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MORPHOLOGICAL AND STRUCTURAL ASPECTS OF GaN FILMS GROWN ON SAPPHIRE BY MBE

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Abstract

Transmission Electron Microscopy (TEM) is employed in order to investigate the morphological and structural aspects of GaN films grown on sapphire, by Molecular Beam Epitaxy (MBE). The sapphire surface was nitridated at high temperature and then a 20-25 nm low temperature buffer layer of AlN was deposited. The buffer layer was annealed at high temperature and then the epitaxial GaN was grown under various conditions. The correlation between structural and morphological properties of GaN and MBE grown conditions is investigated at microscopic level. A significant reduction in the GaN surface roughness with increasing Ga/N ratio is observed.

Introduction

During the last years, great progresses have been realized in III-V nitride optoelectronics [1]. In particular, AlN, GaN and InN which can form a continuous direct band gap alloy system from 1.9 eV (InN) through 3.5 eV (GaN) to 6.2 eV(AlN), are suitable for optical devices from red to ultraviolet [2]. This was recently confirmed by a technological breakthrough in III-V nitride semiconductor technology, and now blue light-emitting diodes (LEDs) are commercially available and high efficiency blue laser diodes (LDs) have been fabricated [3, 4]. Bright III-V nitride LEDs can work in spite of many linear and planar defects [5, 6]. The system most commonly used for device material is GaN/sapphire (0001) where the hexagonal wurtzite lattice of GaN (a-GaN) grows with $(0001)_{GaN}//(0001)_{sapphire}$ and $[11\bar{2}0]_{GaN}//[10\bar{1}0]_{sapphire}$. The aim of this study is to correlate the structural and morphological properties of GaN films with the MBE growth conditions, using TEM and in particular, the influence of fluctuations of the Ga/N ratio during the growth process.

Experimental Details

The GaN layers were grown on the (0001) sapphire surface by electron cyclotron resonance (ECR)-MBE. The sapphire surface was nitridated at high temperature and then an 20-25 nm low temperature buffer of AlN was deposited. The buffer layer was annealed at high temperature and then a 3μm epitaxial GaN was grown under various conditions. Specimens for electron microscopy in cross-section (XTEM) and plan-view geometry were prepared using the standard techniques of mechanical thinning followed by appropriate ion-milling. TEM observations were carried out in a Jeol JEM 120 CX electron microscope operated at 120 kV.

Results

Significant morphological and structural changes in the GaN films are observed when the Ga/N stoichiometry changes during the growth process. In specimens grown under N-rich conditions a large number of linear and planar defects are detected. In Figure 1 the sapphire/AlN and the AlN/GaN interfaces are illustrated with the 0002 reflection when the $[11\bar{2}0]$ crystallographic axis is parallel to the electron beam. A high density of threading dislocations and Inversion Domain Boundaries (IDBs) emanating from the sapphire/AlN interface are observed. A highly strained area, ~20 nm thick, just above the AlN layer corresponding to the early stages of GaN growth is also observed. The IDBs transverse the buffer layer and the GaN film running parallel to the [0001] direction and most of them reach the top surface of the film, generating a "flat roof" surface of high roughness (Figure 2). This is probably due to the slower growth rate of the narrow domains between the IDBs that have inverse polarity with respect to the bulk of the film. As a result, by the end of the growth process these domains possess a lower surface level.

In the top 1 μm of the film dense multiple basal stacking faults (SFs) are observed. These are in contrast with the $10\bar{1}0$ reflection shown in Figure 2a. Figures 2b and 2c taken with the 0002 and $11\bar{2}0$ reflections, respectively, depict two overall extinctions of the SFs. Therefore, the displacement vector **p** of the SFs can be readily determined as **p** = $1/3\langle 10\bar{1}0\rangle$ and thus the SFs are characterized to be of the I_2 type [7]. Interactions between IDBs and SFs are also observed (Figure 3). In addition, prismatic domains elongated along the growth direction and near the AlN/GaN interface area are detected (Figure 4). The possible existence of amorphous material inside these domains at the early stages of GaN growth has been argued [8]. In Figure 5, a TEM micrograph of a plan-view N-rich specimen is illustrated, showing domains of bulk material having various surface levels that are bounded by IDBs. The holes (dark regions) that are depicted in Figure 5 correspond to the narrow domains that grow under a slower growth rate.

