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СВОЙСТВА, ДИАГНОСТИКА И ПРИМЕНЕНИЕ ПОЛУПРОВОДНИКОВЫХ МАТЕРИАЛОВ И СТРУКТУР НА ИХ ОСНОВЕ

AlGaN/GaN HETEROSTRUCTURES IN HIGH ELECTRON MOBILITY TRANSISTORS

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AlGaN/GaN heterostructures are of high research and industrial interest for the production of high electron mobility transistors (HEMT) utilizing the two-dimensional electron gas (2DEG) induced at the interface due to polarization effects. In the current work, the effect of AlGaN thickness on 2DEG formation is under discussion. In particular, ultrathin layers of AlGaN (between 2–12 nm thick) are grown on top of GaN. Composition of these layers is studied and variations of surface potential are mapped using Kelvin probe force microscopy (KPFM) to see the evolution of the 2DEG formation in relation to layer thickness and stoichiometry. The obtained results allow concluding about critical thickness of AlGaN layer for the formation of continuous 2DEG at the AlGaN/GaN interface.

Key words: AlGaN/GaN heterostructures; two-dimensional electron gas; Kelvin probe force microscopy.

INTRODUCTION

Wide bandgap semiconductors, such as GaN and SiC, show advanced materials properties for device operation at higher temperatures, voltages and switching speed, thus, making them attractive for power and high-frequency electronics [1, 2]. In particular, GaN, which has much higher breakdown field, thermal conductivity and charge carrier velocity compared to Si, is of high interest for power switching devices and it is already commercialized, for example, in Schottky diodes and HEMT. In HEMT, outstanding performance can be reached due to the formation of 2DEG at the interface with another III-N semiconductor, typically AlGaN, ensuring high electron concentration with high mobility [3–5].

At ideal AlGaN/GaN interface (defect free), the lattice mismatch and difference in coefficient of thermal expansion (CET) lead to the strain formation. Since nitride semiconductors lack centre of inversion symmetry, presence of strain causes piezoelectric polarization (P_{PE}). There is also spontaneous polarization (P_{SP}) due to the difference in electronegativity of the III-N materials. These two phenomena induce polarization charges at the interface. The field direction and polarity depend on GaN termination at the interface, which can be either Ga- or N-faced [6]. For example, for relaxed (by dislocations) GaN buffer and AlGaN layer with tensile strain on the top the polarization would cause positive net charge $+\sigma$

on the AlGaN side requiring "negative" compensation from GaN in the form of 2DEG originated by the donor-like surface states (see Fig. 1).
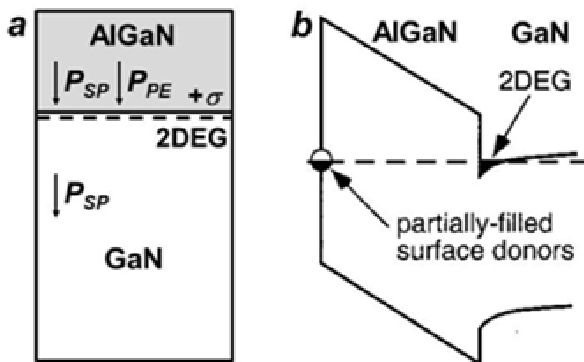
Figure 1. – Schematic representation of (*a*) AlGaN/GaN interface illustrating polarization directions, net charge density and 2DEG and (*b*) band structure at the interface with donor-like surface states

However, crystalline quality of real heterostructures is far from the ideal ones. Bulk crystalline GaN is very expensive and, therefore, the films are produced either by molecular beam epitaxy or metalorganic chemical vapour deposition (MOCVD) on Si, SiC and sapphire substrates. Due to the lattice and CET mismatches, the synthesised GaN films suffer from high concentration of threading dislocations (TD). Strain relaxation through TD also causes unintentional n-type doping of the semiconductor. The dislocations are terminated at the surface forming so-called V-defects which also affect crystalline quality of epitaxial AlGaN layer and 2DEG, in particular, decrease electron mobility [7]. Additionally to crystallinity, one needs to consider composition and thickness of AlGaN films. Both parameters were found to affect charge carrier concentration and mobility [8, 9]. Therefore, there is a continuous research to improve quality of the heterostructures in order to reduce TD density as well as to optimise parameters of interfaces for better HEMT performance [10–12].

In the current work, the emphasis is put on the study of how AlGaN composition and thickness affect the 2DEG. One of the key used methods is Kelvin probe force microscopy (KPFM) allowing to get insights into the polarization phenomena and related band bending at the heterostucture interface.

