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Structural characterisation of GaAlN/GaN HEMT heterostructures

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Abstract

(GaN/GaAlN/GaN)//Al_2O_3(00.1) HEMT heterostructures have been studied by X-ray scattering techniques, transmission electron microscopy and atomic force microscopy. X-ray reflectometry has been used to determine with a high accuracy both the individual layer thicknesses and the interfacial roughness, in spite of the weak electronic density contrast between layers. From the Fourier inversion method and using a simulation software, the roughness of the interface corresponding to the two-dimensional electron gas location has been determined equal to 0.5 nm. Both high resolution X-ray diffraction and transmission electron microscopy experiments have shown the excellent crystallinity of the heterostructures. Finally, the surface morphology has been inferred using atomic force microscopy experiments.

Keywords: X-ray reflectometry; GaAlN/GaN heterostructures; High electron mobility transistors; Thickness determination; Fourier inversion method

1. Introduction

Wide band gap semiconductors, such as SiC and GaN, exhibit many attractive properties far beyond the capabilities of Si and GaAs: an unique combination of the wide band gap, a high breakdown field (over 2 MV/cm), a high saturation velocity and the ability to form high quality GaAlN/GaN heterostructures with good transport properties make them ideal candidates for high power, high frequency applications [1]. Due to the piezoelectric properties of the nitrides, a positive polarisation charge is formed at the GaAlN/GaN interface. As a result, a dense two-dimensional electron gas (2DEG) is formed even in the absence of any intentional doping of the barrier. GaAlN/GaN high electron mobility transistors (HEMTs) with very impressive power densities up to 30 W/mm at 4 GHz have been reported by Cree research [2].

In this paper, we report on a comparative study of the structural properties of GaAlN/GaN HEMT heterostructures on sapphire substrates using X-ray reflectometry (XRR), high resolution X-ray diffraction (HRXRD), TEM and AFM experiments.

2. Experiment

GaAlN/$GaN_{1.2\ \mu m}$ HEMT heterostructures under study were grown by low pressure metalorganic chemical vapor deposition (LPMOCVD). They consisted of a thick (1.2 μm) insulating GaN buffer layer followed by 25–30 nm undoped or Si doped GaAlN layer with Al content varying from 22% to 29% and finally, a GaN cap layer with thickness varying from 0 to 5 nm. Introducing a GaN cap layer modify the band diagram of the heterostructure. Indeed, adding such a GaN cap layer to the GaAlN/$GaN_{1.2\ \mu m}$ heterostructure introduces a negative polarization charge at the upper heterointerface, causing increased electric fields in the GaAlN layer and a decrease in 2DEG density [3]. In the following, the (GaN/GaAlN) heterostructure refers to the bilayer stacking on top of the thick GaN buffer layer.

XRR experiments were carried out using a Seifert MZ-IV Bragg–Brentano $\theta/2\theta$ goniometer equipped with a back-curved graphite monochromator selecting the K_α wavelength from a Cu sealed tube. X-ray reflectometry [4] has been used to infer the individual layer thicknesses of both the AlGaN layers and the (GaN/GaAlN) heterostructures. Basics of XRR experiments and Fourier data-inversion procedure applied to XRR profiles, expressed in terms of the refraction-corrected diffraction-vector S_{corr}, has been described in other references [5,6]. The geometry of an XRR experiment is the well-known specular $\theta/2\theta$ one, θ being the grazing angle of incidence and 2θ the angle between the detector and the incident beam. In the following, the corrected XRR profiles are referring to the $[S_{corr}^4 I(S_{corr})]$ curves, i.e. the intensity expressed versus S_{corr} and multiplied by S_{corr}^4 (correction by the substrate reflectivity). Applying a Fourier

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transform procedure, usually called Fourier inversion method, to a corrected XRR profile gives the autocorrelation function (ACF) of the electronic density derivative, leading to distances between interfaces [5–7].

