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Growth of GaN on SiC(0001) by Molecular Beam Epitaxy

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GaN films are grown by plasma-assisted molecular beam epitaxy on 6H-SiC(0001) substrates. Suitable substrate preparation and growth conditions are found which greatly improve the structural quality of the films. Threading dislocation densities of about 1×10^{9} cm^{-2} for edge dislocations and 1×10^{7} cm^{-2} for screw dislocations are achieved in GaN films of 1 μm thickness grown under optimal conditions. Reverse leakage is observed near some dislocations, although the majority of dislocations do not produce leakage.

Introduction The large band gap, high breakdown field, and high electron saturation velocity of GaN makes it ideal for use in visible-to-UV optoelectronic devices and in high speed, high power electronic applications. Most GaN epitaxial films used for devices have been deposited on sapphire, which despite its large lattice mismatch to GaN (≈16%) has nevertheless produced epitaxial GaN of relatively high quality [1]. Silicon carbide has a much better lattice match to GaN (3.4%), and has gained in popularity in recent years as a substrate for both molecular beam epitaxy (MBE) and metal-organic vapor phase epitaxy of GaN. In our prior work we have discussed the properties of GaN films grown by plasma-assisted MBE under optimal conditions [2]. Here we present additional results, illustrating the importance of various aspects of the substrate preparation and growth technique.

Experimental GaN films of typically 1 μm thickness are deposited by MBE on Si-face on-axis 6H-SiC(0001) substrates. Activated nitrogen is supplied by an RF-plasma source, and effusion cells are used for Ga and various dopants. The Ga flux is measured with a crystal thickness monitor, and the active N flux is calibrated by defining the Ga/N flux ratio to be unity at the point where a transition between streaky and spotty behavior occurs in the reflection high energy electron diffraction (RHEED) pattern [3]. The SiC substrates are hydrogen-etched at a temperature of 1600–1700°C [4]. Following H-etching, the substrates are transferred through air to the MBE chamber where they are outgassed at about 800°C for 30 minutes. To remove the surface oxide formed during transfer through air, several monolayers of Si are deposited on the substrate while it is near room temperature. It is then annealed at 1000°C until the RHEED pattern reveals a 3×1 pattern indicative of a $\sqrt{3}\times\sqrt{3}$-R30° surface reconstruction [2].

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Results & Discussion As noted above, our 6H-SiC substrates are prepared by H-etching. Detailed atomic force microscopy (AFM) images [4] of the resulting surface reveals steps arising from an unintentional miscut of the wafer. The surface morphology actually breaks up into low-angle facets (with the facet angles being less than the miscut angle) since the steps all prefer a particular orientation, namely, <1 –1 0 0>. On a given facet the step heights are all 15.2 Å, corresponding to a full unit-cell of the 6H-polytype, and at the intersection of facets half unit-cell high steps occur. The presence of single bilayer steps in the 6H substrate leads to a stacking mismatch between neighboring grains in wurtzitic GaN [2,5], and similarly for half unit-cell high steps of 4H-SiC. Full unit-cell high steps of 4H or 6H-SiC will not lead to stacking mismatch, and neither will half unit-cell high steps of 6H material.

TEM images reveal the type of stacking disorder described above; previously we have demonstrated that films grown on 6H-SiC in which the H-etching preparation step was *not* used display a thin region of cubic stacking near the GaN/SiC interface, whereas films grown on H-etched 6H-SiC do not display the cubic stacking. Here we present TEM results for GaN grown on 4H-SiC, for which H-etching *was* performed, as shown in Fig. 1. Mixed stacking (cubic and wurtzite) occurs near the interface. The images also display a planar stacking mismatch defect, presumably arising from interface steps, extending up from the interface.

