phys. stat. sol. (a) **176**, 447 (1999)

Subject classification: 68.55.Jk; 78.55.Cr; 78.66.Fd; S7.14

Properties of Homoepitaxial and Heteroepitaxial GaN Layers Grown by Plasma-Assisted MBE

M.A. SÁNCHEZ-GARCÍA[1]), F.B. NARANJO (a), J.L. PAU (a), A. JIMÉNEZ (a), E. CALLEJA (a), E. MUÑOZ (a), S.I. MOLINA (b), A.M. SÁNCHEZ (b), F.J. PACHECO (b), and R. GARCÍA (b)

(a) Departamento de Ingeniería Electrónica, ETSI Telecomunicación, UPM, Ciudad Universitaria s/n, E-28040 Madrid, Spain

(b) Departamento de Ciencia de los Materiales e Ingeniería Metalúrgica y Química Inorgánica, Universidad de Cádiz, Apdo. 40, E-11510 Puerto Real (Cádiz), Spain

(Received July 4, 1999)

This work presents a comparative study of the growth by plasma-assisted molecular beam epitaxy (MBE) of GaN layers on four different substrates: Si(111), Al_2O_3(0001), GaN/Al_2O_3 and ELOG GaN/Al_2O_3 templates. Optimization of the growth parameters for the case of growth of GaN layers on silicon substrates leads to smooth films with surface roughness below 5 nm, intense low temperature photoluminescence (PL) (15 meV FWHM) and X-ray diffraction (XRD) values of 8.5 arcmin. (FWHM). The quality of the material clearly improves when growing on sapphire substrates obtaining intense low- and-room temperature PL (10 and 54 meV FWHM, respectively) and XRD values of 6.5 arcmin (FWHM). The best GaN epilayers (intense low-temperature PL emissions with FWHM of 4 meV) are obtained when growing homoepitaxially on high quality GaN/Al_2O_3 templates, reproducing the optical and structural properties of the template underneath. Finally, the dislocation density decreases drastically from (6 to 10) $\times 10^9$ cm^2 for the case of silicon substrate to $<10^6$ cm^{-2} for the GaN layers grown on the ELOG templates.

1. Introduction

One of the main problems in the field of group III nitrides is the lack of a commercially available substrate which would be lattice and thermally matched to Ga(Al)N. Although most of the current achievements in the device area have been obtained by metalorganic epitaxial techniques (MOVPE) using Al_2O_3 and SiC substrates [1], the advantages of molecular beam epitaxy (MBE) should play an important role when dealing with GaN homoepitaxy. This work presents a comparative study of the growth by plasma assisted MBE (PA-MBE) of GaN layers on four different substrates: Si(111), Al_2O_3(0001), GaN/Al_2O_3 and ELOG GaN/Al_2O_3 templates.

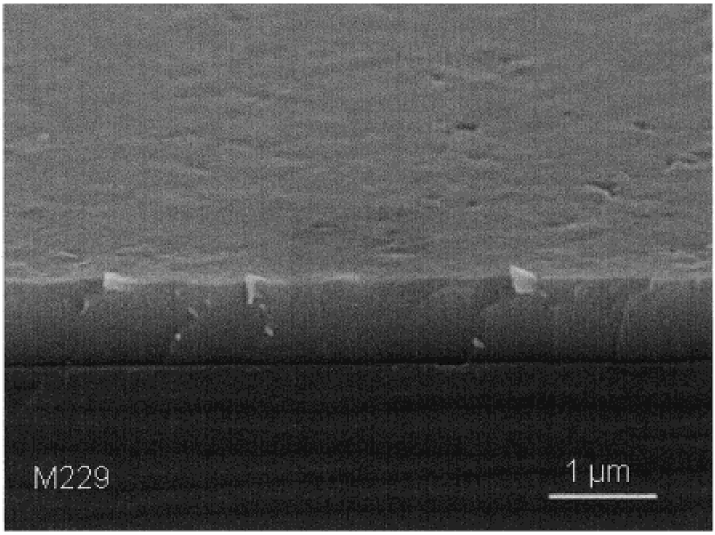
2. Experimental

The growth of all the GaN layers was carried out by PA-MBE using a radio-frequency (RF) source to activate the nitrogen and a standard Knudsen effusion cell for the gallium. More details about the growth system can be found elsewhere [2].

[1]) Corresponding author; Phone: 34 91 549 5700 (x334); Fax: 34 91 336 7323; e-mail: sanchez@die.upm.es

Optimization of the growth parameters used in the growth on Si(111) substrates indicated that an initial coverage of the Si surface with a few monolayers of Al was necessary to prevent the formation of amorphous Si_xN_y at the interface [3]. Following this procedure, GaN layers were grown at 750 °C using high-temperature (800 °C) AlN buffer layers [4] of 150 nm thickness.