HRXRD rocking-curves measurements have been performed using a Philips goniometer equipped with a Bartels double-Ge(2 2 0)-crystals monochromator, which selects the $\lambda_{K_{\alpha 1}}$ (0.1540562 nm) wavelength, and without any rear optics. TEM experiments have been carried out using a TOPCON EM002B (Cs = 0.4 mm) operated at 200 kV. Cross-sections were obtained by mechanical thinning and ion milling (PIPS-Gatan) with 2.5 keV Ar^+ ions. Surface morphologies have been determined by atomic force microscopy (AFM) with a VEECO D3100 operated in tapping mode.

3. Structural study of GaAlN/GaN HEMT heterostructures by X-ray reflectometry

3.1. Individual layer thicknesses determination

A $[GaN_{3\ nm}/Ga_{0.78}Al_{0.22}N_{25\ nm}]/GaN_{1.2\ \mu m}//Al_2O_3(00.1)$ heterostructure has been first studied by the Fourier inversion method applied to the XRR profiles, in order to determine the individual layer thicknesses inside the (GaN/GaAlN) bilayer. Indeed, applying directly a simulation procedure is not relevant due to the weak electronic density contrast between the GaAlN ($\rho_{e^-} = 1471\,e^-/nm^3$) and the GaN ($\rho_{e^-} = 1613\,e^-/nm^3$) layers, leading to a weak contrast of the corresponding fringes (Fig. 1a). It can be noticed that the thickness of the 1.2-μm thick GaN is too large to be inferred by XRR experiment. As shown in Fig. 1b, the corrected XRR profile displays two oscillations, a long-period one and a short period one. The long-period oscillation refers to the 3-nm nominally thick GaN layer (see the arrows in Fig. 1b) and the small-period oscillation refers to the (GaN/GaAlN) bilayer thickness. It can be noticed that the corrected profile (profile on top in Fig. 1b) has been filtered by removing a 5-order polynomial function from the corrected profile in order to enhance the contribution from these two oscillations. In the following ''corrected-profile'' is referring to the corrected-profile which has been filtered (bottom profile in Fig. 1b). Fig. 1c shows the ACF spectrum from the corrected XRR profile. The first peak is related to the GaN layer thickness, and the second one to the (GaN/AlGaN) bilayer thickness. Their positions give 25.2 ± 0.2 nm for the GaAlN layer thickness and 4.0 nm for the GaN one.

3.2. Interfacial roughnesses

The roughness at the ($AlGaN/GaN_{1.2\ \mu m}$) interface is an important parameter to be determined since it corresponds to the 2DEG location. To this end, the electronic density profile (EDP) has been determined using a simulation software [8], starting from the results of the Fourier inversion method and fixing the (GaN/GaAlN) thicknesses values, i.e. varying only the interface and surface roughness σ parameters. Simulation has given the following result: $(Ga, N, O)_{1.2\ nm}/\sigma = 0.3$ nm/$GaN_{4\ nm}/\sigma = 0.2$ nm/$AlGaN_{25.2\ nm}/\sigma = 0.5$ nm/$GaN_{1.2\ \mu m}$. In particular, the roughness of the ($AlGaN/GaN_{1.2\ \mu m}$) interface, i.e. in the vicinity of the 2DEG location, has been determined equal to 0.5 nm. A comparison between the ACF spectra from both the experimental XRR profile and the simulated one has been performed (Fig. 2). The excellent agreement between both the corrected XRR profiles (Fig. 2(b)) and the ACF spectra (Fig. 2(c)) validates the main results from the simulation, in particular the individual layer thickness values and the ($AlGaN/GaN_{1.2\ \mu m}$) interfacial roughness.

