

AlN buffer layer thickness influence on inversion domains in GaN/AlN/Si(111)

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Abstract

The AlN buffer layer thickness influence on the inversion domains (IDs) in GaN/AlN/Si(111) grown by plasma assisted molecular beam epitaxy (MBE) is studied by transmission electron microscopy (TEM). The GaN layer polarity is determined by convergent beam electron diffraction (CBED). The AlN buffer layer thickness notably affects to the IDs density and the GaN epilayer polarity. Moreover the threading dislocation distribution existence also depends on such thickness. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Transmission electron microscopy (TEM); GaN; Molecular beam epitaxy (MBE); Inversion domains (IDs); AlN buffer; Si (111); Surface polarity

1. Introduction

Nitride heterostructures are being successfully employed for optoelectronics applications in the short wavelength range and in transistors [1,2]. The thermal properties and resistance in hostile atmosphere also make them ideal candidates for high temperature and high power devices [3].

The GaN heteroepitaxial growth onto sapphire by Metal Organic Chemical Vapour Deposition using a two step procedure is the most commonly used method to solve the lack of suitable substrates [4,5]. On the other hand, Silicon is an attractive substrate because its properties, crystal quality, doping capability, thermal stability as well as the well-known Si technology. Nevertheless, an amorphous layer appears at the interface by the direct epitaxial growth of GaN films on Si(111), which is not desirable for good epitaxy [6,7]. The deposition of AlN buffer layer was found to

improve the GaN quality [8]. There are many parameters of the buffer layer growth process that play a key role in the attainment of high-quality materials. It seems that the AlN buffer layer thickness is not so critical in GaN/AlN/Al₂O₃ heterostructure, and good results have been obtained in the range from 30 to 100 nm of AlN thickness [9].

In this work, GaN/AlN/Si(111) heterostructures grown by plasma assisted molecular beam epitaxy (PA-MBE) have been studied by transmission electron microscopy (TEM) and convergent beam electron diffraction (CBED) to analyse the AlN buffer layer thickness influence on the GaN epilayer crystal quality.

2. Experimental procedure

Two GaN films with (0001)-oriented surface were grown on AlN buffered Si(111) substrates by PA-MBE. The AlN-buffer layer thickness was 15 and 35 nm in samples S15 and S35, and the GaN thickness was 0.9 and 1.2 μm, respectively. In both cases, the AlN buffer layers were grown at 820 °C, and the GaN epilayers at

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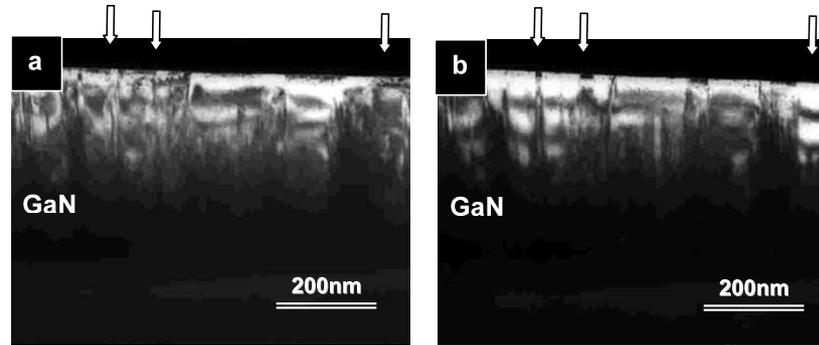


Fig. 1. Dark field XTEM images with (a) $g = 0002$ and (b) $g = 000\bar{2}$ near the $\langle 11\bar{2}0 \rangle$ zone axis from sample S35. The opposite contrast shows ID s (arrows).

760–780 °C. Further growth details on the studied samples are described in [10].

The microstructure of the layers was characterized by conventional TEM in a JEOL 1200-EX transmission electron microscope operated at 120 kV and CBED in a JEOL 2010 working at 200 kV. Both plan view TEM (PVTEM) and cross-sectional TEM (XTEM) specimens were thinned down to 100 μm by mechanical grinding and dimpled down to 10 μm followed by ion milling with a LN_2 cold stage at 4.5 kV to electron transparency. A final step at 3 kV was used to reduce ion beam damage.

