Heteroepitaxial Growth of GaN on Si Substrate Coated with a Thin Flat SiC Buffer Layer

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The III-V semiconductors, GaN, has great potential for use in optoelectronic and high-temperature electronic devices due to its wide band gap and high-temperature stability. In recent years, much effort has been made to grow high-quality GaN films by using various growth methods. A lot of work has concentrated on GaN growth on sapphire substrate.[1] Due to the large lattice mismatch and thermal-expansion-coefficient difference between GaN and sapphire, high threading-dislocation densities (10^8 -10^{10} cm^{-2}) as well as large basal-plane stacking fault densities have been observed in GaN films.

We previously reported that cubic GaN film can be epitaxially grown on a Si (001) substrate coated with a 2.5-nm-thick cubic SiC layer.[2] Direct growth of GaN on a Si substrate results in either polycrystal growth or a substantial diffusion of Si into GaN films. In this paper we report the results of our recent study on the growth of cubic (β) and hexagonal (α) GaN on Si (001) and Si (111) coated with a thin flat SiC buffer layer under Ga- and N-rich growth conditions.

The SiC buffer layers were grown through carbonization of the Si(001) and Si(111) substrates in C_2H_2 (pressure of 5×10^{-6} Torr) for about 3 min at a substrate temperature of 910 ~ 970^{o}C. The thickness of SiC was about 2.5 nm. The details of SiC growth have been shown in reference 3. The surface roughness of SiC was 0.3-0.5 nm. GaN films were grown in a MBE chamber equipped with an RF-activated nitrogen plasma source. The N_2 flow rates were 0.1 and 2 sccm which correspond to MBE chamber pressures of $7.6{\times}10^{-5}$ (Ga-rich condition) and $4.4{\times}10^{-4}$ Torr (N-rich condition) respectively.

Figure 1 shows the β-SiC surface topography observed by atomic force microscopy (AFM) and a high-resolution TEM micrograph. The SiC was prepared on Si (001) at 970^{o}C. At the SiC/Si interface, misfit dislocation arrays (pure edge type) about 1.5 nm apart were generated in the SiC film. The lattice mismatch between β-SiC and Si is fully relaxed by misfit dislocation arrays. The surface roughness is 0.3 nm. A flat SiC surface is necessary to reduce the structure defects in GaN film because stacking faults and threading dislocations can originate from rough regions of the SiC surface. The substrate temperature and C_2H_2 pressure greatly affected the surface topography of the SiC buffer layers. If SiC is prepared at 1070^{o}C the surface roughness is as large as 3.0 nm[4].

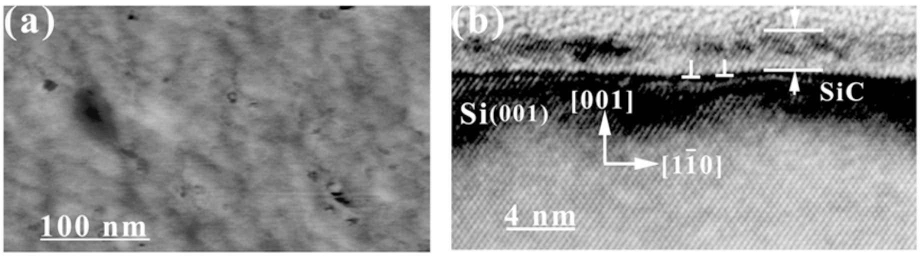

Fig. 1. (a) AFM image and (b) high-resolution cross-sectional TEM micrograph of β-SiC film, about 2.5 nm thick

GaN films were grown under different growth conditions. Under the N-rich growth condition, the surface roughness (R) measured by AFM increased with the film thickness (t), and was proportional to $t^{1/2}$ for both α- and β-GaN films. This indicates a statistical roughening of the surface and a characteristic columnar structure. It is plausible that a low Ga/N flux ratio results in a (partly) nitrogen-terminated surface, which has a high sticking coefficient for Ga atoms, but low surface mobility. The morphology then evolves by statistical roughening. Under Ga-rich growth condition cubic- and hexagonal-GaN films showed different growth mode. For β-GaN, after the beginning of GaN growth, the streaky SiC RHEED (reflection high energy electron diffraction) pattern immediately became spotty, which corresponds to three-dimensional diffraction from a surface that is rough on a nanometer scale. This kind of RHEED pattern was observed under both Ga- and N-rich growth conditions in our experiments. Poor wetting of GaN on SiC leads to pure 3D nucleation favoring the formation of dislocations at the island edges[3]. As the growth time was increased, the grains grew up and then laterally coalesced. This coalescence began after the films grew about 100 nm thick. The RHEED pattern became gradually streaky, and its intensity became more and more stronger. Figure 2 shows the AFM surface topography and high-resolution cross-sectional TEM image of a 0.82 μm thick β-GaN film grown under Ga-rich condition. The atomically flat areas are (001) GaN surfaces with sizes of about 0.05-0.40 μm. The main defects are stacking faults and microtwins. Near the interface, the GaN film is highly defected due to the lattice mismatch. The density of stacking faults and microtwins decreases with the distance from the interface. Stacking faults are a common form of strain relief in f.c.c crystal structures because their formation energy is fairly low. Careful examination showed that many stacking faults originated from the rough interface regions.