A high density of linear and planar defects is also present in specimens grown under Ga-rich conditions. In Figure 6, the corresponding sapphire/AlN and AlN/GaN interfaces are depicted with the $[11\bar{2}0]$ crystallographic axis parallel to the electron beam. The highly strained area of the early stages of GaN growth just above the buffer layer exists here too. The IDBs emerging from the sapphire/AlN interface transverse the GaN film along the [0001] direction reaching the top surface of the film. Here, both domain types exhibit similar growth rates, and this is probably due to the significant increase in the width of the inverse polarity domains. This results in a rather smooth top surface of the GaN film with low roughness compared to the roughness of the N-rich specimens (Figure 7).

Significantly less multiple basal SFs near the surface area compared to the N-rich specimens, are detected (Figure 8). These are also visible with the $10\bar{1}0$ reflection (Figure 8) and are extincted with the 0002 (Figure 7b) and $11\bar{2}0$ reflections, as in the previous case; thus they are of the same I_2 type with a **p**=$1/3\langle 10\bar{1}0\rangle$ displacement vector. No prismatic domains near the AlN/GaN interface are observed in the Ga-rich specimens.

Concluding Remarks

GaN films epitaxially grown on (0001) sapphire by MBE suffer significant morphological and structural changes that are strongly dependent on the Ga/N ratio fluctuations during growth. A high density of linear and planar defects is detected in all cases. Specimens grown under N-rich conditions present a "flat roof" top surface resulting from the different growth rates of narrow and wide domains between the IDBs. On the other hand, in Ga-rich specimens a low roughness surface is observed. I_2 type SFs near the surface area is detected in both cases, which are significantly denser in the N-rich conditions. In addition, prismatic domains containing amorphous material near the AlN/GaN interface are observed only in N-rich specimens.

Acknowledgments

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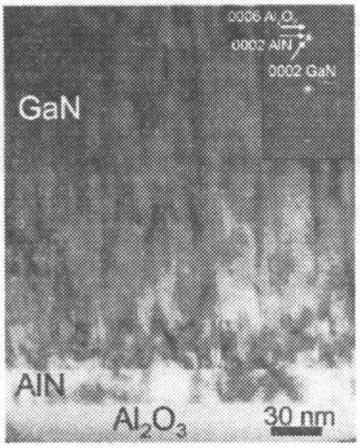

Figure 1. TEM micrograph depicting the Sapphire/AlN and AlN/GaN interfaces in a N-rich specimen.The corresponding diffraction pattern is given as an inset.

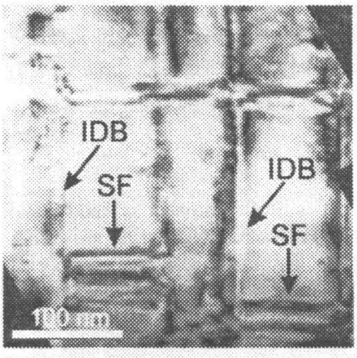

Figure 3. TEM micrograph illustrating interactions between IDBs and multiple I_2 basal Sfs in the N-rich specimens.

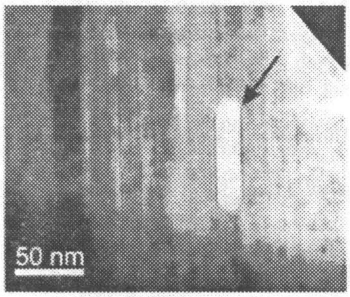

Figure 4. TEM micrograph showing a prismatic domain near the AlN/GaN interface elongated along the growth