3. Experimental results and discussions

In the characterized samples, inversion domains (IDs) are present in the GaN epilayers. Multiple dark field technique was used to establish the inversion character of these domains in XTEM [11,12] and PVTEM [11] specimens. The Fig. 1 shows a complementary contrast in images recorded with $g = 0002$ and $000\bar{2}$ reflections with the beam along the $\langle 11\bar{2}0 \rangle$ direction. The IDs characterization in PVTEM specimens was carried out using the $g = 1\bar{1}01$ and $\bar{1}10\bar{1}$. The asymmetry between both reflections has been previously used [11,13] to

determine the IDs in GaN layer. Using this method a much higher IDs density reaching the GaN surface has been observed in S15 compared with S35 as can be seen in Fig. 2.

The polarity of growth for the epitaxial layers has been determined by CBED technique applied in different regions inside the GaN films. Fig. 3 shows CBED patterns recorded at the $\langle 1\bar{1}00 \rangle$ axis from both samples. By comparing the (0002) and $(000\bar{2})$ diffraction disks with simulated ones the layer polarity can be determined [14]. Sample S35 seems to present Ga-polarity as shown the fit between the experimental and the simulated CBED patterns for a GaN layer thickness of 95 nm (Fig. 3b). In sample S15, we have examined many areas inside two XTEM samples and as can be seen in Fig. 3a, the CBED results seems to correspond to N-polarity with a GaN layer thickness of 110 nm. Each time we have used a 25 nm beam diameter and formed the CBED pattern in areas which exhibited homogeneous contrast. The CBED patterns are perfectly reproducible.

Previous characterizations [10] based on a wet etching method with KOH and reflection high energy electron diffraction (RHEED) patterns for both GaN layers were also used to determine the surface polarity. The RHEED surface reconstruction during the growth points to a N-face surface or mixed polarity for sample

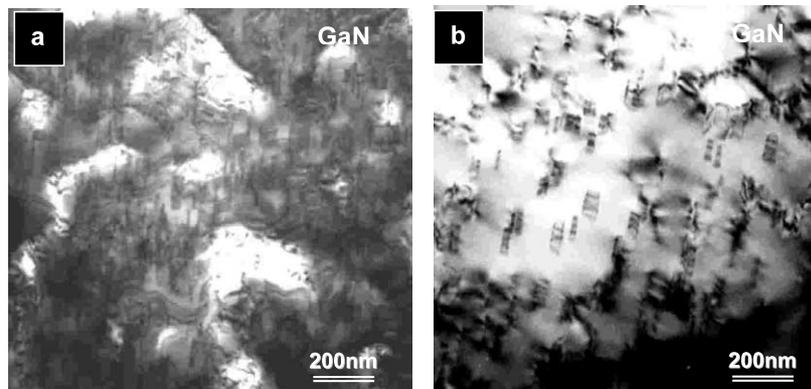


Fig. 2. Two beam condition PVTEM image with $g = 01\bar{1}\bar{1}$ reflection at the $\langle 12\bar{1}\bar{3} \rangle$ one axis from samples (a) S15 and (b) S35, revealing the ID s with Ga polarity presence at the GaN epilayer surface.

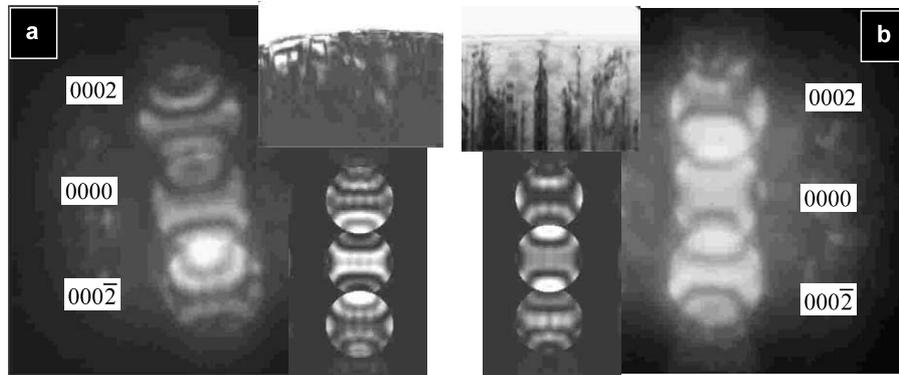


Fig. 3. CBED patterns recorded along the $\langle 1\bar{1}00 \rangle$ from GaN epilayers of samples (a) S15 (N-polarity) and (b) S35 (Ga-polarity).