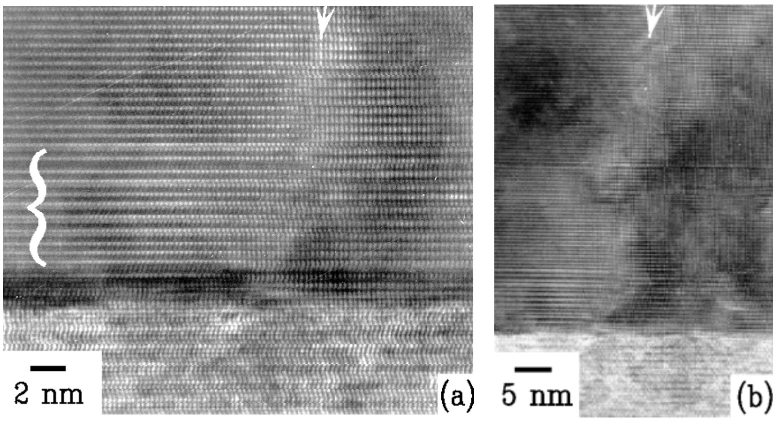

Fig. 1 High-resolution TEM images of GaN film on 4H-SiC. The same region is imaged, at two different magnifications. The curly bracket in (a) indicates a region of cubic stacking. Arrows indicate a stacking mismatch boundary.

Following H-etching, transfer to ultra-high-vacuum, and Si-cleaning, GaN films are deposited on the SiC as described above. A dislocation network arises in the film because of the lattice mismatch between GaN and SiC. For growth at > 700°C, the GaN grows initially as three-dimensional islands, which then strain relax by the formation of misfit dislocations with Burgers vector of 1/3 <1 1 –2 0> [2,6]. When the islands coalesce the misfit dislocations either join or annihilate with each other, or they produce a threading edge dislocation. Annihilation of a threading dislocation may occur when it meets another one with oppositely oriented Burgers vector, but for films grown with high Ga/N flux ratio (≈1.5) the threading dislocations generally extend straight up through the film and do *not* annihilate.

Typical dislocation densities for a films grown with high Ga/N ratio (≈1.5) are around 1×10^{10} cm^{-2} for the edge dislocations intersecting the surface of a 1.0 μm thick film. Figure 2(a) shows a plan view image of a sample grown at 750°C and with Ga/N ratio of 1.5. All the dislocations seen there have edge character, and their density in this image is 2×10^{10} cm^{-2}. Concerning screw dislocations, cross-sectional images [2] generally do not reveal any screw dislocations, implying a density of < 1×10^{8} cm^{-2}. AFM images can be used to count screw dislocations since they give rise to growth spirals on the surface [3]; Fig. 2(b) shows a typical example. The growth spirals can be seen by the small raised (white) features on the surface, the density of which is found to be $\approx 2\times10^6$ cm^{-2}. Typically we find a spiral density in the range $10^6 - 10^7$ cm^{-2} in our films. It may be possible that not all screw dislocations will give rise to growth spirals (i.e. depending on the location at which they intersect the surface), but even allowing for an order of magnitude correction factor for this effect we would estimate a screw dislocation density of $10^7 - 10^8$ cm^{-2}, consistent with the estimate from TEM above.

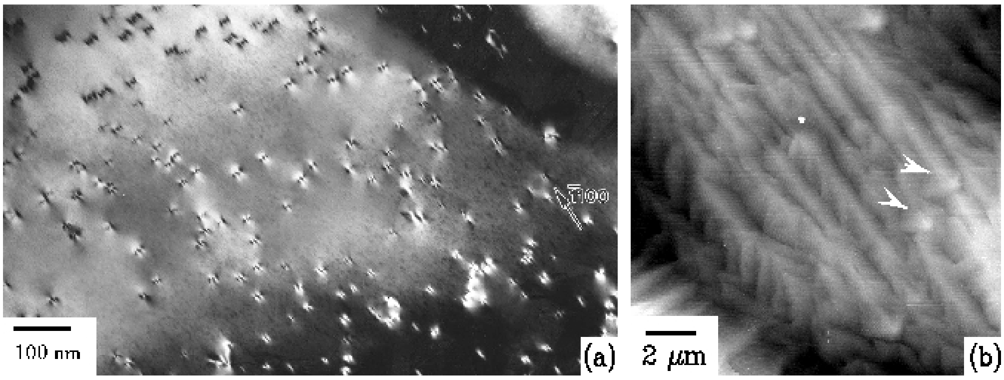

Fig. 2. Image of GaN films grown at 750°C with Ga/N ratio of 1.5. (a) Plan-view TEM image revealing edge dislocations. (b) AFM image revealing growth mounds arising from screw dislocations, two of which are marked by arrows. Gray scale range is 8 nm.

