phys. stat. sol. (b) **234**, No. 3, 935–938 (2002)

Origin of Inversion Domains in GaN/AlN/Si(111) Heterostructures Grown by Molecular Beam Epitaxy

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(Received July 22, 2002; accepted October 1, 2002)

PACS: 68.37.Lp; 81.15.Hi

Using high-resolution electron microscopy, the formation of inversion domains inside GaN layers grown by molecular beam epitaxy (MBE) on Si(111) was investigated. It was shown that when the buffer layer thickness is small (15 nm), the inversion domains form inside a nitrogen polar layer at the steps on the Si(111) surface. As the thickness of the AlN buffer layer is increased to 35 nm, the MBE GaN layer polarity switches to gallium polarity, but inversion domains still form. In this situation they originate at the GaN/AlN interface.

Introduction Over the last few decades III–V nitride semiconductors have become very promising materials for optoelectronic and power device applications. Most of the successful devices have been obtained with layers heteroepitaxially grown on Al_2O_3 and SiC by metalorganic chemical vapor deposition (MOCVD). Nevertheless, the epitaxial growth of III–N semiconductor films on Si substrates is an interesting alternative to Al_2O_3 and SiC, due to the availability of large and high-quality wafers. Moreover, this kind of growth should make possible the integration of GaN optoelectronic properties with the well-known silicon technology.

Si(111) substrates have the necessary hexagonal symmetry for GaN growth, but with a large lattice mismatch and high thermal expansion coefficient difference with respect to the epilayer, making epitaxial growth difficult. An amorphous SiN_x layer at the GaN/Si(111) interface can be observed during the direct growth of GaN on Si(111) substrates, which is not desirable for a good epitaxy [1, 2]. AlN buffer layers were found to improve the overgrown GaN film; however, a high density of extended defects, including threading dislocations, inversion domains and stacking faults, has been determined in GaN/AlN/Si(111) heteroepitaxies [3, 4]. In contrast to GaN epilayers grown on Al_2O_3 and SiC substrates to which much work has been devoted, inversion domains in GaN/AlN/Si(111) have received less attention.

The existence of inversion domains in GaN/AlN/Si(111) systems was previously characterized using techniques described in work on GaN/sapphire. Experimental investigations carried out by conventional transmission electron microscopy (CTEM) and convergent beam electron diffraction (CBED) revealed the presence of inversion domains

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 0370-1972/02/23412-0935 $ 17.50+.50/0

at the GaN surface, even in Ga-polarity layers [5]. Moreover, the characterization of GaN/AlN/Si(111) indicated that the AlN buffer layer thickness influences the inversion domain density. High-resolution transmission electron microscopy (HRTEM) analysis of IDBs showed that two different atomic configurations coexist inside the same layer by interacting with a basal stacking fault [6].

In this work we focus on the origin of inversion domains in GaN/AlN/Si(111) heterostructures grown by molecular beam epitaxy (MBE). Earlier reports on inversion domains in systems grown on sapphire showed that these defects are generated mostly at small surface steps [7]. We have attempted to make a connection between these defects to the Si(111) substrates through the characterization of the AlN/Si(111) interface.

Experimental Two (0001)GaN films grown by plasma-assisted MBE (PA-MBE) on AlN-buffered (111)Si substrates have been characterized. The AlN buffer layers were grown at 820 °C and the GaN epilayers at 760–780 °C. The main difference between the samples is the nominal AlN buffer layer thickness: 15 nm and 35 nm for samples A and B, respectively. TEM specimen preparation was carried out by mechanical grinding up to 100 μm and dimpling down to 10 μm, followed by ion milling to electron transparency. The HRTEM studies were performed using Jeol 2000-EX and TOPCON 0002B electron microscopes, both operating at 200 kV.

Results and Discussion Although the existence of inversion domains and the atomic structure of their boundaries have been previously demonstrated [5, 6], the origin of these defects in GaN/AlN/Si(111) is still a matter of debate. Previous studies have showed a connection between the (0001) sapphire surface and the formation of the inversion domains in the GaN epilayer related to the surface steps in the GaN/sapphire system [7]. Geometrical analysis and experimental results obtained from HRTEM indicated that the inversion domain boundaries originated on *c*/6 and *c*/3 steps in order to relax the shift along the *c* axis introduced by such steps. The inversion domains were not observed on stepless surface substrates, confirming the relationship between these defects and the substrate configuration.

