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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

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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. [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 cm^2/Vs,[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[1,6] and superior interface control[7] 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 5×10^8 and $10^9\ cm^{-2}$, with the majority being screw and mixed types. Capacitance–voltage measurements show a background net donor concentration below $10^{15}\ cm^{-3}$ 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 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

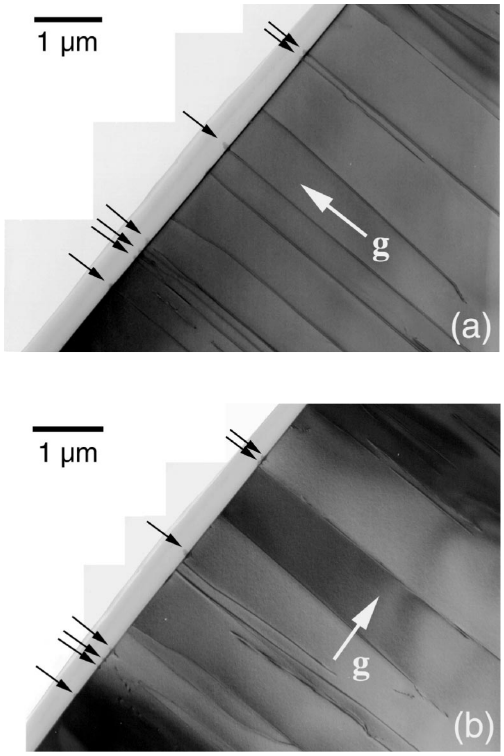

FIG. 1. Cross-sectional TEM images of a MBE GaN grown under Ga-rich condition. Micrographs were taken at the same sample position under different diffraction conditions to show dislocations with a screw component in (a) and those with an edge component in (b). Arrows indicate extra materials in a form of small particles on the surface. The arrows in the two images correspond to the same positions.

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[12] and have reduced barrier heights[13] 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[14,15] and confirmed experimentally by high-resolution TEM images.[16] Deep acceptors, hence electron traps for *n*-type materials, are predicted to accompany these edge dislocations.[17] On the other hand, comparably little is known about threading screw dislocations. Theoretically, Elsner *et al.* found an open core

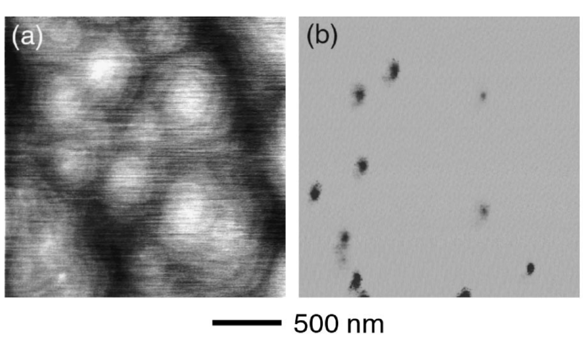

FIG. 2. 2 μm$\times$2 μm (a) topographic images and (b) simultaneously taken SIVM image under-6 V reverse bias of a GaN film grown under Ga-rich conditions. Grayscale represents 3 nm in (a) and 6×10^{-11} A in (b). The dark spots in (b) are conducting regions. They correlate with hillocks in (a).

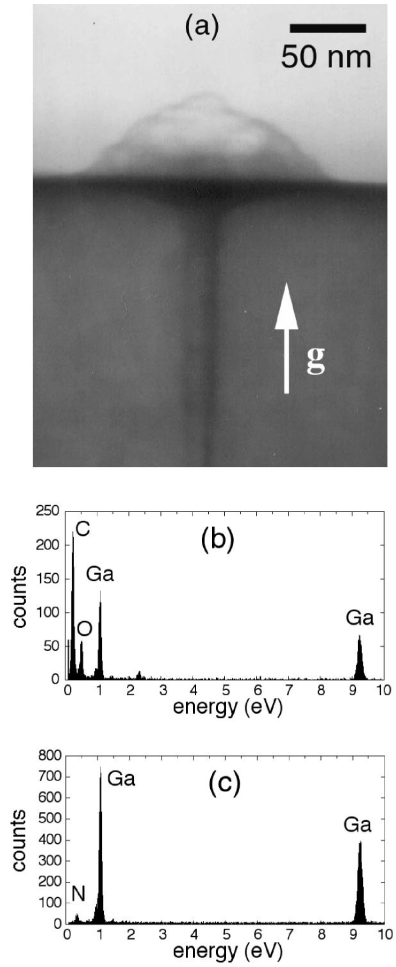

FIG. 3. (a) Cross-sectional TEM micrograph of the same sample as in Figs. 1 and 2 to show extra materials at the surface termination of a screw dislocation. EDS spectra taken on the TEM specimen with the beam focused (b) on the surface bump and (c) on GaN films away from the surface.

