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The Elimination of Inversion Domains in MBE-GaN Grown Using Low Temperature Nitridation

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1. Introduction

In the absence of suitable GaN substrate, the hetroepitaxial growth of GaN on sapphire (0001) substrate carried out by any technique contain high dislocation density as well as other classes of defects such as voids and inversion domain boundaries (IDBs). Inversion domains (IDs), consisting of regions of GaN with opposite polarity to primary matrix, resulting in different surface morphologies are observed [1,2]. The formation of IDs is not an intrinsic property of MBE growth of GaN, but is apparently related to nucleation conditions [1,3]. A key characteristic of wurzite GaN is its polarity due to the lack of inversion symmetry in the (0001) plane give rise to two possible polarities, Ga and N polarity. In addition, Ga-polar GaN films have smoother surface morphology, stable chemical and thermal properties, etc. [4,5]. It is well-known that Ga-polar GaN is believed to be typical of MOCVD. However, GaN grown by RF-MBE was reported to predominately exhibit N polarity which is not suitable for electrical devices [6]. Recently, High temperature (HT) AlN buffer and intermediate layer or Al insertion layer has been used to convert favorable N polarity to Ga polarity films in MBE [4,7,8]. Our original motivation is to realize high quality Ga-polar GaN bulk on sapphire (0001) and improve surface morphology by eliminating IDs in RF-MBE. Several groups have demonstrated that the nitridation of sapphire substrate have developed the homogenous GaN leading to better structural and optical qualities [9,10]. Performing sapphire nitridation in the initial growth condition forms a very thin AlN layer which also competes with NO formation [11]. Specifically, nitridation at 200℃ causes a very thin AlN layer with 90% coverage is able to surpass the formation of IDs [5,12]. In this study, IDs free GaN layer with Ga polarity has been obtained through 200℃ nitridation and HT AlN buffer layers.

2. Experiments

GaN was grown on sapphire (0001) substrate by RF-MBE (ULVAC MBE system) attached with high-energy electron diffraction (RHEED). Before initiation of growth, the sapphire was first heated to 850 ℃ and hold for 1 hr for thermal cleaning. In order to investigate influence of sapphire nitridation on IDs, we prepare two samples for comparison. Only sample 2 was nitrided at 200℃ for 1 h under rf-power of 350W and N_2 flow rate of 1.5 sccm; The other one, sample 1, was not. Next, a thin AlN buffer layer of about 10nm was subsequently deposited at 850℃ to convert complete the conversion from N polarity to G polarity. Finally, a 2 μm thick GaN epilayer was grown under Ga-rich condition at 800℃ with 0.5 μm/h growth rate. Wet etching of GaN films was carried out using a KOH solution (2M KOH) about 30 min at room temperature. The in-situ RHEED, transmission electron microscopy (TEM), and scanning electron microscope (SEM) were used to study surface morphology and its relation to the mircostructure of GaN epilayer.

3. Results and discussion

The evolution of in-situ RHEED patterns of sample 2 along the sapphire <11-20> azimuth during the sapphire nitridation process are presented in Figure 1. It is found that after 20 min of nitridation at 200℃ streaky AlN patterns appear obviously while sapphire streak looked vague as shown in Figure 1(b). The modification of surface reconstruction imply that the formation of the thin AlN [3]. The coming nitridation enhance the intensity of AlN streak till sapphire streaky patterns have vanished. The RHEED pattern shown in Figure 1(c) indicates homogenous AlN consisting complete coverage is produced during nitridation at 200℃.

The main differences between nitrided and non-nitrided sapphire were which kinds of the surface terminal atoms in the initial growth condition. Figure 2(a) shows that the sapphire exhibits complete N-terminated surface after low temperature nitridation. It is believed that the very thin AlN nucleation layer, acting as a superior template to prevent from the presence of IDs and also enhance the lateral growth of following HT AlN buffer and GaN film. On the other hand, Figure 2(b) shows the sapphire exhibits Al-rich terminated and some oxygen-terminated surface after thermal cleaning at 850℃. Subsequently, we start to grow HT AlN buffer and then open Nitrogen (N) and Al shutter in order. When N adatoms diffuse to surface, two kinds of bonding configuration, N-O and Al-N, will be obtained. The presence of NO at sapphire/AlN interface causes polarity inversion.

Surface morphologies after KOH chemical wet etching of GaN film were characterized, respectively. Clearly, Figure 3(a) presents several hexagonal inversion domains on the top surface, which are typical three dimensional (3D) island growth with rough surfaces; this finding is also observed by M. Sumiya *et al* [13]. From the point of view of lattice polarity, smooth matrix of 2D growth mode possesses Ga polarity, whereas hexagonal IDs of rough 3D growth mode are N terminated [14]. In Figure 3(b), IDs free GaN layer with Ga polarity has been demonstrated through 200℃ nitridation, resulting to smooth surface.

