Effect of growth stoichiometry on the electrical activity of screw dislocations in GaN films grown by molecular-beam epitaxy

J. W. P. Hsu(a) and M. J. Manfra
Bell Laboratories, Lucent Technologies, Murray Hill, New Jersey 07974

S. N. G. Chu
Agere Systems, Murray Hill, New Jersey 07974

C. H. Chen and L. N. Pfeiffer
Bell Laboratories, Lucent Technologies, Murray Hill, New Jersey 07974

R. J. Molnar
Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, Massachusetts 02420-9108

(Received 27 February 2001; accepted for publication 25 April 2001)

The impact of the Ga/N ratio on the structure and electrical activity of threading dislocations in GaN films grown by molecular-beam epitaxy is reported. Electrical measurements performed on samples grown under Ga-rich conditions show three orders of magnitude higher reverse bias leakage compared with those grown under Ga-lean conditions. Transmission electron microscopy (TEM) studies reveal excess Ga at the surface termination of pure screw dislocations accompanied by a change in the screw dislocation core structure in Ga-rich films. The correlation of transport and TEM results indicates that dislocation electrical activity depends sensitively on dislocation type and growth stoichiometry. © 2001 American Institute of Physics. [DOI: 10.1063/1.1379789]

During the past year, the quality of AlGaN/GaN heterostructures has improved dramatically. AlGaN/GaN heterostructures grown on GaN templates by molecular-beam epitaxy (MBE) have been shown to display extremely high mobilities.1–3 The low temperature mobility of the two-dimensional electron gas (2DEG) confined at the AlGaN/GaN interface has reached 75 000 cm2/V·s,4 limited by charged dislocation scattering.1,5 These advances can be attributed to the reduction of dislocation density in the GaN templates, and the low background impurity incorporation and superior interface control inherent to the MBE growth. Despite the improvement in low-temperature 2DEG mobility, excess reverse bias leakage is a still a major impediment for commercialization of III-nitride electronic devices. For films grown by MBE, growth stoichiometry has a pronounced impact on the surface morphology and the electrical activity of defects.8,9 Ga-rich films are smooth with monolayer steps and dislocations appear as hillocks. Ga-lean films display a pitted morphology. The smooth morphology of the Ga-rich growth is known to enhance 2DEG mobility. On the other hand, Schottky diode measurements show that reverse bias leakage at a fixed bias is 2–3 orders of magnitude larger for Ga-rich samples than for Ga-lean samples.10 In this work, we elucidate the origin of excess reverse bias leakage in MBE grown films and illustrate the impact of growth stoichiometry on dislocation electrical activity.

The GaN films were grown by nitrogen plasma assisted MBE on GaN templates prepared by hydride vapor phase epitaxy (HVPE). The HVPE templates were nominally 15 μm thick. The MBE growth temperature was 750 °C and growth rate was 0.25 μm/h. The Ga-rich growth conditions refer to having visible Ga droplets on the surface. Figure 1 shows cross-sectional transmission electron microscopy (TEM) images of a sample grown under Ga-rich conditions. (No surface cleaning was done prior to making the cross sectional TEM specimen, i.e., the excess surface Ga was not removed.) The MBE/HVPE interface is invisible, indicating good control of our MBE growth. Since no new dislocations were generated in the MBE layer, the dislocation density and type are determined by the HVPE template. The total dislocation density in these samples varies between $5 \times 10^8$ and $10^9 \text{ cm}^{-2}$, with the majority being screw and mixed types. Capacitance–voltage measurements show a background net donor concentration below $10^{15} \text{ cm}^{-3}$ in the MBE GaN layer.

Scanning current–voltage microscopy (SIVM) was employed to map the spatial distribution of reverse bias current. For these measurements, the excess surface Ga was removed with concentrated HCl. In the SIVM experiment, a voltage bias is applied between the tip and sample while current that flows through the conducting tip is detected using a current preamplifier. The tip acts as a microscopic Schottky contact to the GaN sample.11 All data were taken using a boron-doped conducting diamond tip, and the experiment was performed in air at room temperature. Figure 2(a) shows a topographic image of a MBE GaN films grown under Ga-rich conditions. The spiral hillocks correspond to the presence of pure screw or mixed dislocations. Figure 2(b) shows the SIVM image taken simultaneously with Fig. 2(a) under $-6 \text{ V}$ reverse bias. The reverse current is defined with a negative sign; thus, current is nonzero in dark regions of Fig. 2(b). Evidently, the reverse bias current flow concentrates on small isolated regions. The locations of most leakage spots correspond to spiral hillocks, suggesting that the leakage occur at screw/mixed dislocations. Further confirmation comes from the similar density between the leakage spots and screw/mixed dislocation density determined by TEM.

(a)Electronic mail: jhsu@lucent.com
The SIVM results indicate that screw/mixed dislocations contribute significantly more to gate leakage than pure edge dislocations. Previously, screw/mixed dislocations were reported to be more effective recombination centers and have reduced barrier heights compared to pure edge dislocations in GaN. One interesting question is why screw/mixed dislocations are more electrically active than pure edge dislocations. The structure of threading edge dislocations in GaN have been studied extensively theoretically and confirmed experimentally by high-resolution TEM images. Deep acceptors, hence electron traps for $n$-type materials, are predicted to accompany these edge dislocations. On the other hand, comparably little is known about threading screw dislocations. Theoretically, Elsner et al. found an open core structure that is energetically more favorable. Experimentally, both full core and open core structures have been reported for threading screw dislocations. Furthermore, the calculation showed no deep levels associated with this core structure. This is inconsistent with experimental results showing screw/mixed dislocations are more electrically active than pure edge dislocations.

