Study of the interaction of atomic hydrogen with GaN surfaces monitored by spectroscopic ellipsometry

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ABSTRACT

A key issue in the growth of wurtzite GaN films is the polar nature of the films arising from the absence of a symmetry center making the (0001) and (000−1) surfaces inequivalent. The morphology, optical, and electrical properties of GaN films with Ga− and N−polarity have been demonstrated to be significantly different, and strongly impact device performance. Furthermore, which reaction occurs on each polarity surface, (0001) and (000−1) has been unclear yet.
The present work aimed at providing further insight into the reactivity of GaN epitaxial films by investigating the interaction of GaN polar surfaces with atomic hydrogen produced by a remote r.f. H_2 plasma in order to distinguish not only film polarity, but also to discriminate different inversion domains (IDs) densities present in films with the same polarity. It is found that the surface reaction of atomic hydrogen with GaN epilayers is sensitive to GaN polarity and is useful for distinguishing films of mixed polarity, and with different densities of inversion domains (ID). This is because a different reaction rate and reaction extent is found for N− and Ga−polar GaN with atomic hydrogen, with N−polar GaN exhibiting greater reactivity. The reactivity has been in−situ monitored in real time by spectroscopic ellipsometry that measures the change of the GaN dielectric function during the exposure to hydrogen atoms.

INTRODUCTION

GaN and its alloys have emerged as important semiconductor materials for applications as emitters of yellow, green, blue, and ultraviolet light, as detectors and for high power electronics [1]. Because it is difficult to produce large bulk crystals of GaN for homoepitaxy [2], it is necessary to grow epitaxial layers on foreign substrates. Due to the polar wurtzite structure of GaN there exist two distinct {0001} planes. GaN(000−1) and GaN(0001) polar films, which are related to the stacking sequence of atomic structure, show differences in their physical and chemical properties. The [0001] orientation is known as Ga−face, while the [000−1] orientation is known as N−face. It is important to underline that polarity is a bulk property and not a surface property. These two different orientations cause, in addition to line defects, some kinds of planar defects, e.g., double positioning boundaries (DPB), stacking mismatch boundaries (SMB) and inversion domain boundaries (IDB).
The morphology, optical, and electrical properties of GaN films with Ga− and N− polarity have been demonstrated [3] to be significantly different, and strongly impact device performance. Nevertheless it is expected that Ga−face and N−face surfaces of GaN should have quite different chemical properties, which reaction occurs on each polarity surface has been unclear yet.
In this work, we present a process based on the interaction of GaN films with H−atoms from a remote plasma source to determine GaN film polarity. The efficacy of this process results from the different stability of the etching products (NH_x or GaH_x) and from the different reaction rate of the two polar faces. The reactivity has been in−situ monitored in real time by spectroscopic ellipsometry that measures the change of the GaN dielectric function during the exposure to hydrogen atoms.
The ellipsometric results combined with Kelvin probe microscopy (KP−EFM) measurement allows us to differentiate not only between films with opposite polarity, but also between epilayers with the same polarity but with a different density of IDs.

EXPERIMENTAL DETAILS

n−type GaN epitaxial layers with a thickness of ~ 1μm were grown under Ga−rich conditions on buffer layers on (0001) sapphire. In order to study the effect of the buffer layer engineering on the GaN bulk polarity, samples

grown by various techniques (MOCVD, Remote plasma MOCVD and MBE) and with various buffers of GaN and AlN have been tested. Further details can be found in other works [4].
To study the reactivity of GaN films, the samples were exposed to an atomic hydrogen flux produced by a remote r.f. H_2 plasma operated at 60 W, 1 Torr, and with an hydrogen flux of 800 sccm. All remote−plasma treatments were performed at a temperature less than 650 °C in order to avoid any effect due to thermal decomposition of GaN (threshold for GaN thermal decomposition has been reported to be 750 °C [5−7]
To evaluate change in surface and bulk composition and to detect change in surface roughness and morphology, the samples were analyzed by spectroscopic ellipsometry (SE). The kinetic of the surface reaction of atomic hydrogen with GaN epilayers was monitored in real time by ellipsometry operating in kinetic mode, i.e., by acquiring variation of the GaN dielectric function at the photon energy of 3.5 eV as a function of exposure time to atomic hydrogen with a time sampling interval of 500 msec. SE spectra of the real and imaginary parts of the pseudodielectric function are acquired in the energy range 1.5 − 5.5 eV and analysed in terms of the Bruggeman effective medium approximation (BEMA). Below the fundamental absorption edge, where GaN is transparent, multiple reflection at the sapphire substrate/GaN interface results in the interference fringes from which the film thickness can be deduced. Hence, the analysis of the variation of the fringes numbers and position is used to obtain film thickness variation due to an etching process,
The assignment of the H−atoms interactions behaviour to the polarity is also achieved by the analysis of surface potential maps by scanning Kelvin probe microscopy (KP−EFM). Kelvin probe EFM is one of the powerfull tools used to probe the surface potential distribution and its applicability to investigate GaN polarity and IDs has been already demonstrated by Jones et al [8].

