Defect investigation in Al$_{0.87}$In$_{0.13}$/AlN/GaN heterostructures by scanning force microscopy methods

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Abstract. AlInN/AlN/GaN heterostructures were characterized by atomic force microscopy (AFM) in semi-contact and conductive mode. These indium-related alloys contain threading dislocations (TDs) with a density around $10^8$ ~ $10^9$ cm$^{-2}$, originating from the GaN (0001) substrate grown on sapphire. The TDs, with screw or mixed components, terminate at the surface of overgrown layers as V-defects. Using semi-contact AFM (phase-imaging) mode, we traced sites of indium segregation at the V-defects. These sites in V-defects were found to be highly conductive by current-AFM and could be a possible cause for the leakage current in Schottky diodes.

1. Introduction
Research on III-nitride semiconductors with a wide band gap varying between 0.63 eV (InN) and 6.2 eV (AlN) is achieving new heights due their potential wide range of applications in photonics and electronics. Heterojunctions based on III-Nitrides with high band-offsets have allowed Multiple Quantum wells (MQWs) (AlN/GaN or InN/GaN) based devices like Light Emitting Diodes (LEDs) and Laser Diodes (LD). They have shown promising results in terms of high emission efficiency, lifetime and have also realized red to UV/blue emission [1]. In the field of electronics, Heterojunction Field Effect Transistors (HFET) like High Electron Mobility Transistors (HEMT) based on AlGaN/GaN or AlInN/GaN have shown promising results in high frequency, high power operating-regime [2, 3] as they inherit properties like high electron saturation velocity and high breakdown voltage. However, these devices suffer from short lifetime and poor efficiency because of the presence of defects, poor surface/interfaces and phase-separation at inversion domains produced during their fabrication (growth) [4]. Due to availability of very few studies on their effect on optical and electrical properties, realization of high quality devices is hindered. Nanoscale investigation would be of considerable interest in determining their effect on the device electrical and optical properties [5]. Here, from the perspective of electronic devices (AlInN/GaN and AlInN/AlN/GaN HEMT structures), defects like threading dislocations (TDs) could be one of the deciding factors of device lifetime and efficiency. We have studied the electrical effects of these defects by tapping-mode AFM and conductive-AFM.
2. Methods

2.1. Current-Atomic Force Microscopy (contact mode)

Current AFM is operated in contact-mode with a constant bias voltage either applied to the AFM tip (with respect to the sample) or to the sample (with respect to the AFM tip). Here, as the AFM tip scans the surface, current is measured simultaneously. The image obtained providing details on spatial distribution of current, is called current-map. On a conductive sample where the AFM tip makes an ohmic contact with the surface, a current-map would give a one-to-one relation with the spatial distribution of resistivity as current is inversely proportional to the resistance. This is often called spreading resistance map (SSRM). However, when dealing with semiconductors, current-maps may not be proportional to spatial resistivity. Due to the inhomogeneity from phase-separation, clustering or defects, various factors like barrier height, band-gap, localized states and potential barrier would contribute to the current-map.

2.2. Phase-contrast image (semi-contact mode)

Nowadays, an AFM is often fitted with a cantilever oscillating at its resonant frequency, which is driven by piezoelectric crystal. During the scan, alteration in the oscillation amplitude (smaller than the free amplitude) from the surface features acts as a feedback signal to the electronic controller, which maintains the preset oscillation amplitude by adjusting the height of the scanner (piezoelectric crystal). This height is used to image the surface topography. Simultaneously alongside topography, the phase difference between cantilever oscillation and the driving signal applied to the piezoelectric crystal can also be monitored (phase-contrast image). This carries additional and complimentary information relating to certain surface properties including friction, adhesion and visco-elasticity, as they would affect the phase. One needs to be careful when associating phase-contrast with surface properties as above as it may be related to nanoscopic topographical artifacts, arising from enhanced adhesion due to an increased interacting area (e.g. at a grain boundary) or acting lateral forces at a step-feature. All the effects could be fundamentally described as an elastic/inelastic interaction of the AFM tip with the surface when operated at constant-amplitude [6, 7]. The surface energy of any material will vary spatially with a different chemical composition (originating from presence of oxide/aqueous layer, inhomogeneity and defects, not excluding contamination). In a real case situation, there will always be an inelastic interaction, and this loss of energy between the tip and surface can be summarized as the cause of phase-contrast. This type of imaging is a very powerful technique in providing surface properties.

2.3. Error mode image (semi-contact mode)

In semi-contact mode, during scanning the current value of the signal related to cantilever oscillation is the “error signal” of the feedback loop system. In this mode, feedback loop gain is adjusted in such a way that the feedback loop is able to follow the smooth features of the surface topography but not the abrupt features. Abrupt features in surface topography may occur from adsorbed nano-particles, structural defects or fabricated structures like trenches on the surface. So, abrupt features will appear with high contrast and smooth features with low contrast in error mode image. Therefore, error mode imaging is a useful method to enhance the contrast of very small (nm range) abrupt features.

3. Results and discussion

3.1. GaN

3 µm-thick GaN layers (000-1) were grown on sapphire at 1050 °C using LT (low temperature) GaN nucleation layer. This leads to the formation of semi-insulating (non-intentionally doped) n-type GaN. Semi-contact AFM topographical (fig. 1a) and phase-mode maps (fig. 1b) [8] show inverted pyramidal
shaped facets that could also be distinguished in phase contrast mode. These features can be related to inverted pyramidal shapes (V-pits), as it was found that in n-type GaN substrates, threading dislocations open as N-terminated V-pits (V-defects) [9, 10]. From the corresponding phase-contrast image, it is seen that the facets of these pyramidal structures show a phase different from other regions.