S15 and a typical (2×2) of Ga-face layer for sample S35. Ga-face and N-face surfaces of GaN have different chemical properties [15] and this fact has been checked in the characterized samples. Our polarity determination by CBED is in good agreement with these previous results.

On the other hand, the GaN layers present a mosaic structure with slightly misoriented subgrains. Selected area electron diffraction patterns taken from areas of about $65 \mu\text{m}^2$ of PVTEM specimens revealed this structure. The diffraction spots in these patterns, recorded at the $\langle 0001 \rangle$ zone axis, are elongated due to the in-plane misorientation between the subgrains. At the upright corners of images in Fig. 4 high indices diffracted spots are shown. The measurement of the arc that such curved spots occupy is related to this misorientation, being considerably higher in sample S15. In the PVTEM micrograph from sample S15 of Fig. 4 the subgrain boundaries are notably better defined than those in sample S35. In these images threading dislocations reaching the free surface in both samples are evident. The density of dislocation with an edge-component was measured after analyzing low magnification PVTEM images recorded under two beam conditions with $g = 11\bar{2}0$ near the $\langle 0001 \rangle$ zone axis (Fig. 4). This density ($\rho_D \sim 1.5 \times 10^{10} \text{ cm}^{-2}$) results to be similar in both samples although a different

dislocation arrangement has been observed. While the dislocation distribution is rather random in sample S35, the dislocations form low angle boundaries in sample S15.

PVTEM micrographs taken along $\langle 0001 \rangle$ axis as well as scanning electron microscopy images revealed the presence of cavities in the GaN epilayer surface in sample S15. They are faceted and exhibited an irregular hexagonal shape. This fact constitutes another difference between the studied samples.

4. Conclusions

The GaN/AlN/Si(111) characterization by TEM has pointed out the AlN buffer layer thickness influence on the IDs density inside the GaN epilayers, being higher in the sample with a smaller buffer layer thickness. Moreover, CBED was used to determine the GaN layer polarity, it is different for both GaN films. The N-polarity observed in sample S15 leads to a higher IDs density reaching the GaN surface. Nevertheless, IDs are present in sample S35 (with a larger buffer layer thickness) in spite of the Ga-polarity of the epilayer. The AlN buffer layer thickness also affects the threading dislocation distribution and the existence of cavities.

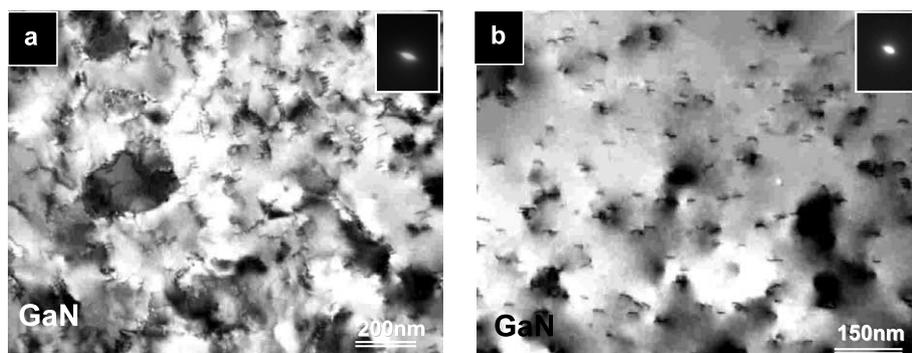


Fig. 4. Two beam condition PVTEM images with $g = 11\bar{2}0$ reflection at the $\langle 0001 \rangle$ zone axis from samples (a) S15 and (b) S35 showing the mosaic structure and threading dislocations

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