For the growth on sapphire substrates, *c*-axis oriented 1in diameter Al_2O_3 wafers were employed. Different growth initiations have been studied, i.e. low-temperature (450 °C) GaN and high-temperature (800 °C) AlN buffer layers. The GaN epilayer is grown on top of one of these buffers at 750 °C.



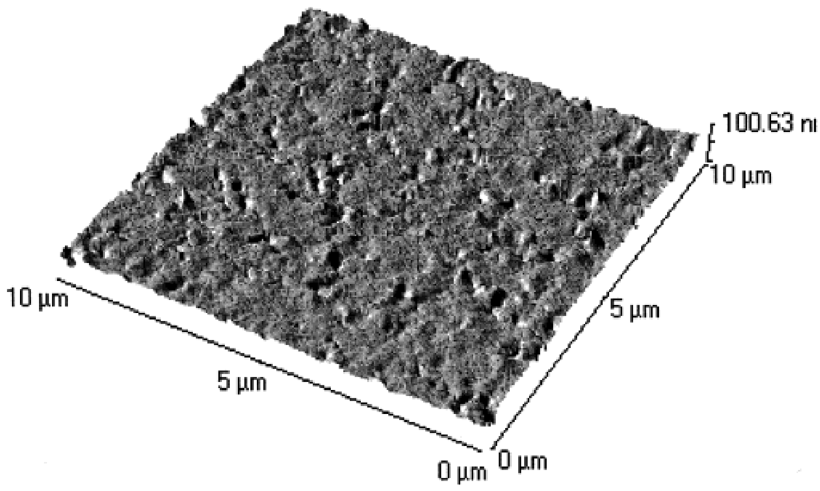


Fig. 1. Atomic force (AFM) and scanning electron microscopy (SEM) photographs of a GaN layer grown on AlN-buffered Si(111) substrate. Surface roughness of 5nm (rms value)

Two different types of GaN/Al_2O_3 templates are used in this study. The *standard template*, provided by Aixtron, consists of a GaN layer grown on sapphire by MOCVD, while the second one (*ELOG template*), provided by CHREA (Valbonne), included an ELOG process giving rise to a high quality GaN layer on top [5]. Outgassing of these templates takes place at a low temperature (760 °C) to avoid possible decomposition of the GaN layer in the vacuum atmosphere of the system [6]. Growth initiates at 750 °C activating the nitrogen plasma source and opening the shutter of the gallium cell.

3. Results and Discussion

GaN layers grown on Si substrates exhibited surface roughness below 5 nm and XRD values of 8.5 arcmin (FWHM) [3]. Fig. 1 shows AFM and scanning electron microscopy (SEM) photographs of one of these layers. Fig. 2a shows a plan view transmission electron microscopy (PVTEM) image, obtaining a dislocation density in the range (6 to 10) $\times 10^9$ cm^{-2}. This density can be decreased down to 8×10^8 cm^{-2} with heavy Si doping (above 1×10^{18} cm^{-3}) [7]. The low-temperature optical properties (PL) in Fig. 3b reveal an emission at 3.466 eV (sample under tensile residual strain) with a FWHM of 15 meV.

Growth on sapphire substrates has been carried out using two types of buffer layers, as can be seen in the XTEM images of Fig. 4. The high-temperature AlN buffer layer

