Materials Science Forum Vols. 433-436 (2003) pp. 1003-1006
online at http://www.scientific.net

Structural Study of GaN Layers Grown on Carbonized Si(111) Substrates

F.M. Morales[1], A. Ponce[1], S.I. Molina[1], D. Araújo[1], R. García[1], J. Ristic[2]
M.-A. Sánchez-García[2], E. Calleja[2], V. Cimalla[3] and J. Pezoldt[3]

[1]Dpto. de Ciencia de los Materiales e Ingeniería Metalúrgica y Química Inorgánica
Universidad de Cádiz, Apdo. 40, Puerto Real, ES-11510 Cádiz, Spain

[2]Dpto. de Ingeniería Electrónica, ETSI Telecomunicación, Universidad Politecnica de Madrid
ES-28040 Madrid, Spain

[3]FG Nanotechnologie, Zentrum für Mikro- und Nanotechnologien, Postfach 100565
DE-98684 Ilmenau, Germany

Keywords: GaN, MBE, RTCVD, Si Carbonization, SiC

Abstract: A structural study of a fabricated GaN/AlN/SiC/Si structure is reported. The GaN layer is grown by molecular beam epitaxy (MBE) on carbonized Si substrates where SiC is covered by a thin AlN buffer layer before GaN deposition. Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Selected Area Electron Diffraction (SAED) studies allow evaluating the structural quality of the obtained SiC and GaN. As a first step, Si carbonization in a rapid thermal chemical vapor deposition reactor (RTCVD) is used to obtain ultra-thin β-SiC(111)//Si(111) structures where SiC exhibits good crystalline orientation, homogeneity and structural quality. The latter allows to obtain a thin SiC buffer between the Si substrate and the GaN layers. The grown GaN layer is thicker than one micron and results of electron diffraction indicate that the GaN layer is well aligned with the Si(111) substrate. The measured surface dislocation density is in the range of $10^9 cm^{-2}$, thus SiC/Si templates improve the GaN structural quality compared to pure silicon substrates.

Introduction

The emergence of new wide band-gap semiconductors results from their attractive characteristics in terms of semiconducting (high open circuit voltage, high breakdown field, etc.) and thermomechanical (thermal conductivity, mechanical resistance, etc.) behaviors. Among them, silicon carbide demonstrates to be a powerful candidate in microelectronics world for high power applications even in aggressive environments. In addition, SiC is also used as substrate for group III-Nitride (III-N) heteroepitaxial growth due to its relatively low lattice mismatch and its similar thermal expansion coefficient. However, the limited wafer diameter and the high price of SiC substrates motivate to search alternative substrates for growing III-N layers.

Thin SiC on Si pseudo-substrates support both III-N feasible growth and the low cost development of these structures within the well-known Si technology. Most of the attempts on direct growth of III-N films on Si often demonstrated three dimensional growth of GaN islands due to the combination of large mismatches, difference in surface energy and chemical reactivity of Si surface with the subsequent generation of a high threading dislocation densities. These dislocations limit the performance of devices due to increased carrier recombination, leakage currents increment and loss in breakdown strength, efficiency and lifetime of optical devices [1,2]. Thin SiC and AlN buffer layers not only reduce the large mismatch between Si and GaN but also act as masks to protect Si substrates against active nitrogen supplied during GaN growth. The aim of this contribution is to demonstrate that with a short and simple thermal treatment before GaN growth on Si, a reduction of one order of magnitude in dislocation density can be obtained with respect to direct growth of GaN on Si.

Experimental

Si wafer (111) orientation was carbonized in a RTCVD system [3] using a mixture of 0.15 % of propane in H2 during 60 s with a final temperature of 1280° C and a ramp rate of 50 K/s. Later on, SiC is covered by a thin AlN buffer layer before GaN deposition. The AlN and GaN layers were grown by plasma-assisted molecular beam epitaxy (MBE), using a radio-frequency plasma source to activate the N2, and standard Knudssen effusion cells for Ga and Al. The substrate temperature is determined with an optical pyrometer. More details about the system configuration are given in reference [4]. The growth of the GaN layer was performed at 700-730°C while the AlN layer was grown at 760°C.

TEM, HREM and SAED were the techniques used to study the inner crystalline structure of the samples. Specimens were prepared for cross section TEM (XTEM) and plan view TEM (PVTEM) using mechanical thinning and Ar^+ milling at 4.5 KV in a Gatan Dual Ion Mill system. Conventional TEM was carried out in a JEOL JEM-1200EX electron microscope and a JEOL JEM-2000EX/THR was used for HRTEM.