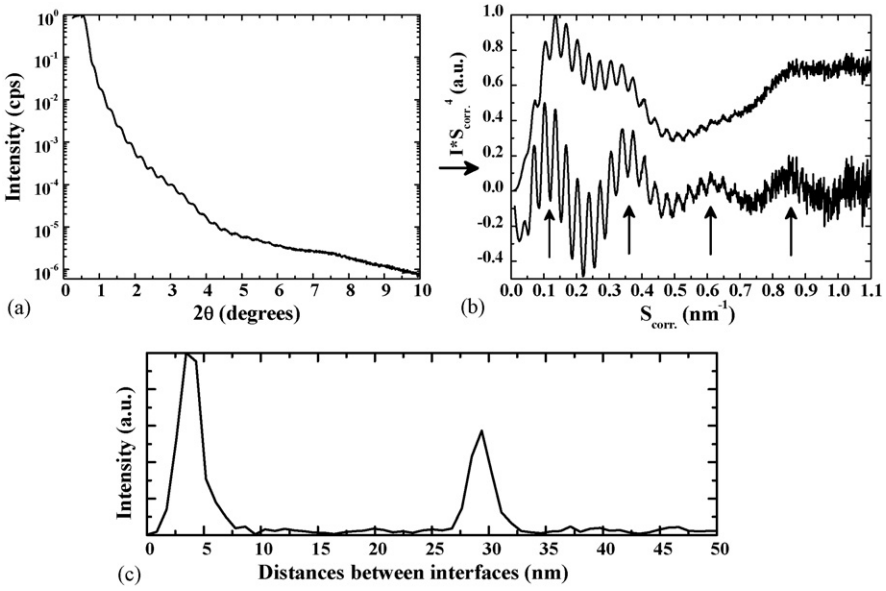


Fig. 1. (a) Experimental XRR profile from the $[GaN_{3\ nm}/GaAlN_{25\ nm}]/GaN_{1.2\ \mu m}//Al_2O_3(00.1)$ heterostructure. (b) Top: corrected XRR profile; bottom: corrected XRR profile after filtering by a polynomial component. The arrows show the fringe positions related to the GaN top layer thickness. (c) ACF spectrum of the corrected XRR profile after filtering.

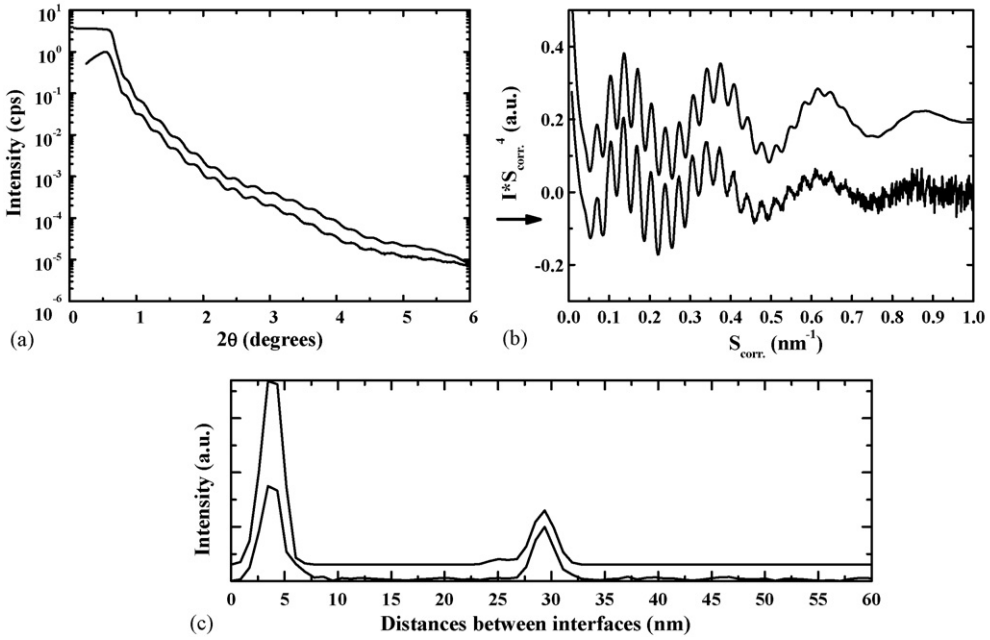


Fig. 2. (a) Experimental XRR profile (bottom) and simulated XRR profile (top) from the (GaN/GaAlN)/$GaN_{1.2\ \mu m}$//Al_2O_3(00.1) heterostructure. (b) Corrected experimental XRR profile (bottom) and corrected simulated one (top). (c) Corresponding ACF spectra.