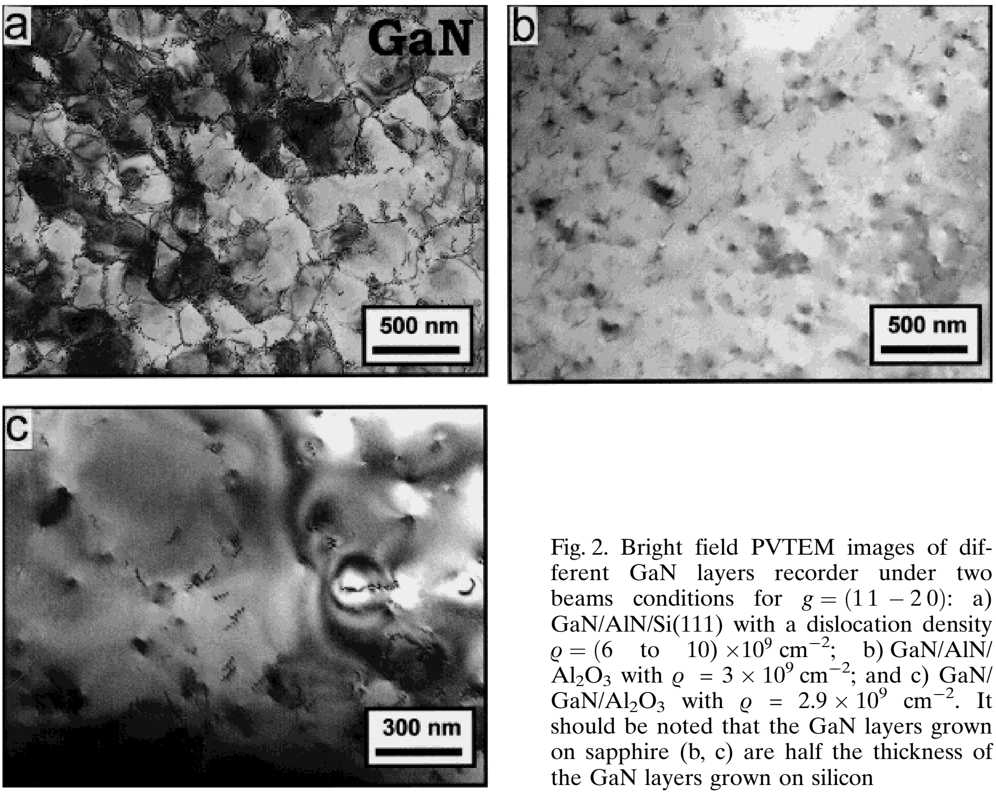


Fig. 2. Bright field PVTEM images of different GaN layers recorder under two beams conditions for $g = (1\,1\,-2\,0)$: a) GaN/AlN/Si(111) with a dislocation density $\varrho = (6$ to $10) \times 10^9$ cm^{-2}; b) $GaN/AlN/Al_2O_3$ with $\varrho = 3 \times 10^9$ cm^{-2}; and c) $GaN/GaN/Al_2O_3$ with $\varrho = 2.9 \times 10^9$ cm^{-2}. It should be noted that the GaN layers grown on sapphire (b, c) are half the thickness of the GaN layers grown on silicon

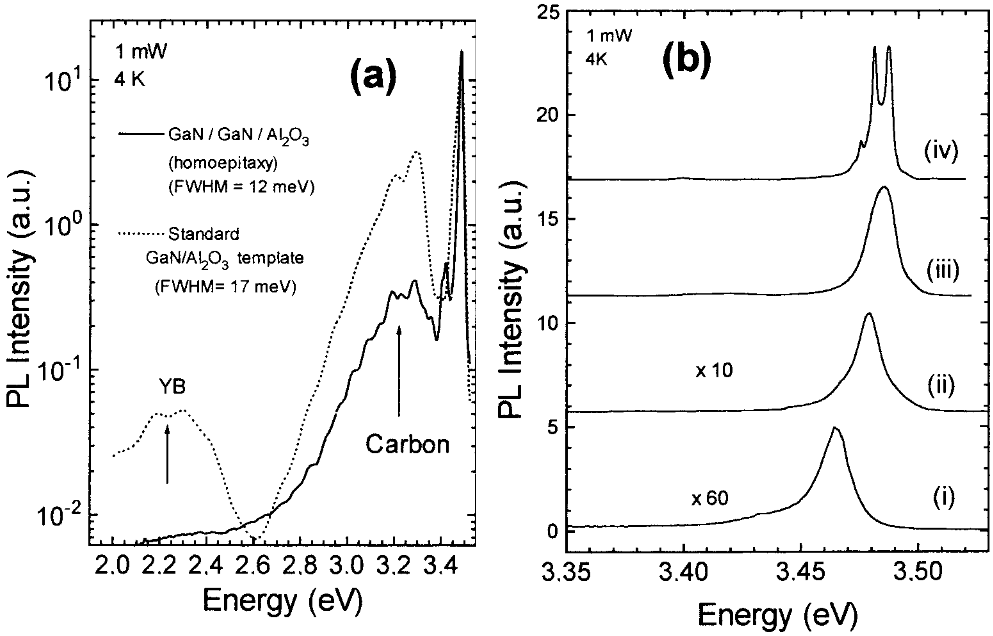


Fig. 3. Low-temperature photoluminescence spectra of: a) standard GaN template and GaN layer grown on standard GaN template; b) GaN layers on different substrates: (i) GaN/AlN/Si(111), (ii) GaN/AlN/Al_2O_3, (iii) GaN/GaN standard template, and (iv) GaN/GaN ELOG template

presents a better AlN/GaN interface quality as compared with the low-temperature GaN buffer, which presents more interface roughness and a large number of planar defects which do not propagate towards the top GaN layer and that could act as dislocation filters. The dislocation densities (Figs. 2b and c) measured in these layers are very similar (around $3 \times 10^9\ cm^{-2}$ for both types of buffers) but represent a considerable improvement with respect to the growth on silicon substrate, if we consider that the thickness of the GaN layers grown on sapphire are almost half the value of the GaN on silicon ones. The structural (XRD values of 6.6 arcmin) and optical properties (intense low- and room-temperature PL with 10 and 54 meV FWHM, respectively) are also improved, especially for the case of the low-temperature GaN buffer layer, and in spite of not being fully optimized.