Results and discussion

In a first stay, well-defined homogeneous and continuous flat SiC layers were visualized from XTEM images of the sample studied. This structures mainly consisted of ultra-thin β-SiC(111)/Si(111) with an average measured thicknesses of 2.1 nm for a 3 inches wafer. More details about this structure can be found elsewhere [5]. Since the atomic arrangement of (0001) plane of 6H-SiC is equivalent to (111) plane of 3C-SiC, the deposition of good quality hexagonal AlN (0001) buffer layers for further hexagonal (0001) GaN overgrowth is possible. Moreover, SiC buffer layers thickness in combination with growth temperature of GaN plays a very important role in growing a good epitaxial GaN film and thin SiC films are needed [6]. The AlN buffer layer between SiC and GaN structures has an estimated measured thickness of 25 nm and the grown GaN layer is about 1.35 μm in thickness measured from XTEM and SEM micrographs. Electron diffraction results indicate that the GaN layer is well aligned with the Si(111) substrate.

GaN thickness and roughness. The GaN/SiC structure is studied by SEM and TEM. The roughness was measured to be about ± 25 nm from XTEM images of surface profiles (fig 1 (a)). These kinds of images are registered in [110] zone axis from not affected surfaces where glue of specimen preparations persists and only show topography but not the whole GaN layer. SEM micrographs show a continuous GaN layer with certain surface roughness as it is shown in the cross-section images of fig. 1 (b) or in the plan view image of fig. 1 (c).

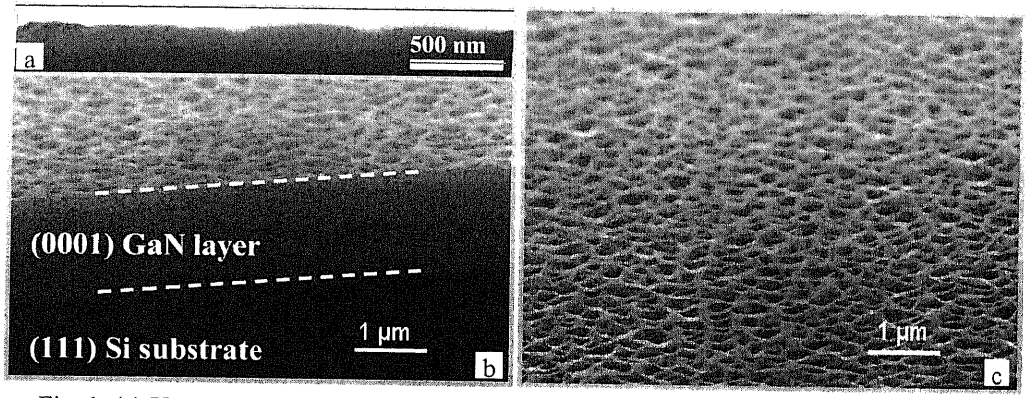

Fig. 1. (a) XTEM roughness profile. SEM micrographs in cross-section (b) and plan view (c).

Well-aligned crystalline GaN. SAED patterns registered from all samples prepared indicate that the grown GaN layers are well aligned with respect to the Si (111) substrate. Fig. 2 (a) corresponds to the diffraction associated to the specimen prepared for XTEM registered along the [1 1 0] zone axis of Si. The good crystalline quality of the formed GaN is demonstrated since no other diffraction spots related to polycrystalline inclusions appear. SiC and AlN diffraction do not appear due to their small contribution to the diffraction. The net of spots encircled is associated to Si diffraction while the other spots correspond to the diffraction of hexagonal GaN along the [1 1 $\bar{2}$ 0] zone axis. Indeed, SAED patterns in PVTEM were indexed to correspond to the [0 0 0 1] zone axis of GaN.

