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Surface and defect microstructure of GaN and AlN layers grown on hydrogen-etched 6H–SiC(0001) substrates

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Abstract

Hydrogen-etching of 6H–SiC(0001) substrates removed mechanical polishing damage and produced an array of parallel, unit cell high steps. The initial stage of AlN deposition on these etched substrates occurred via island nucleation, both on step edges and on terraces. Coalesced AlN films did not show scratch-induced undulations observed on the surfaces of AlN films deposited on as-received substrates. The films also had a lower density of growth pits. The majority of threading dislocations (TDs) observed in these films were of **a** type. Jagged networks of misfit dislocations were seen on the terraces in the 15 nm thick AlN/hydrogen-etched SiC composite. GaN islands nucleated primarily at undulations in AlN layers and at hillocks on the AlN surface of as-received and hydrogen-etched substrates, respectively. Complete coalescence of these islands occurred at thicknesses close to 20 nm, and subsequent growth occurred via the step-flow mechanism. Strain measurements showed more strain relaxation in GaN films grown on the hydrogen-etched substrate. On- and off-axis X-ray rocking curves revealed statistically similar full width at half maximum values for both on- and off-axis reflections, indicating similar densities of TDs in the two types of films. The majority of TDs in GaN epi-layers resulted from defective regions observed contiguous to the GaN/AlN interfaces.

Keywords: Group III-nitrides; Dislocations; Heteroepitaxy; AFM; MOCVD

1. Introduction

The Si-terminated basal plane of 6H–SiC(0001) has been investigated by several groups [1,2] as a potential substrate for heteroepitaxial growth of AlN and GaN layers. The thermal conductivity along the [0001] direction is 4.9 W cm^{-1} K^{-1} [3] at room temperature and the material can be cleaved along the $[11\bar{2}0]$ direction. The former property appears to contribute to the improved performance of group III nitride-based ultraviolet light emitting diodes [4] and heterojunction field effect transistors [5,6] deposited on SiC. Despite the apparent benefits of SiC substrates, GaN films grown on AlN have yet to demonstrate lower defect densities than those observed in films of comparable thicknesses deposited on sapphire. This is attributed to the damaged surface of as-received SiC wafers, resulting from slicing, lapping and polishing. As shown in the atomic force microscopy (AFM) image in Fig. 1, the surfaces of SiC(0001) substrates show numerous randomly oriented scratches due to mechanical polishing, with widths ranging from 100 to 800 nm and depths of 12 nm. The scratches are commonly observed on surfaces of as-received SiC wafers since the mechanical hardness and chemical inertness of this material makes polishing difficult [7]. The polishing process can result in damage extending to

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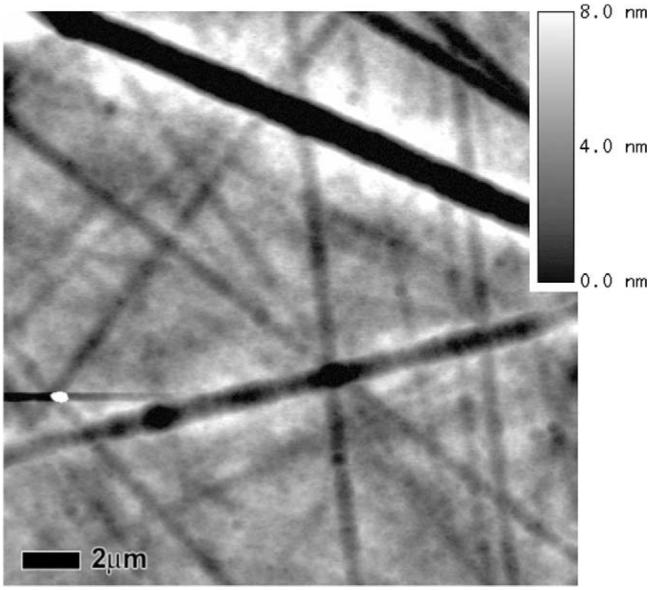

Fig. 1. 10×10 μm AFM height image of as-received 6H–SiC(0001) wafer showing polishing scratches present on the surface. The vertical height scale is given in the upper right corner of the image.

a depth of micron beneath the surface [8]. Even with a highly optimized polishing process, subsurface damage extends up to 8 nm in the regions of the scratches [9]. Several researchers studying homoepitaxial growth of SiC have observed locally higher densities of edge and screw threading dislocations (TDs) [10,11], film surface defects [12] and inclusions believed to correspond to the 3C polytype [13]. These defects were in areas directly over a polishing scratch or damaged surface region of the substrate. In an effort to improve the surface of SiC substrates, chemomechanical polishing [14], oxidation and subsequent oxide removal [15], sublimation etching [16] and various gaseous etchants including H_2, H_2 + hydrocarbon (C_2H_4 or C_3H_8) and H_2 + HCl [17] have been used. Of these processes, etching in H_2 is perhaps the most intriguing since it involves relatively simple equipment and could in principle be incorporated into a system for the growth of homoepitaxial SiC or heteroepitaxial group III-nitrides.