4. Complementary structural studies by HRXRD, TEM and AFM experiments

Complementary to the XRR experiments, HRXRD rocking-curves have been performed to investigate the heterostructure crystallinity on a ($GaN_{5.5\ nm}$/$GaAlN_{25.6\ nm}$)/GaN HEMT heterostructure, in which thicknesses have been determined by XRR. Fig. 3 shows both the experimental and the corresponding simulated X-ray rocking curves related to the mentioned GaN/GaAlN/GaN HEMT heterostructure, performed around the GaN (00.6). A fair superposition of the experimental and calculated X-ray rocking curves is observed which indicates a high degree of crystalline perfection of the GaAlN layer. This means that there is no apparent grading of the layer (good homogeneity of the composition) and abrupt structural interfaces. The "structural" term refers here to the (00.*l*) crystallographic planes. The observation of Pendellösung fringes in the experimental spectrum allows a very good correlation between measured and expected layer thicknesses (GaAlN: 25.6 nm; GaN cap: 5.5 nm), in good agreement with the XRR results. Since HRXRD is mainly sensitive to the structural interfaces and XRR is sensitive to the chemical interfaces, it means that both the structural and the chemical interfaces coincide. Hence, according to the good fringe contrasts in both the XRR and HRXRD profiles, this means no rugosity at the interfaces (that is a two-dimensional growth). The large full-width at half-maximum of the thick GaN buffer layer integrates both the effect of the underneath GaN nucleation layer and the mosaïcity induced by the threading dislocations. From the fit of the experimental X-ray rocking curves, Al content of the high band gap layer has also been extracted.

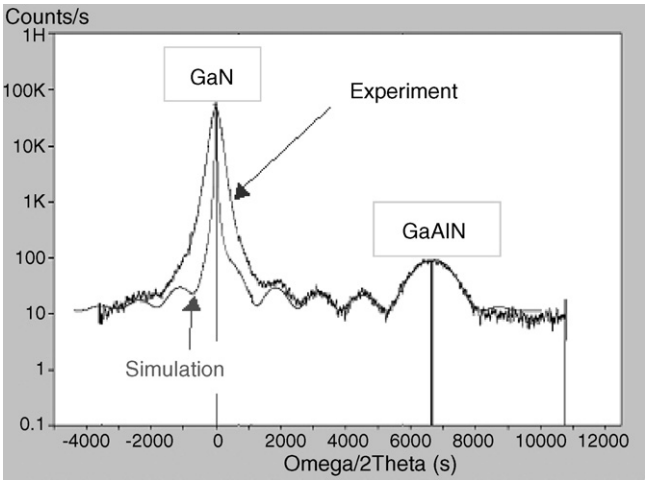


Fig. 3. X-ray rocking curves of a GaN/GaAlN/GaN heterostructure with GaN cap layer = 5.5 nm, around the GaN(00.6).