The growth of GaN layers using GaN templates has led to the best results of this study. Fig. 3a shows the low-temperature PL spectra of a standard GaN template (with no MBE layer grown on top) and that of a GaN epilayer grown on top of the same template. Although the intensities of the dominant emission at 3.481 eV are very similar in both cases, there is some improvement in terms of FWHM, from 17 meV for the standard template down to 13 meV for the GaN epilayer. There is also a substantial decrease (close to one order of magnitude) in the intensity of the emission centered around 3.25 eV for the case of the MBE-grown GaN epilayer, which can be assigned to carbon contamination and which is normally higher in MOCVD material as compared with MBE. Another characteristic of the MOCVD-grown material is the appearance of the yellow band, which can also be observed in the spectrum of the standard template.

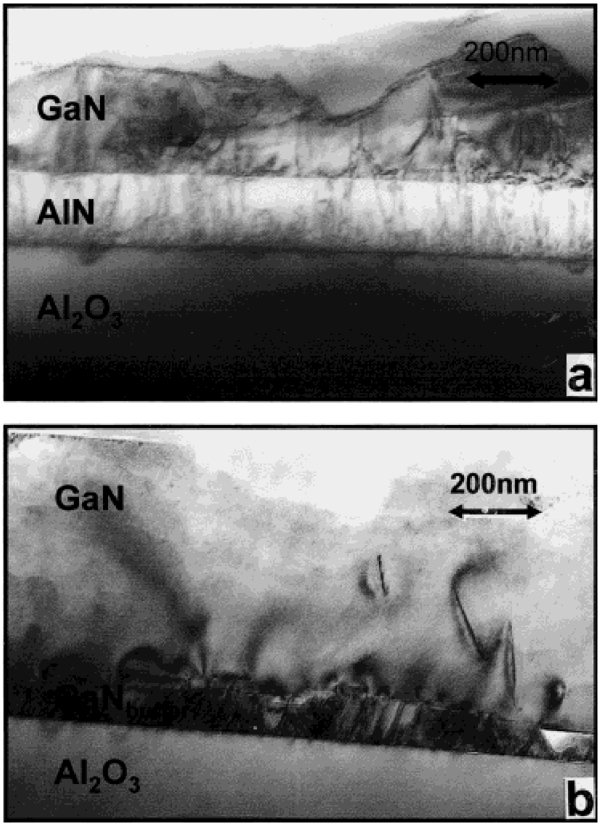


Fig. 4. Low magnification XTEM images near the $\langle 1\,1\,{-2}\,0\rangle$ zone axis under two beams conditions with the reflection (0002), showing different defect structures in GaN epilayers grown on (0001) sapphire substrates with: a) a high-temperature AlN buffer layer, and b) a low-temperature GaN buffer layer

Fig. 3b (iv) shows the PL spectrum of a GaN layer grown on ELOG template with two much narrower emissions (4 and 3 meV FWHM) than previous layers. The exact origin of each one of these two emissions is still under study. The dislocation density for the case of the layers grown on standard templates was 1.5×10^9 cm^{-2} and $<10^6$ cm^{-2} for the layers grown on ELOGs. This extremely low density value is obtained in regions of the GaN layer located above the SiO mask from the ELOG process reproducing the high structural quality of the initial template.

In summary, GaN epilayers grown homoepitaxially by PA-MBE on high quality GaN/Al_2O_3 templates (ELOG) reproduce the optical and structural properties of the substrate underneath leading to intense low-temperature PL emissions with FWHM of 4 meV and dislocation densities below 10^6 cm^{-2}. With these results, it is proved that MBE techniques can produce epilayers of the same quality as MOVPE whenever growth is started on a suitable high crystal-quality GaN substrate. The advantages of MBE over MOVPE can now be exploited for the fabrication of complex semiconductor structures.

Acknowledgements This work has been supported by ESPRIT LAQUANI 20968 Project and ALDUV Project ENV4-CT97-0539. The group from Cadiz wishes to acknowledge the financial support by CICYT Project MAT98-0823-C03-02 and Junta de Andalucía (Group PAI TEP 0120).

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