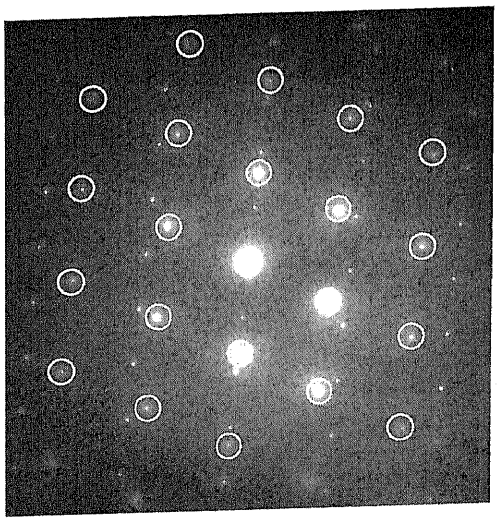

Fig. 2. SAED pattern of a XTEM preparation where GaN and Si diffraction are evidenced. Encircled spots correspond to Si-

Defect structure (dislocations). Threading dislocations (TD) have been characterized from both XTEM and PVTEM preparations micrographs. The density of these dislocations in our sample is estimated to be $3.7 \pm 0.7 \times 10^9$ cm^{-2}. Fig. 3 is a PVTEM image in two beam conditions obtained with the (1 1 $\bar{2}$ 0) reflection registered near the [0 0 0 1] zone axis of GaN. Dislocations reaching the GaN surface that are visible in this image have Burger vectors b=1/3 [1 1 $\bar{2}$ 0] and 1/3 [1 1 $\bar{2}$ 3]. Some of these dislocations coming to the GaN surface are pointed out with arrows. Other related defects such as grain boundaries or micropipes are detected. The dislocation density measured is smaller or in the range than other reported before in GaN/carbonized Si or GaN/Si [1,6-9].

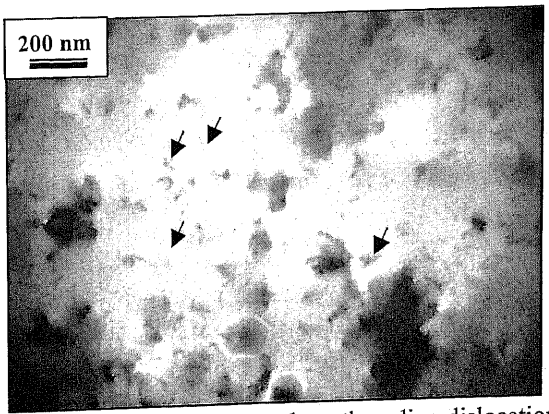

Fig. 3. PVTEM micrograph of GaN surface where threading dislocations are revealed.

Fig. 4 is a weak beam (WB) XTEM image obtained with the (0 0 0 2) reflection working near the [1 $\bar{1}$ 0 0] zone axis. The layer structure of the sample is shown in this image. GaN is not complete in thickness due to the specimen preparation. Dislocations can also be visualized in cross section; TD or characteristics semi-loops in GaN on the AlN layer are the common defect patterns on

different regions. TDs mainly propagate to the surface but some of them bend laterally contributing to the dislocation density decreasing.

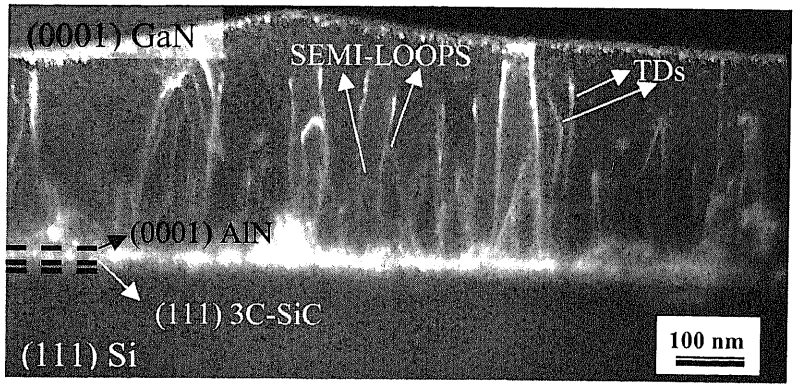

Fig. 4. WB XTEM image of the studied sample.

Conclusion

An epitaxial hexagonal GaN layer with a dislocation density in the range of 10^9 has been achieved on AlN-buffered carbonized Si (111) wafers by MBE. This result confirms that SiC/Si pseudosubstrates are promising templates to improve the GaN quality with respect to the reached by direct growth on silicon substrates.

Acknowledgements

This work has been financed by the project MAT2000-0478-P4-02 and the Junta de Andalucía (Group TEP-0120). TEM measurements were carried out at the "División de Microscopía Electrónica, SCCYT, Universidad de Cádiz".

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