Hydrogen-etching of SiC was first reported by Chu and Campbell in 1965 [18]. Since then, other investigators have used thermodynamic calculations to predict that the reaction pathway for hydrogen etching proceeds via the dissociation of SiC into liquid silicon, which evaporates, and reaction between solid carbon and atomic hydrogen to form hydrocarbons [19,20]. Owman et al. [16] showed that hydrogen etching of on-axis 6H–SiC(0001) resulted in an array of regular straight terraces separated by steps with a height equal to the 6H unit cell (15.12 Å). These steps were subsequently shown to be aligned along the $\langle 1\bar{1}00\rangle$ directions, with etching proceeding by an inverse step-flow mechanism [21]. Etching in HCl/H_2 results in similar stepped surfaces [22]. The use of H_2 [12,23] or HCl/H_2 [12] etching prior to homoepitaxial SiC growth results in reduced defect density and smoother film surfaces.

In addition to the benefits of removing surface damage, it was predicted that the formation of unit cell height steps on 6H–SiC wafers will reduce the density of two-dimensional threading defects in heteroepitaxial group III-nitrides. As-received SiC wafers show surface steps with random heights and orientations, resulting in terraces terminated with different bilayers of the ···ABCA′C′B′···6H(0001) stacking sequence [16]. In the deposition of group III-nitrides on the (0001) surface of 2H SiC, the stacking sequence of islands growing on adjoining substrate terraces is determined by the stacking of the underlying SiC. Therefore, when two islands coalesce across a surface bilayer step, a two-dimensional threading defect known as a stacking mismatch boundary (SMB) can form [24,25]. For example, for two SiC terraces terminated with ···ABC and ···BCA stacking and separated by a bilayer step, the resulting group III nitride islands would have the stacking sequences of BCBC··· and CACA···, respectively, resulting in an SMB at their coalescence fronts, since the "B" and "A" bilayers will not align. These SMBs have been predicted to be bounded by stacking faults and/or dislocations parallel to the surface. The calculations indicate that they may introduce energy states in the bandgap corresponding to the commonly observed yellow luminescence in GaN [26]. Hydrogen etching of 6H–SiC results in unit cell height steps separated by terraces of the same stacking termination [27]. Since the 2H III-nitrides have a stacking sequence that is an integral multiple of the 6H–SiC substrate, islands which coalesce across a unit cell height step will have the same stacking sequence and SMBs will not form.

The growth of AlN on H_2- or HCl/H_2-etched SiC has been studied by several groups. Using high-resolution transmission electron microscopy (TEM), Torres et al. [27] observed a very disordered AlN/SiC interface with as-received SiC substrates and a smooth interface devoid of SMBs using H_2-etched substrates. The latter films also demonstrated a higher degree of crystalline order, as seen by Rutherford backscattering spectroscopy. Cross-sectional TEM also demonstrated reduced contrast, which was attributed to defects in AlN films deposited on HCl/H_2-etched SiC [28]. Other studies [29,30] also showed reduced X-ray rocking curve full width at half maximum (FWHM) values for AlN on H_2- or HCl/H_2-etched SiC.

GaN deposition on H_2- or HCl/H_2-etched SiC has not been examined as thoroughly as AlN deposition. Lantier et al. [31] reported lower X-ray rocking curve FWHM for GaN with an AlN buffer layer on H_2-etched SiC, but cross-sectional TEM showed approximately equal densities of edge and screw TDs. Plan-view TEM was not performed to confirm the dislocation densities. In addition, photoluminescence spectra at 10 K showed similar features and line widths, irrespective of substrate preparation. Xie et al. [32,33] deposited GaN films with high-temperature AlN and low-temperature GaN buffer layers on 6H–SiC substrates etched with H_2, H_2/C_2H_4 and H_2/HCl. They observed fewer pinholes, smoother surfaces and decreased