RESULTS AND DISCUSSION

Figure 1 shows SE spectra of some GaN samples grown using different buffers layer that result in a different GaN epilayer/sapphire interface; the SE best−fit BEMA models from which the structure of films is derived are also shown. The different substrate/film interface results in GaN epitaxial layers with different structura, morphological and polarity properties. The AFM surface morphology and corresponding KP−EFM images of the surface potential and line profiles of the same GaN epitaxial layers are reported in Figure 2.

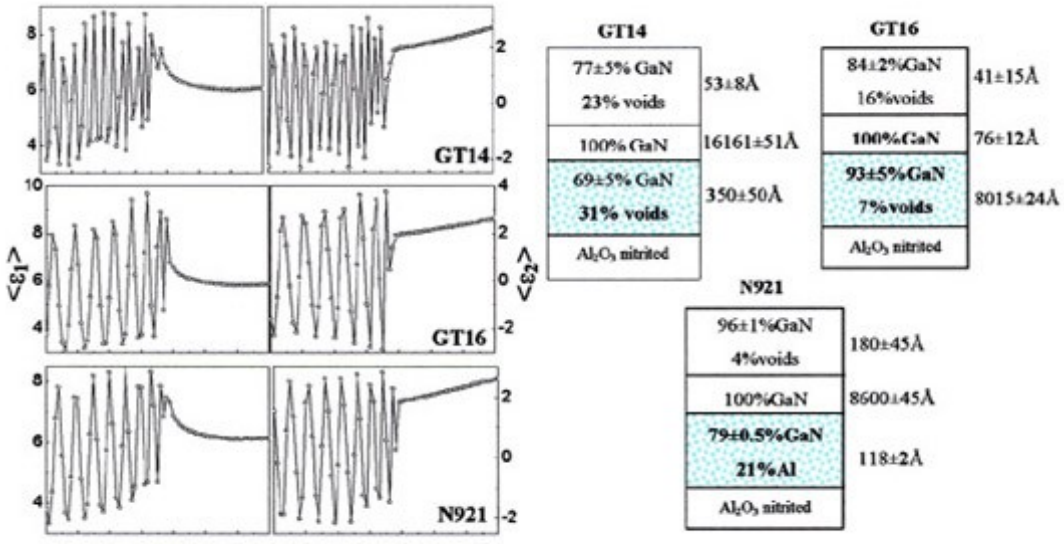

Figure 1: SE spectra of the real, $<\varepsilon_1>$, and imaginary, $<\varepsilon_2>$, parts of the pseudodielectric function recorded for the GaN samples grown using different buffer layers.

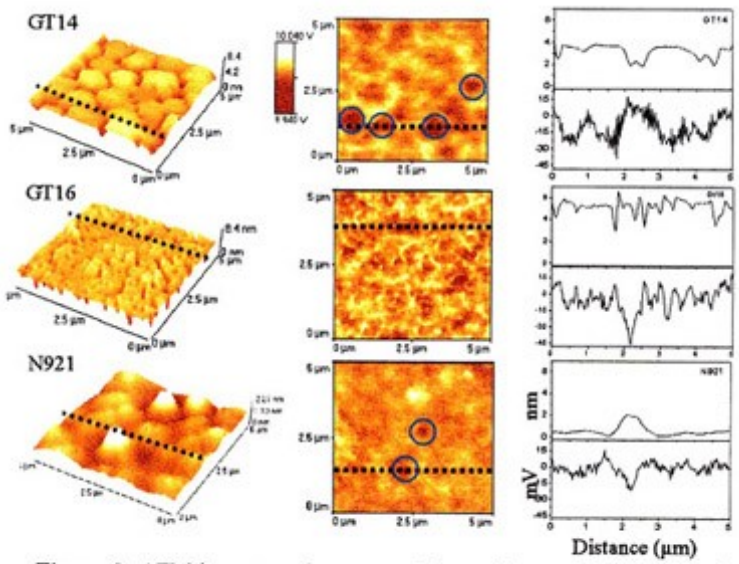

Figure 2. AFM images and corresponding surface potential maps of the as-grown GaN samples