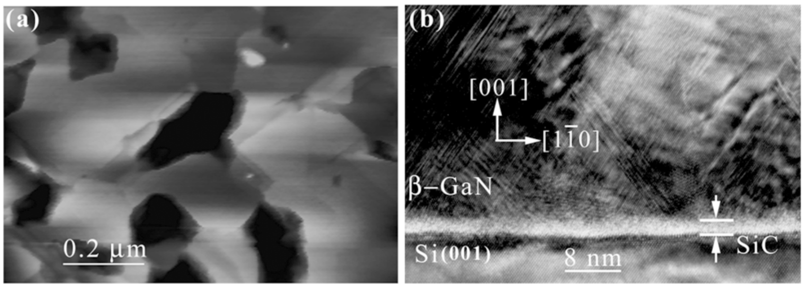

Fig. 2. (a) AFM image and (b) high-resolution XTEM micrograph of β-GaN film prepared under Ga-rich condition.

For α-GaN growth under Ga-rich condition, the RHEED pattern remained streaky during the growth, indicating a two-dimentioanl growth mode. At the first initial 5 nm thick film growth, the RHEED pattern was streaky but its intensity was very weak, indicating the GaN crystal quality was not good due to the lattice mismatch between α-GaN and α-SiC. As the growth time was increased, the RHEED pattern became more and more streaky and stronger, indicating a flat GaN surface which was confirmed by AFM observations. Figure 3 shows the AFM surface topography and high-resolution cross-sectional TEM image of a 500 nm thick GaN prepared under Ga-rich condition.

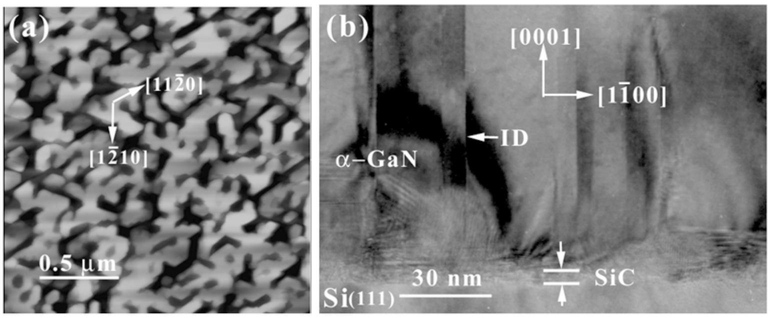

Fig. 3. (a) AFM image and (b) high-resolution XTEM micrograph of α-GaN film prepared under Ga-rich condition.

The flat surfaces in Fig. 3(a) are the (0001) GaN planes. The main defects in films observed by cross-sectional and plan-view TEM are dislocations and inversion domain boundaries (IDBs) along [0001] direction. It is clear from Fig. 3(b) that the IDBs are very flat and remain parallel to the [0001] growth direction. These planar defects begin at the interface of α-GaN/α-SiC and run throughout the entire epilayer. The IDBs were formed by shifting one side of an IDB by c/8 along the [0001] direction. It is interesting to note that there are no stacking faults in the basal (0001) planes, while in α-GaN films prepared under N-rich condition the density of stacking faults in basal planes is high. Both the stacking faults and IDBs do not induce electronic states in the band gap and therefore would not adversely impact photoluminescence efficiency.

Photoluminescence (PL) spectrums of β-GaN prepared under both Ga- and N-rich conditions showed only the near-band-edge peak at 3.22 eV or the yellow-band luminescence (YL) was very weak, while that of α-GaN prepared under Ga-rich condition showed both the near-band-edge and a strong YL. The origin of YL is not fully understood. It is a defect-induced transition associated with widely spread energy levels deep within the band gap. From our TEM observations we believe that the YL may be related to screw and/or mixed dislocations in the GaN grains.

In summary, high quality α- and β-GaN films were successfully grown on Si (001) and Si (111) coated with a thin flat SiC. The thin flat SiC layer was an effective buffer layer for GaN growth. The reduction in SiC surface roughness reduced the defect density in the GaN films. Under Ga-rich condition, flat and better crystal quality GaN films were obtained.

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