structure that is energetically more favorable.[14] Experimentally, both full core[16] and open core[18] structures have been reported for threading screw dislocations. Furthermore, the calculation[14] 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.[10,12,13]

Close examination of our TEM images reveals nanometer size particles at the surface termination of pure screw dislocations [arrows in Fig. 1 and Fig. 3(a)]. The TEM contrast of this material is different from that of GaN. To obtain chemical information, we perform energy dispersive x-ray spectroscopy (EDS) on the cross sectional TEM samples using a detector sensitive to low *Z* elements. The beam size is ~15 nm. Figure 3(b) is a spectrum taken with the electron beam focused on a small particle at the surface termination of a screw dislocation. The only elements detected were Ga, O, and C. No N signal was detected, indicating that the particle is not GaN. The carbon comes from contamination buildup during data acquisition and not from the sample. Thus, these particles are comprised of Ga and O. For comparison, the spectrum of the GaN film was shown in Fig. 3(c). The N signal is distinctly evident while the O signal is not detectable. Hence, the excess materials at the surface termination of screw dislocations are microscopic size

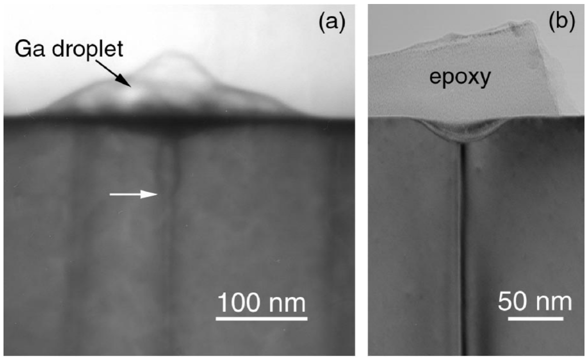

FIG. 4. Cross-sectional TEM micrographs taken under $\vec{\mathbf{g}}=[0002]$ diffraction condition showing the difference in screw dislocations between (a) a Ga-rich sample and (b) a Ga-lean sample.

(~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. It is evident that the dislocations in the two samples display a different strain contrast under the [0002] imaging condition. Screw dislocations in the Ga-rich sample [Fig. 4(a)] appear in general to have a wider and weaker contrast, suggesting a relaxed core structure. Moreover, the apparent width of the dislocation core contrast in the Ga-rich film widens as they approach the surface Ga droplet, while in Ga-lean sample [Fig. 4(b)] the dislocation line contrast remains sharp all the way to the surface. These results directly indicate that excess Ga induced change in dislocation core structure. In Fig. 4(a), the white arrow marks the position at which a sudden change in dislocation core contrast diameter from 12 to 22 nm. Such diameter changes were observed for many screw dislocations in the Ga-rich samples.

Combining TEM and SIVM results, a self-consistent picture of excess reverse bias leakage emerges. In addition to the reverse bias current in GaN being predominantly carried by dislocations with a screw component, we found that excess Ga accumulated at or near screw dislocations has a profound effect on the dislocation core structure and strain field. TEM images taken under kinematic conditions further indicate composition variation near screw/mixed dislocations in the Ga-rich sample. Evidently, these structural changes induced by excess Ga significantly affect the dislocation electrical activity. Since surface nano-Ga droplets were found only on pure screw dislocations, the amount of excess Ga depends on the screw component. Hence, the electrical activity should also depend on the type of dislocations and is expected to be largest for pure screw dislocations. This is particular to Ga-rich MBE growth conditions and is consistent with the lower reverse bias leakage found in MBE samples grown under Ga-lean conditions. We do not believe that impurities gettered at dislocations are the origin of dislocation electrical activity because the background impurity in our MBE material is well below $10^{15}\,\mathrm{cm}^{-3}$. Recent first-principles total energy calculations show that screw dislocations with a Ga-filled core has a lower formation energy in Ga-rich growth environments and dislocations with this core structure is expected to be electrically active.[19]

From SIVM measurements we found that reverse bias leakage occurs predominantly at dislocations with a screw component. This leakage depends sensitively on the growth soichiometry and is 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.

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