Dislocation reduction in MOVPE grown GaN layers on (111)Si using SiN\textsubscript{x} and AlGaN layers

M Haeberlen, D Zhu, C McAleese, MJ Kappers and CJ Humphreys

Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, UK

E-mail: mh544@cam.ac.uk

Abstract. Growth of GaN on Si(111) potentially enables cost efficient manufacturing of optoelectronic devices due to the possibility of using cheap large area substrates. However, GaN layers grown on Si(111) substrates suffer from high tensile stress that can lead to cracking at layer thicknesses exceeding 1 µm. Another challenge is the high dislocation density of GaN layers grown on Si(111) which is detrimental to device performance. In this paper we show that a step graded AlGaN buffer layer can compensate tensile stress, avoiding cracking, and at the same time reduce the dislocation density. An additional SiN\textsubscript{x} interlayer in the GaN layer is shown to further reduce the dislocation density down to the high 10\textsuperscript{8} cm\textsuperscript{-2}. Weak beam dark field TEM was used to study the dislocation reduction in cross sectional samples and for comparison of the step graded AlGaN buffer layer structure to a continuously graded one. STEM ADF was used to determine the exact location of dislocation bending with respect to the position of the interface.

1. Introduction

The potential cost reduction by successful growth of GaN based LEDs on large diameter (111) oriented silicon substrates is thought to give solid state lighting a boost towards replacing incandescent lighting [1]. However, in order to achieve this, a few obstacles still have to be overcome. The large mismatch in thermal expansion coefficients (46%) can lead to large tensile stresses resulting in cracking of the GaN layer. High dislocation densities in GaN grown on silicon of typically 10\textsuperscript{10} cm\textsuperscript{-2} originate from a large lattice mismatch of 17%. For comparison, LED structures on sapphire substrates are deposited on GaN layers which exhibit a typical dislocation density of ~5x10\textsuperscript{8} cm\textsuperscript{-2}.

Build-up of tensile stress can be addressed by the integration of AlN interlayers deposited at low temperatures [2] or the use of an AlGaN buffer layer which results in compressive stress counteracting the tensile stress generated upon cooling in the top GaN layer [3]. In order to reduce dislocation densities, the in-situ deposition of SiN\textsubscript{x} interlayers has been found to be effective [4].

In this paper we studied the propagation of dislocations through continuously or step graded AlGaN buffer layers by means of weak beam dark field TEM. Simultaneous imaging of compositional variations in the step graded AlGaN buffer together with residual contrast from dislocations in STEM ADF allows for exact determination of regions of dislocation interaction near interfaces. The results found in this study suggest that dislocation bending occurs at or very close to the interfaces between AlGaN layers of different composition. Dislocation bending in a continuously graded AlGaN buffer is much less pronounced indicating the presence of a threshold in strain for the bending over of...
dislocations as proposed for example in [5]. The combination of stress management layers with SiN$_x$ interlayers is found to reduce the threading dislocation density significantly.

2. Experiment

2.1. Sample structures

Two different sample structures were grown on Si(111) for the study presented in this paper. Growth was carried out in a Thomas Swan close coupled showerhead MOVPE reactor. The sample structures are shown schematically in Figure 1. Sample A contains a continuously graded AlGaN strain management layer, whereas sample B employs a step graded AlGaN layer for compensation of tensile strain. A SiN$_x$ interlayer for dislocation reduction was grown after 330 nm and 100 nm of GaN growth in sample A and sample B, respectively.

![Figure 1. Schematic of sample structures grown for this study. Sample A: Continuously graded AlGaN strain management buffer with a thin SiN$_x$ interlayer 330 nm above the AlGaN/GaN interface and Sample B: Step graded AlGaN strain management buffer with thicker SiN$_x$ interlayer for dislocation reduction.]

2.2. Experimental details

Cross sectional TEM samples were prepared so that both the [10-10] and [11-20] zone axes of the GaN film could be accessed in one sample. Sample preparation was carried out employing mechanical grinding followed by dimpling and ion beam thinning. Weak beam dark field images were taken in a Philips CM30 TEM operating at 300 kV along the [10-10] zone axis using (0002) and (11-20) reflections to reveal dislocations with a screw and edge component, respectively.

STEM ADF images were acquired along the [11-20] zone axis of sample B in a Tecnai F20 TEM operating at 200 kV equipped with an ADF detector with an inner diameter of 35 mrad and an outer diameter of 105 mrad. A camera length of 100 mm was chosen to enable Z contrast imaging together with imaging of residual diffraction contrast from dislocations as outlined for stacking faults in [6].

3. Results and Discussion

Figure 2 shows the WBDF images obtained from the samples containing a continuously graded (a) and, (b) a step graded strain management layer, respectively.
Figure 2. WBDF TEM images of sample (a) containing a continuously graded AlGaN layer and sample (b) with a step graded AlGaN layer. Screw dislocations annihilating by the formation of loops are marked with “l”, misoriented grains visible in the (11-20) WBDF images are marked with “m”, respectively.

It is apparent from the TEM images in figure 2 that significant differences in the dislocation structure exist in both samples. It can be seen that the formation of loops leading to annihilation of screw type dislocations is much more pronounced in sample B compared to sample A. Screw type dislocations are found to be bent slightly at each AlGaN/AlGaN interface leading to an increased likelihood of two dislocations annihilating. This way, the step graded AlGaN layer reduces screw type dislocations more efficiently than the continuously graded layer. The same observation can be made for edge type dislocations. Bending of edge type dislocations in sample A only occurs very close to the AlGaN/GaN interface, whereas dislocation bending can be noticed at each interface between AlGaN layers of different composition in sample B. The influence of the thickness of the in-situ deposited SiNx layer can also clearly be seen in figure 2. It is found that the thicker SiNx in sample B reduced the dislocations significantly, whereas the SiNx layer in sample A hardly affects the dislocations at all. Misoriented grains, which can be seen in the (11-20) WBDF images of both samples, are efficiently reduced within both the continuously and step graded AlGaN layer. However, lower contrast from these misoriented grains after the AlGaN/AlGaN interfaces also indicates that dislocations are reduced in the step graded buffer layer structure.

In order to study dislocation bending in the step graded buffer layer in more detail STEM ADF images were acquired. A typical STEM ADF image of the uppermost portion of the step graded AlGaN layer is shown in Figure 3.
Figure 3. STEM ADF image of sample A. Z-contrast as well as residual contrast from dislocations is visible.

It can clearly be seen that the majority of dislocations (mainly edge type) bend over by angles of less than 10° at or very near the interfaces of the step graded AlGaN layer. Bending over of dislocations in AlGaN layer of different composition has already been reported in the literature [5,7] and occurs in order to reduce strain energy in the system. A threshold energy for the bending of dislocations of 10 eV has been proposed in [5]. Further experiments will be conducted to optimise the AlGaN buffer layer design for both dislocation reduction and strain management purposes.

4. Conclusions
MOVPE grown GaN layers on Si(111) with either a continuously or step graded AlGaN buffer layer for strain management have been investigated by means of weak beam dark field TEM and STEM ADF. It has been found that step graded AlGaN layers can lead to significant bending of edge type dislocations and that annihilation of screw type dislocations by loop formation is also favoured. Dislocation bending was only observed near the GaN/AlGaN interface of the continuously graded buffer layer sample.

References
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