**Figure 1.** (a) Topography of GaN surface obtained in semi-contact mode. Pyramidal facet of TD (V-pit) is encircled. In the inset, its semi-contact error-signal image showing V-pits in GaN obtained at low feedback gain is shown and the corresponding phase-image (b) of the topography shown in (a). (c) Phase-profile and topography profile across the V-pit show a phase-difference between facets and GaN-surface.

**Figure 2.** (a) Topography of GaN surface obtained in contact mode. TD with screw-component is encircled (b) its corresponding current-map obtained at an applied bias of -6.5 volts to AFM probe. Reprinted with permission from [9]. Copyright [2008], American Institute of Physics.
This indicates that facets of TDs can be distinguished from their different surface energy. N-termination at the TD-facets due to surface reconstruction [9, 10] could explain the change in surface energy and hence, the contrast in phase-image.

It was already shown by Lochthofen et al. that N-terminated surfaces would also increase the electron affinity, which would lower the barrier locally [9]. In their current-map, here reproduced in fig. 2, it is seen that the TD facets show a relatively high current density compared to TD free surface (see figs. 2a & 2b). The same result has been also confirmed by the present analyses [11].

### 3.2. AlInN/AlN/GaN heterostructures

Alloys of AlN and InN (Al\(_{x}\)In\(_{1-x}\)N) grown on c-plane GaN-buffer have played a very important role in further improving HEMT devices. The association of polarization fields, both spontaneous and piezoelectric, with AlInN and GaN allows the induction of polarization charges, which is compensated by formation of a two-dimensional electron gas (2DEG) [3]. For an indium concentration of 17\%, AlInN is in lattice-match with GaN, allowing pseudomorphic-growth [12] and the presence of strong polarization fields in AlInN alone itself could cause high 2DEG density (~10\(^13\) cm\(^{-2}\)). However, the large difference in lattice-constants and thermal decomposition of AlN and InN prevent good quality growth of AlInN.

AlInN (33 nm)/AlN (1nm)/GaN (3 \(\mu\)m) heterostructures were grown on sapphire. The density of V-pits associated to TDs was found to be ~10\(^7\) cm\(^{-2}\). As shown in figure 3(a), two different features related to TDs can be distinguished, V-pits and channels. Channels are a series of V-pits situated in proximity and as a result appear continuous. It is known that indium preferentially segregates at the core of threading dislocations on the GaN surface [1, 13, 14]. As the AlInN layer grows, threading dislocations propagate towards the surface forming an In-rich or metallic indium nano-pipe extending from the AlInN/GaN interface to the AlInN surface. Interestingly, threading dislocations with screw-component terminate at the surface with inverted pyramidal structures consisting of 6-facets due to surface construction as a part of strain relaxation (called V-defects). Migration of In-adatoms is strain driven and as a result In-N bonds (weaker bonds) occupy low-coordinated sites like the edges of these pyramidal structures, while Al-N bonds (stronger bonds) occupy high-coordinated sites like the bulk and the surface of V-defects [1].

While fig. 3a shows a topography map of the sample surface, fig. 3b is a phase contrast image of the surface, the dark contrast appearing at the edges of threadlike features and pits whereas bright contrast in their interior. As in phase imaging the contrast could be related to compositional variations [6, 7], this dark contrast at the edges of TDs can be related to In, where In is expected to be localized.

Figure 3. (a) Topography image of AlInN surface obtained in semi-contact mode. A pit is marked as 1 and channel is marked as 2. (b) Phase-contrast image of AlInN surface showing phase-contrast change around pits and threadlike features. There is dark contrast around the edges of threadlike features and pits whereas bright contrast in their interior. (c) Depth-profile and the corresponding phase-contrast profile across a channel and a pit marked in (a) and (b). Solid-line and dashed-line indicate channel and pit, respectively. Reprinted with permission from [15]. Copyright [2010], American Institute of Physics
One could also expect a localized increase or decrease of band-gap of AlInN due to the formation of Al-rich or In-rich regions, respectively (by Vegard’s law). The indium segregated could also show a metallic behavior. Current-map obtained by applying 10 volts between the tip and the surface shows that the edges of V-defects, where dark-contrast in phase-image is also seen, shows a high current density compared to other regions (see fig 4a and 4c). The presence of high indium concentration, which would reduce band gap locally or would act as shunt between the surface and 2DEG could explain the high current density.

Figure 4. (a) Topography image of AlInN surface obtained in contact mode focusing on V-defects marked as 1 and channels marked as 2 in its insets. (b) Current-map of AlInN surface corresponding to (a) showing the presence of high conductivity along the edges of channel and pit. Bias voltage = 10 V. (c) Depth-profile and the corresponding current-profile across a channel and a pit marked in (a) and (b). Solid-line and dashed-line indicate channel and pit, respectively. Reprinted with permission from [15]. Copyright [2010], American Institute of Physics

4. Conclusion
From phase-contrast and C-AFM analyses of GaN and AlInN, compositional variation in V-defects and their effect on electrical properties have been inferred. Phase contrast image shows a different chemical composition on the facets of V-defects in GaN and at the edges of V-defects in AlInN. In these regions, C-AFM shows higher conductivity due to the increase of electron affinity in the case of GaN and due to the high indium content at the edges of the V-defects in the case of AlInN. The presence of such conductive channels and V-defects would facilitate high gate leakage current in AlInN/GaN heterostructure based HEMT devices.

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