EXPERIMENTAL

The structures are grown on 2-inch single side polished (0001)-oriented sapphire substrates using the AIX 200/4 RF-S MOCVD reactor. Trimethylaluminium, trimethylgallium and ammonia are used for the synthesis. For all samples, about 750 nm thick AlN buffer layer is grown on the substrate followed by ca. 1 μm thick GaN film which is covered by AlGaN layer with nm-scale thickness. The samples are studied by atomic force microscopy and KPFM [13]. To reveal composition and stoichiometry of the samples, Rutherford Back-scattering (RBS) and X-ray Photoelectron Spectroscopy (XPS) combined with sputtering are utilized. Al 2p, Ga 3d and N 1s peaks are used for the analysis. Due to overlap of Ga LMM (Auger electrons) peak with N 1s one, it is hardly possible to accurately deconvolute the spectra that leads to possible underestimate of N content.

RESULTS AND DISCUSSION

RBS measurements carried out on the GaN buffer (without AlGaN) suggest that the Ga/N stoichiometry is 1/1. This information is used to calibrate the XPS and avoid the

above-mentioned underestimate of nitrogen. Nevertheless, the XPS analysis is only reliable for thicker AlGaN because in the case of thin layers the photoelectrons are emitted not only from them but also from the underlying GaN, thus, corrupting the data about composition. The results obtained from XPS are presented in Table showing more or less constant stoichiometry of thicker layers why in layers thinner than 5 nm, Al concentration is found to be lower most probably due to the Ga contribution from GaN buffer.

Table

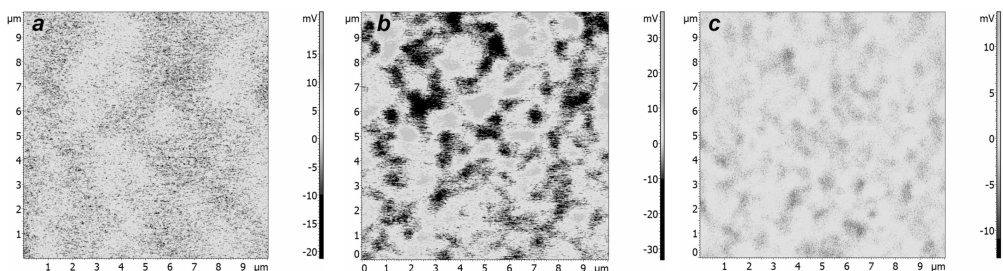**Composition and thickness of AlGaN layers obtained from XPS measurements**

Thickness (estimated from growth), nm	Al, %	Ga, %	N, %	Thickness from XPS, nm	Thickness from XPS + sputtering, nm
1–2	3.6	44.0	52.4	1.4	1.6
3–4	7.7	42.3	50.0	3.3	3.2
5–6	9.8	40.1	50.1	4.7	4.9
7–8	10.0	36.5	53.5	> 5	7.4
10	9.0	34.5	56.5	> 5	–
12	10.4	37.7	51.9	> 5	–

From XPS peak intensity one can also calculate thickness of the analyzed layers using following equation:

$$\frac{I_{Al}}{I_{Ga}} = \frac{I_{Al}^{\infty}}{I_{Ga}^{\infty}} \left(e^{d/\lambda \cos\theta} - 1 \right),$$ (1)

where I_{Al}/I_{Ga} is the ratio of XPS peak intensities for a particular layer, the ratio with ∞ sign corresponds to the thickest film in our case and equals to 0.28, d is the film thickness, λ is the mean free pass of electron in AlGaN (2.1 nm) and θ is the experimental angle. The calculated data presented in column "Thickness from XPS" agree well with those estimated from the growth parameters. Further study of the layer thickness is carried out by combining XPS with sputtering of the AlGaN films. Results of these measurements are presented in the last column of Table also showing good correspondence to both previous columns of the thickness. The XPS under sputtering data reveal that N concentration is almost constant through the AlGaN layers while Ga and Al contents change in dependent manner: there is higher concentration of Ga and lower of Al close to the GaN buffer while Ga content decreases and Al increases close to the surface.

KPFM is used to study variations of surface potential depending on AlGaN thickness (see Fig. 2). Pure GaN samples show homogeneous potential distribution across the surface and this map does not show any relation to the topography. Growth of thin (ca. 2 and 4 nm) layers of AlGaN leads to a mosaic-like potential distribution which is interpreted as variations in electron density at the interface due to poor stoichiometry of ultrathin films. Homogeneity of the surface potential maps increases with layer thickness allowing to conclude about a critical thickness of AlGaN for the formation of continuous 2DEG, which is in our case is estimated to be around 7–8 nm. Overall, the measured contact potential difference rises from pure GaN to AlGaN/GaN following the theoretical estimates for these compound semiconductors.

**Figure 2. – KPFM images of (*a*) GaN buffer, (*b*) AlGaN(3.5 nm)/GaN
and (*c*) AlGaN(10 nm)/GaN**

CONCLUSION

The obtained results show that thickness and composition of AlGaN layer formed on top of GaN buffer are critical parameters for the formation of 2DEG at the interface. One requires to overcome a critical thickness to form stoichiometric AlGaN in order to obtain continuous 2DEG across the interface. Further study of crystalline quality of AlGaN and parameters of charge carriers (concentration and mobility) are in progress.

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