Figure 4 is the cross section view of the sample 1 where an area around the hexagonal inversion domain was shown. The center area A on the TEM image with only a few dislocations corresponded to the N-terminated surface while the area B area showed high density of dislocations, corresponding to the Ga-terminated surface. It is known that a large compressive stress will be induced to the GaN film when it is grown on the sapphire due to the huge lattice mismatch (~16%). The grown of N-polar GaN as in our sample was believed to be initiated on the 3D nucleation islands and merged with each other. The 3D growth characteristic was able to accommodate much of the stress in the GaN film and resulted in an area with only a few dislocations. However, the final surface of the N polarity was much rougher than that of the Ga polarity. In contrast, the Ga-polarity GaN grown layer-by-layer suffering the huge misfit stress and therefore a high density of dislocation was generated.

4. Conclusions

GaN film grown on the non-nitrided sapphire was mainly Ga-polar and a few-percentage of N-polar, i.e. mixed polarities. Further, it has been shown that the N-polar GaN with much lower dislocation density can be achieved under certain growth condition. However, the N polarity GaN is not appropriate for the fabrication of high quality electronic devices. For this purpose, Ga polarity GaN is desired. Using nitridation at 200℃, we can eliminate IDs in GaN grown by MBE. It is believed that a high quality Ga-face GaN can be grown with the used of some effective dislocation reduction methods such as the insertion of a proper AlN interlayer.

Acknowledgements

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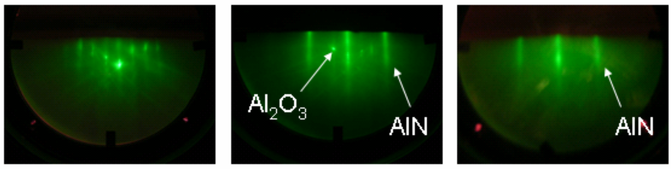
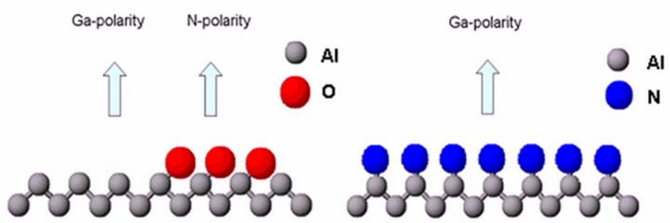


(a) (b) (c)

Figure 1. The evolution of RHEED patterns of sample 2 along the sapphire <11-20> azimuth during the 200℃ sapphire nitridation process: (a) prior to nitridation, (b) at 20 min nitridation, (c) at 1 hr nitridation.



(a) non-nitrided substrate (b) nitridaed substrate

Figure 2. Schematic models to illustrate the surface terminal atoms in different initial growth conditions.

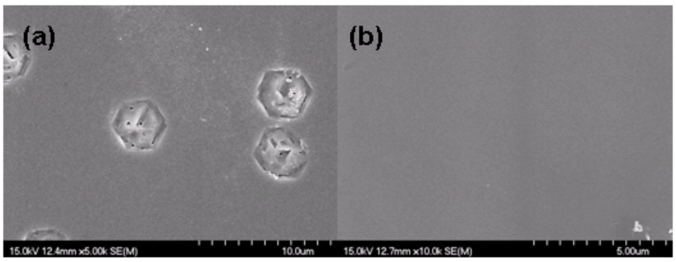


Figure 3. Surface morphologies of GaN epilayer after KOH etching observed by SEM: (a) sample 1, (b) sample 2.

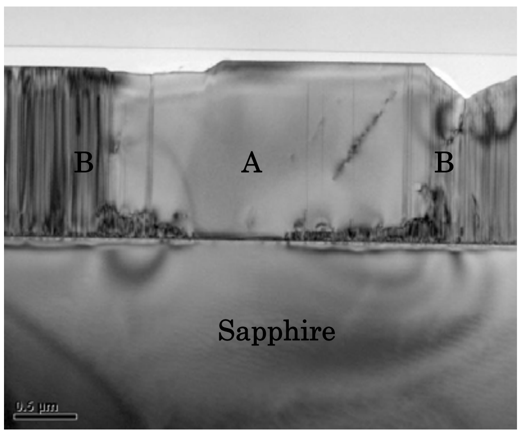


Figure 4. Cross-sectional TEM image of sample 1.