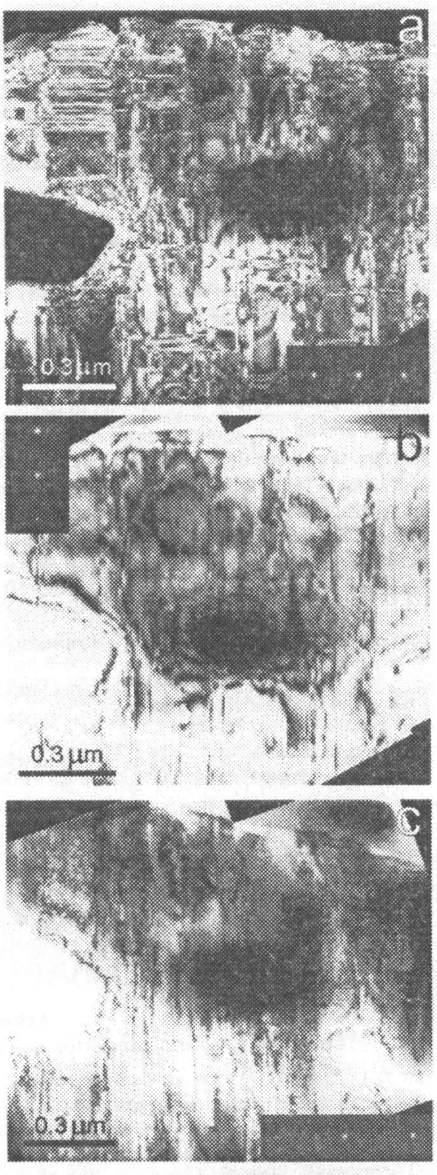

Figure 2. a) Dark Field (DF) TEM micrograph with the $10\bar{1}0$ reflection, depicting the I_2 basal SFs and the "flat roof" morphology of the top surface of the GaN film. b, c) Bright Field (BF) micrographs of the same area with the 0002 and the $11\bar{2}0$ reflections, respectively, where SFs are in overall extinction.

Figure 5. N-rich specimen in plan-view geometry. Bright regions correspond to domains of bulk material bounded by IDBs, whereas dark "holes" correspond to narrow domains growing under slower growth rate.

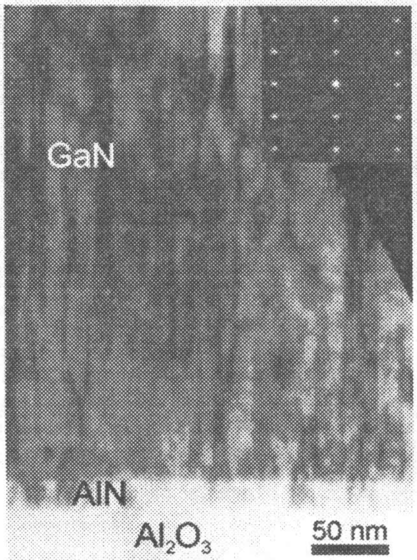

Figure 6. TEM micrograph depicting the Sapphire/AlN and AlN/GaN interfaces in a Ga-rich specimen. The corresponding

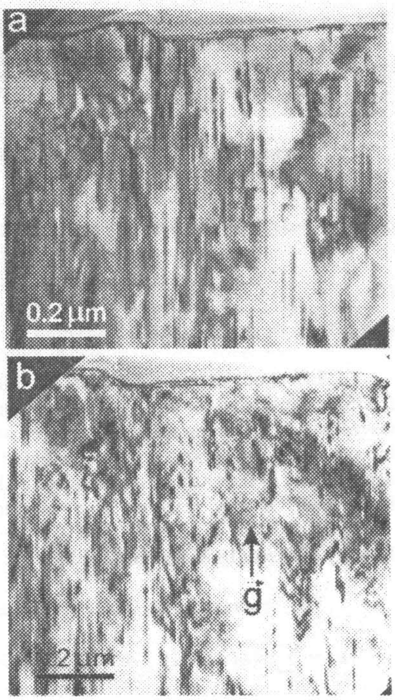

Figure 8. TEM micrographs depicting the wider inverse polarity domains between IDBs and the smoother top surface of the GaN film, in a Ga-rich specimen. a) With the $11\bar{2}0$ pole. b) With the 0002 reflection, where basal SFs are in extinction.

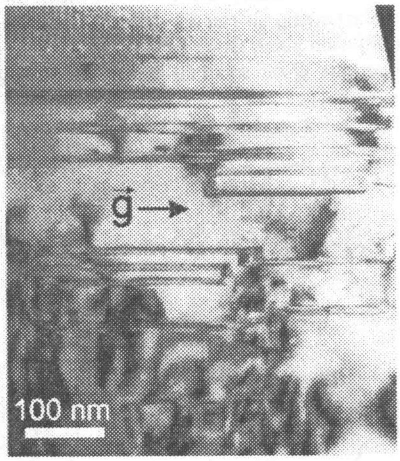

Figure 7. TEM micrograph of the top surface of GaN in a Ga-rich specimen illustrating the existence of basal SFs, with the