Close examination of our TEM images reveals nanometer size particles at the surface termination of pure screw dislocations [arrows in Fig. 1 and 2 to show extra materials at the surface termination of a screw dislocation. EDS spectra taken on the TEM specimen with the beam focused on a small particle at the surface termination of screw dislocations. The dark spots in (b) are conducting regions. The arrows in the two images correspond to the same positions.](Fig. 1)

The SIVM results indicate that screw/mixed dislocations contribute significantly more to gate leakage than pure edge dislocations. Previously, screw/mixed dislocations were reported to be more effective recombination centers and have reduced barrier heights compared to pure edge dislocations in GaN. One interesting question is why screw/mixed dislocations are more electrically active than pure edge dislocations. The structure of threading edge dislocations in GaN have been studied extensively theoretically and confirmed experimentally by high-resolution TEM images. Deep acceptors, hence electron traps for $n$-type materials, are predicted to accompany these edge dislocations. On the other hand, comparably little is known about threading screw dislocations. Theoretically, Elsner et al. found an open core structure that is energetically more favorable. Experimentally, both full core and open core structures have been reported for threading screw dislocations. Furthermore, the calculation showed no deep levels associated with this core structure. This is inconsistent with experimental results showing screw/mixed dislocations are more electrically active than pure edge dislocations.

Close examination of our TEM images reveals nanometer size particles at the surface termination of pure screw dislocations [arrows in Fig. 1 and 2 to show extra materials at the surface termination of a screw dislocation. EDS spectra taken on the TEM specimen with the beam focused on a small particle at the surface termination of screw dislocations. The dark spots in (b) are conducting regions. The arrows in the two images correspond to the same positions.](Fig. 1)

The SIVM results indicate that screw/mixed dislocations contribute significantly more to gate leakage than pure edge dislocations. Previously, screw/mixed dislocations were reported to be more effective recombination centers and have reduced barrier heights compared to pure edge dislocations in GaN. One interesting question is why screw/mixed dislocations are more electrically active than pure edge dislocations. The structure of threading edge dislocations in GaN have been studied extensively theoretically and confirmed experimentally by high-resolution TEM images. Deep acceptors, hence electron traps for $n$-type materials, are predicted to accompany these edge dislocations. On the other hand, comparably little is known about threading screw dislocations. Theoretically, Elsner et al. found an open core structure that is energetically more favorable. Experimentally, both full core and open core structures have been reported for threading screw dislocations. Furthermore, the calculation showed no deep levels associated with this core structure. This is inconsistent with experimental results showing screw/mixed dislocations are more electrically active than pure edge dislocations.

Close examination of our TEM images reveals nanometer size particles at the surface termination of pure screw dislocations [arrows in Fig. 1 and 2 to show extra materials at the surface termination of a screw dislocation. EDS spectra taken on the TEM specimen with the beam focused on a small particle at the surface termination of screw dislocations. The dark spots in (b) are conducting regions. The arrows in the two images correspond to the same positions.](Fig. 1)

The SIVM results indicate that screw/mixed dislocations contribute significantly more to gate leakage than pure edge dislocations. Previously, screw/mixed dislocations were reported to be more effective recombination centers and have reduced barrier heights compared to pure edge dislocations in GaN. One interesting question is why screw/mixed dislocations are more electrically active than pure edge dislocations. The structure of threading edge dislocations in GaN have been studied extensively theoretically and confirmed experimentally by high-resolution TEM images. Deep acceptors, hence electron traps for $n$-type materials, are predicted to accompany these edge dislocations. On the other hand, comparably little is known about threading screw dislocations. Theoretically, Elsner et al. found an open core structure that is energetically more favorable. Experimentally, both full core and open core structures have been reported for threading screw dislocations. Furthermore, the calculation showed no deep levels associated with this core structure. This is inconsistent with experimental results showing screw/mixed dislocations are more electrically active than pure edge dislocations.

Close examination of our TEM images reveals nanometer size particles at the surface termination of pure screw dislocations [arrows in Fig. 1 and 2 to show extra materials at the surface termination of a screw dislocation. EDS spectra taken on the TEM specimen with the beam focused on a small particle at the surface termination of screw dislocations. The dark spots in (b) are conducting regions. The arrows in the two images correspond to the same positions.](Fig. 1)
(~100 nm) Ga droplets that were oxidized when the surface was exposed to air. By comparing Figs. 1(a) and 1(b), we notice that these microscopic Ga droplets are associated exclusively with pure screw dislocations. No Ga droplets were found at the termination of mixed or edge dislocations.

To examine the effect of excess Ga might have on dislocations with a screw component, TEM was done on a Ga-rich and a Ga-lean sample using both [0002] and kinematic diffraction conditions. Figure 4 shows TEM images taken under the [0002] diffraction condition showing the difference in screw dislocations between (a) a Ga-rich sample and (b) a Ga-lean sample.

From SIVM measurements we found that reverse bias leakage occurs predominantly at dislocations with a screw component. This leakage depends sensitively on the growth stoichiometry and is of orders of magnitude larger for MBE samples grown under Ga-rich conditions. Cross-sectional TEM images and local EDS reveal microscopic Ga droplets at the surface terminations of pure screw dislocations in these samples. We show that excess Ga drastically changes the screw dislocation core structure. Consequently, dislocation electrical activity depends not only on the type of dislocation, but also upon growth stoichiometry.

The authors would like to thank S. Richter, R. N. Kleiman, and A. M. Sergent for their technical assistance. The Lincoln Laboratory portion of this work was sponsored by the Office of Naval Research under Air Force Contract No. F19628-00-C-0002. Opinions, interpretations, conclusions and recommendations are those of the authors and not necessarily endorsed by the United States Air Force.