During epitaxial growth of the AlN buffer layers on the Si(111) substrates, the symmetry is broken at the AlN/Si(111) interface. The Si(111) substrate, although this orien-

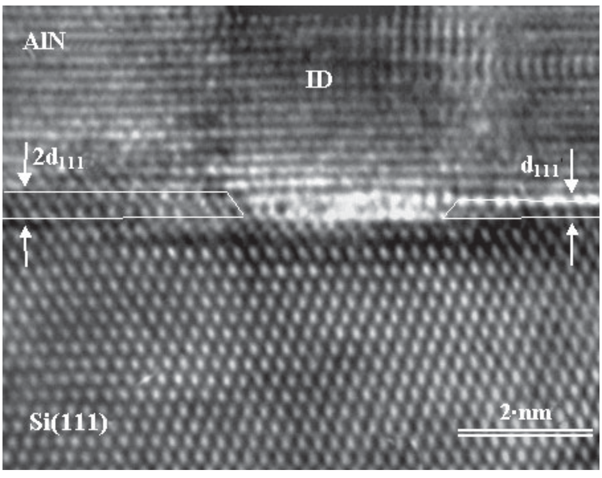

Fig. 1. $\langle 11\bar{2}0 \rangle$ HREM image at the AlN/Si(111) interface in the GaN/AlN/Si(111) system

tation presents the required hexagonal symmetry, is cubic and centrosymmetric whereas the AlN has hexagonal and non-centrosymmetric symmetry. Therefore, one has to analyze the AlN/Si(111) interface in order to determine the possible origin of the inversion domains previously observed in the GaN epilayer. In Fig. 1, corresponding to sample A, an inversion domain is shown to originate at the AlN/Si interface. This inversion domain is directly connected to the substrate surface, without any amorphous layer at the interface with Si(111). As can be observed in this image, the inversion domain has a small diameter at the interface with Si. In this area two steps with different height have been determined in the substrate. Steps with heights of d_{111} and $2d_{111}$ nm on the right and left side of the inversion domain, respectively, form a small terrace, $\sim$3 nm, where this defect has nucleated. This is in good agreement with previous studies carried out on GaN/sapphire systems where steps introduce a shift along the *c* axis that may be minimized by the introduction of inversion domain boundaries if these steps form a small terrace. In the growth direction, the difference in the lattice parameter between the AlN and Si substrate ($\sim$20%) leads to an even larger mismatch than in the GaN/sapphire system, and the inversion domain boundary generation probably helps in the relaxation along the growth axis [7]. There is another fact to consider: the coexistence of two atomic configurations of the inversion domain boundaries (Holt and IDBV) in the GaN epilayer. The Holt-type configuration was shown to be present in very small domains, so in this case the steps in the Si substrate could be one of the factors leading to Holt inversion domain formation in the GaN film.

However, in GaN/AlN/Si(111) another origin of these defects has been observed. Figure 2 shows an inversion domain in the GaN epilayer arising from the AlN buffer layer in sample B. In this case, the inversion domain contrast does not continue down to the Si substrate surface. As can be seen, the inversion domain appears on top of a misorientated grain in the AlN buffer layer. Unfortunately, the misorientation of this grain of AlN with respect to the GaN epilayer makes it quite difficult to determine the interface position. It is still not clear if the inversion domain formation is due to steps at the AlN/GaN interface or to the buffer grain misorientations.

An AlN buffer layer thickness influence on the polarity of the GaN epilayer was previously determined [5]. The N-polarity in sample A led to a higher inversion domain density in the GaN than in sample B, with Ga polarity. In this case, the AlN buffer layer thickness appears to be an important factor in determining the GaN polarity. The thicker AlN buffer layer in sample B led to a Ga polarity in the layer.

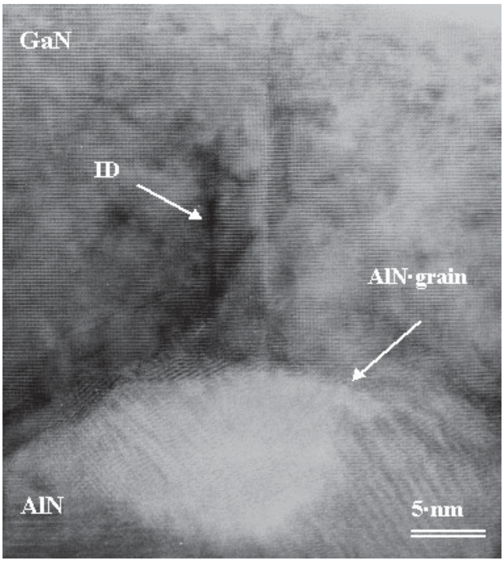

Fig. 2. $\langle 11\bar{2}0\rangle$ HREM image at the GaN/AlN interface in sample B

Summary The formation of inversion domains inside GaN layers grown on Si has been investigated. It is shown that the small 10–20 nm inversion domains originate on steps at the Si surface or on the top of the AlN buffer layers in connection with misorientated grains.

Acknowledgements The authors acknowledge the support of the EU under contract HPRN-CT-1999-00040, the Junta de Andalucia (PAI TEP 0120), the DME-SCCYT-UCA and MCYT (project MAT2000-0478-P4-02). The samples were kindly provided by Professor E. Calleja and his group (Universidad Politecnica de Madrid).

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