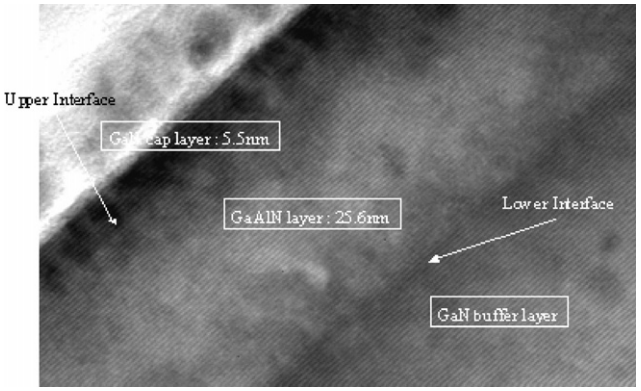
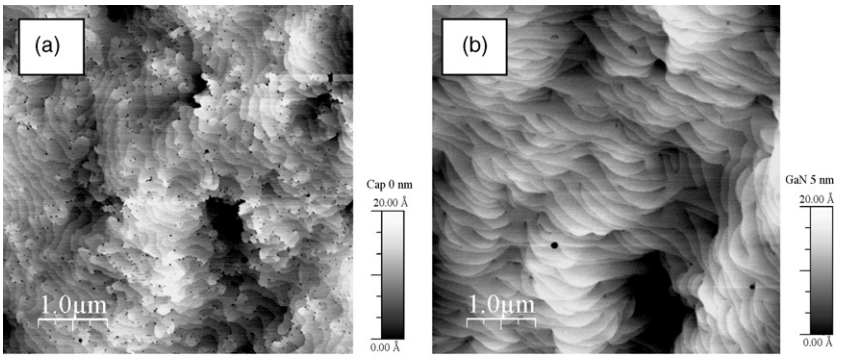


Fig. 4. TEM cross-section of a GaN/GaAlN/GaN HEMT double heterostructure with GaN cap layer thickness equal to 5.5 nm.



(a) x_{Al} = 29.13%
Threading Dislocations = 2.10^{9}cm^{-2}
RMS roughness = 0.488 nm

(b) x_{Al} = 27.96%
Threading Dislocations = 2.10^{8}cm^{-2}
RMS roughness = 0.452 nm

Fig. 5. Surface morphology of 2 in. GaAlN/GaN/Al_2O_3 HEMT structures: (b) with and (a) without GaN cap layer.

The good structural quality of such an heterostructure has been confirmed at the atomic scale by TEM. The upper and lower heterointerfaces GaN/GaAlN and GaAlN/GaN are sharp and perfectly delineated as observed in Fig. 4. The thicknesses of the measured layers fit very well the expected thicknesses already measured by HRD and XRR.

Finally, a comparison of the surface morphology between GaAlN/GaN/Al_2O_3 HEMT structures with and without the GaN cap layer has been performed using atomic force microscopy (AFM). AFM measurements performed on capped heterostructures revealed less defect density (ED), more than an order of magnitude, as compared to HEMT structures without cap layer (as illustrated in Fig. 5). Results concerning a comparative study on the structural and electrical properties of heterostructures with GaN cap layer thicknesses varying from 0 to 5 nm, as determined by XRR, are reported in Ref. [9].

5. Conclusion

A structural study of GaN-capped GaAlN/GaN HEMT heterostructures on sapphire substrates has been performed. In particular, the individual layer thicknesses from the top (GaN/GaAlN) bilayer and the interfacial roughnesses have been determined by XRR technique using a two-steps method which allows to overcome the problem of the weak contrast of electronic density between both the GaN and GaAlN layers. First, the model-independent Fourier inversion method has been applied in order to infer both the thin-GaN cap layer and the GaAlN layer thicknesses. Then, a model-dependant simulation procedure has been used to determine the individual layer thicknesses using the results of the Fourier inversion method and fixing the (GaN/GaAlN) thickness values. The roughness of the (GaAlN/GaN) interface, where is located the 2 DEG, has been determined equal to 0.5 nm. Complementary structural studies by both HRXRD and TEM experiments have confirmed the excellent crystalline quality of these heterostructures. A comparison between surface morphology of both non-capped and GaN-capped GaAlN/GaN HEMT heterostructures by AFM has revealed less surface-defect density for the GaN-capped heterostructure.

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