As seen in Fig. 2(b) and elsewhere [2], the surface morphology for those films grown with high Ga/N ratio near 1.5 is quite flat. In contrast, for Ga/N ratios near 1.3, pits with typical separation of about 1 μm are seen in the morphology. These pits are believed to arise from some sort of preferential film decomposition during growth at threading dislocations. As the Ga/N ratio is reduced to about 1.1 these pits proliferate, and eventually merge into trenches on the surface which separate plateaus of atomically flat morphology. However, even though the morphology for such low Ga/N ratios is worse, the dislocation density (for edge dislocations in particular) is significantly better. Edge dislocation densities of 1×10^9 cm^{-2} are typically found for somewhat rough films grown with Ga/N ratio near 1.1. We believe that the reduction in dislocation density arises from annihilation of edge dislocation due to their effective attraction to valleys in the topography, as will be further discussed elsewhere.

Scanning current-voltage microscopy (SIVM) was performed on a GaN film; an AFM image of the film is shown in Fig. 3(a). Growth spirals can be seen there, with density of about 2×10^7 cm^{-2}. In SIVM, a negatively biased conducting probe tip is brought down on the GaN film (n-type, due to unintentional doping), and the tip is scanned over the surface while monitoring the magnitude of the reverse bias leakage current. Prior measurements of this sort on other GaN films revealed excess leakage near screw dislocations but not near edge dislocations [7]. Figure 3(b) shows the AFM topograph acquired during the SIVM measurement, and Fig. 3(c) shows the associated current measurement. As in Fig. 3(a), growth spirals can be identified in Fig. 3(b) by the raised (white) features in the image, three of which are marked by arrows. The small, isolated dark spots in Fig. 3(c) arise from regions with measurable current. Some of these conducting regions are seen to be associated with growth spirals (i.e. screw dislocations), but others are not. Since the number of edge disloca-

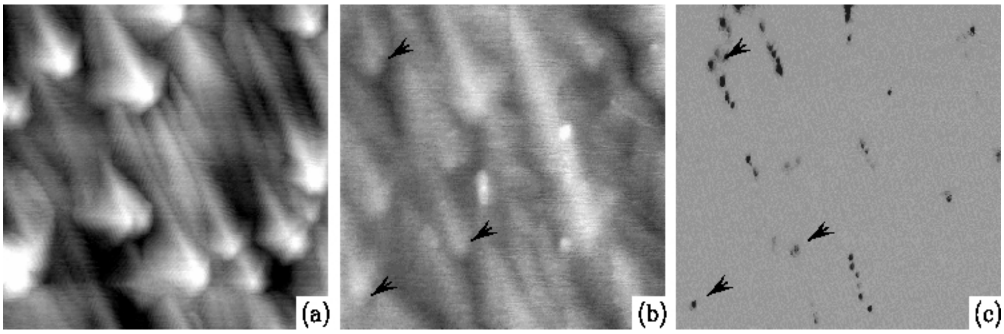

Fig. 3 (a) 10x10 μm AFM topograph of GaN film grown at 750°C with Ga/N ratio of 1.5. Grey scale range is 4 nm. (b) and (c) 5x5 μm simultaneously acquired images of (b) topography and (c) current at tip bias of –8 V. The grey scale range in (c) extends from 0 nA (light grey) to 0.02 nA (black). Arrows mark locations of several spiral growth mounds.

tions in the film ($\approx 10^{10}$ cm^{-2}) is much greater than the number of dark spots seen in Fig. 3(c) ($\approx 2\times10^{8}$ cm^{-2}), we conclude that the vast majority of edge dislocations do *not* give rise to reverse leakage, in agreement with prior studies [7]. However, since many of the darks spots in Fig. 3(c) are *not* associated with growth spirals, we also conclude that there are electrically active defects in the film which are not apparent in the topography. These defects could be a screw dislocations which due to their location at the surface do not give rise to growth spirals, or alternatively they could be some other type of defect.

Conclusions In conclusion we have grown GaN films by plasma-assisted MBE on Si-face SiC(0001) substrates. Relatively good structural quality is achieved in the films, with edge dislocation density of about 10^{10} cm^{-2} for films grown with high Ga/N ratio and 10^{9} cm^{-2} for films grown with Ga/N ratio slightly greater than unity. Screw dislocation densities are 1–2 orders of magnitude lower than the edge dislocation densities. This work was supported by the Office of Naval Research (grant N00014-96-1-0214, monitored by C. Wood).

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