/\square$ . The maximum drain current is 880 mA/mm at a gate bias of +2 V. (b) Transconductance and drain current as a function of gate voltage at  $V_{sd}=8 \text{ V}$ . The maximum measured transconductance is 120 mS/mm.

roughened surface morphology. In accord with the findings of Lee *et al.*<sup>9</sup> for MBE growth of GaN on SiC substrates, we find that a roughened surface morphology during growth aids the reduction of threading dislocations. The 3D growth mode appears to increase dislocation interactions, and thus, reduces the number of dislocations which propagate to the surface. This claim is supported by the bright field cross-sectional TEM image taken with  $g=[0002]$  on a typical sample displayed in Fig. 1. In this image significant bending of threading dislocations is observed throughout the first 750–1000 nm of growth. Many of these dislocations intersect other dislocations where they can annihilate if the dislocations have Burgers vectors with opposite sign. The arrows in Fig. 1 indicate a few of the closed dislocation loops seen in this film. The dislocation loops seen in the first phase of growth are consistent with the coalescence of 3D islands. These results indicate that plasma MBE growth on sapphire substrates under slightly nitrogen stable conditions promotes defect annihilation.

While growth under nitrogen stable conditions appears to enhance threading dislocation interactions, the roughened surface morphology produced by continued growth under these conditions is not optimal for device structures.<sup>9</sup> Smooth AlGaIn/GaN interfaces are needed to reduce interface rough-

TABLE I. Measured room temperature carrier density, mobility, and sheet resistance of eight consecutive MBE growths on sapphire. The average mobility of the eight runs is  $1410 \text{ cm}^2/\text{V s}$ . The average sheet resistance is  $438 \Omega/\square$ .

Sample No.	2DEG density ( $\text{cm}^{-2}$ )	Mobility ( $\text{cm}^2/\text{V s}$ )	Sheet resistance ( $\Omega/\square$ )
1	$9.0 \times 10^{12}$	1340	518
2	$1.0 \times 10^{13}$	1310	456
3	$9.5 \times 10^{12}$	1320	474
4	$1.1 \times 10^{13}$	1430	405
5	$9.0 \times 10^{12}$	1420	490
6	$9.5 \times 10^{12}$	1480	444
7	$1.1 \times 10^{13}$	1535	363
8	$1.2 \times 10^{13}$	1450	352

ness scattering of the 2DEG and to facilitate processing into high electron mobility transistors (HEMTs). Therefore in the second phase of growth of the insulating GaN buffer, the Ga flux is increased to produce metal stable growth. After a few hundred nanometers of Ga-stable growth the RHEED undergoes a rough/streaky transition. The primary reflections become truncated and the entire pattern becomes dimmer. No chevron pattern is observed upon substrate rotation. The remainder of the epilayer is grown under these Ga-stable conditions. The Ga flux is limited such that no metal droplets are observed on the surface. It is important to note that the Ga flux is increased by over 40% from the value used during nitrogen stable growth. Concomitant with the observed changes in the RHEED pattern, at a distance of  $\sim 1 \mu\text{m}$  from the sapphire interface, a fairly abrupt change is observed in the defect structure seen in Fig. 1. From this point, many dislocation loops have closed and the remaining threading defects are seen to propagate straight up to the film surface. The rough/smooth transition appears to minimize dislocation bending. We have taken TEM images with the diffraction condition  $g=[0002]$ , exposing pure screw and mixed dislocations, and with the diffraction condition  $g=[11\bar{2}0]$ , exposing pure edge and mixed dislocations, in order to estimate the total threading dislocation density near the surface in films grown with this two-step process. The total dislocation density in such films is  $\sim 5 \times 10^9 \text{ cm}^{-2}$ .

The surface morphology of our heterostructures was studied by atomic force microscopy (AFM). Atomic steps are visible and the surface is rather flat with a rms roughness of 1 nm over a  $4 \mu\text{m}^2$  area. As seen in Fig. 2, the two-stage MBE growth produces smooth AlGaIn surfaces. In this image, we see the spiral hillocks characteristic of MBE growth around threading dislocations with a screw component. We note that this surface morphology depends critically on the GaN flux used during the growth of the second phase of the GaN buffer layer. Films with morphologies similar to that seen in Fig. 2 must be grown under Ga-stable conditions near the transition to Ga droplet formation. Films grown under slightly less Ga rich conditions, while still quite flat, do not present visible atomic steps. Our results indicate that films nucleated directly via MBE on sapphire can exhibit surface morphologies comparable to those achieved by MBE growth on thick GaN templates.<sup>1,3</sup>

Table I summarizes the room temperature electrical characteristics of eight sequential AlGaIn/GaN heterostructures grown directly on sapphire. We note that other growth stud-

ies on different substrates were interspersed within this series, so that the eight runs actually took place over one month. These results indicate the run-to-run reproducibility and the long-term stability of our process. The average mobility of the eight runs is  $1410 \text{ cm}^2/\text{V s}$ . For comparison, we have grown structures entirely under Ga stable conditions. For such conditions, the RHEED exhibits the rough/smooth transition within the first 50 nm of growth. Heterostructures grown under such conditions routinely yield poorer mobility in the range of  $800\text{--}900 \text{ cm}^2/\text{V s}$  at  $T=300 \text{ K}$ .

We fabricated transistors using contact lithography. The devices are not passivated. Figure 3(a) displays the dc current–voltage ( $I$ – $V$ ) characteristics of a field effect transistor fabricated from sample No. 4 listed in Table I. This unprocessed wafer exhibited a sheet resistance of  $405 \Omega/\square$ . This device has a gate length of  $2 \mu\text{m}$  and a periphery of  $50 \mu\text{m}$ . The source-drain spacing is  $6 \mu\text{m}$  and the source-gate separation is  $1 \mu\text{m}$ . The maximum drain current is  $880 \text{ mA/mm}$  at a gate bias of  $+2 \text{ V}$ . We note that the maximum drain current compares favorably with the best devices grown by MOCVD on sapphire substrates.<sup>7</sup> As shown in Fig. 3(b), the maximum extrinsic transconductance is  $120 \text{ mS/mm}$  at a gate bias of  $-4 \text{ V}$ . Small-signal rf testing gives an  $f_t$  of  $6 \text{ GHz}$ . Large-signal power measurements of a  $100 \mu\text{m}$  wide device at  $1.6 \text{ GHz}$  yielded an output power density of  $2.2 \text{ W/mm}$  at  $3 \text{ dB}$  gain compression in class A operation.

In conclusion, we have demonstrated the importance of precise control of gallium flux for the growth of high mobility  $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{GaN}$  heterostructures by plasma-assisted MBE directly on sapphire substrates. The use of nitrogen stable growth during the early stages of growth is shown to enhance dislocation reduction while Ga stable growth is used to maintain good interface quality at later stages of the epilayer. The room temperature sheet resistance of our material compares favorably with  $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{GaN}$  heterostructures grown by any method.

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