All films have uniform and very smooth morphologies that are typical of Ga−polar surfaces. Inhomogeneities in the surface potential related to defects and inversion domains (IDs) are detected. Indeed, it has been reported [8] that N−polar domains have a surface potential lower than that of Ga−polar films. It si worthy to note in the line scan profiles that regions with lower surface potential do not correspond to a hole in the surface morphology (hence, we are sure that the tip is not retracing the surface morphology); rather, they correspond to hillocks in teh morphology (see for example sample N921) that are due to the different growth rate of the N− and Ga−polar regions. Therefore, the dark regions present in the as deposited GT14 film with a lower surface potential of −20/−30 meV (see profiles in fig. 2) can be associated to N−polar domains. As for film GT16 that is characterized by a higher density of dislocations a more complex surface potential map is recorded. For this sample a local increase of surface potential is found in the vicinity of threading, screw and mixed dislocations. Moreover, dark regions that are confined by threading dislocations are observed. In this case, localized strain will result in piezoelectric charging where the dislocation intersects the surface, as evidenced by the surface potential map. These results indicate that the density of the N−polar domains is higher for sample GT14 than for sample GT16. For sample N921, few N−polar domains are observed on a 5micron x 5micron scan area.

The different line profiles and SP−EFM maps provide evidence of different characteristics of the various GaN films that is expected to correspond to a different reactivity towards H−atoms.
The different kinetics of the variation of the imaginary part of the pseudodielectric function of GaN recorded during exposure of GaN epitaxial layers to H−atoms are compared in Figure 3.

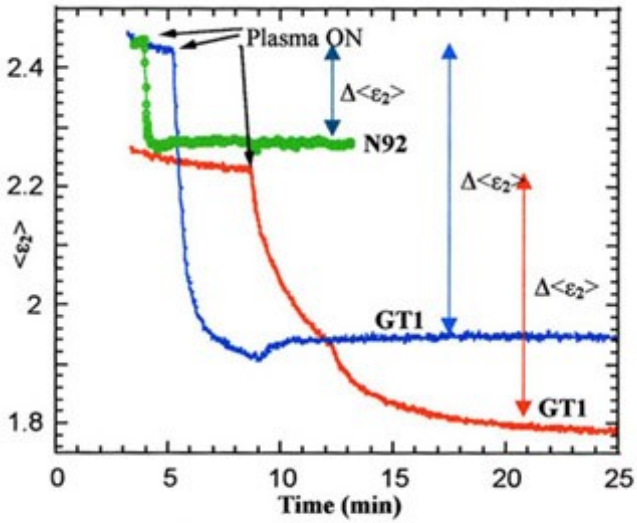

Figura 3. time variation of the real, $\langle\varepsilon_1\rangle$, and imaginary, $\langle\varepsilon_2\rangle$, parts of the pseudodielectric function recorded for the GT16, GT14 and N904 GaN samples

It is found that these kinetics differ in the initial rate, the total variation and in the time they reach a plateau value. In particular, it is found that the faster the initial rate, the shorter time for reaching a plateau and the smaller the overall variation. The observed variation of the imaginary part of the GaN dielectric function during exposure to H−atoms corresponds to a thickness decrease of the film due to etching of the N−polar domains. The thickness is reduced by 160 Å and 65 Å for samples GT14 and GT16, respectively; no thickness variation is found for the N921 sample with very few N−polar domains (see fig. 2). Therefore, a different "chemical reactivity" of H−atoms toward Ga− and N−sites is deduced. In particular, it is found that the larger the density of N−polar domains, the more reactive is the GaN surface to H−atoms and the larger the exent of GaN etching by H−atoms.
The different reactivity observed toward hydrogen treatment, is consistent with the different reactivity of N−polar and Ga−polar surfaces found by M. Eickoff et al [9], that showed the enhanced formation of native oxide on the N−polar surface.

CONCLUSION

In conclusion, it has been reported that the interaction of GaN films with atomic hydrogen depends on the electronic properties of surfaces and that this reactive process allows to discriminate between film with different polarity and density of inversion domains. This is because a different reaction rate and reaction extent is found for N− and Ga−polar GaN with atomic hydrogen, with N−polar films exhibiting greater reactivity.

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