High-temperature AlN interlayer for crack-free AlGaN growth on GaN

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This paper presents a study of the transformation of high-temperature AlN (HT-AlN) interlayer (IL) and its effect on the strain relaxation of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}/\text{HT-AlN}/\text{GaN}$. The HT-AlN IL capped with $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ transforms into AlGaN IL in which the Al composition increases with the HT-AlN IL thickness while the total Ga content keeps nearly constant. During the HT-AlN IL growth on GaN, the tensile stress is relieved through the formation of V trenches. The filling up of the V trenches by the subsequent $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ growth is identified as the Ga source for the IL transformation, whose effect is very different from a direct growth of HT-AlGaN IL. The *a*-type dislocations generated during the advancement of V trenches and their filling up propagate into the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overlayer. The *a*-type dislocation density increases dramatically with the IL thickness, which greatly enhances the strain relaxation of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$. © 2008 American Institute of Physics.
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I. INTRODUCTION

AlN interlayer (IL) has been widely used as a strain engineering technique to achieve crack-free growth of thick GaN films on Si (111) substrate¹ and AlGaN layers on GaN template.² The reduction/elimination of tensile stress in Ga(Al)N overlayer through a low-temperature AlN (LT-AlN) IL is assigned to an incoherent growth of LT-AlN IL on GaN (Refs. 3 and 4) and/or the formation of hexagonal pits in LT-AlN IL.⁵ Interestingly, high-temperature AlN (HT-AlN) ILs are also able to suppress crack formation in AlGaN films grown on GaN template,⁶ although the mechanism of stress reduction via HT-AlN IL is not very clear. The study on HT-AlN growth on GaN by Vennéguès *et al.*⁷ has suggested a mechanism of strain relaxation through the formation of V trenches and misfit dislocations. We have reported the effects of HT-AlN IL thickness on the lateral phase separation of Al composition⁸ and spatial distribution of deep level defects⁹ in the subsequently grown AlGaN layer. It has also been found that the V/III ratio for HT-AlN IL growth can greatly affect the crystal quality and the strain evolution of subsequently grown GaN.¹⁰ However, there is still no direct investigation on HT-AlN IL with the presence of AlGaN cap layer, given the limited volume of ILs. This paper has revealed the transformation of HT-AlN IL into Al(Ga)N IL after $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overgrowth and proposed the related mechanism responsible for the strain relaxation at the two interfaces of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}/\text{HT-AlN}/\text{GaN}$ heterostructure.

II. EXPERIMENT

Five samples were prepared using low pressure metalorganic chemical vapor deposition in a showerhead reactor. Trimethylgallium, trimethylaluminum, and ammonia were

employed as precursors in H_2 carrier gas. $2.5\ \mu\text{m}$ GaN grown by a standard two-step procedure on (0001) sapphire serves as pseudosubstrate. $1.1\ \mu\text{m}$ $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ was grown at $1040\ ^\circ\text{C}$, under a nominally identical condition for all the samples on a HT-AlN IL deposited at $1040\ ^\circ\text{C}$ with nominal thicknesses of 9, 18, 26, and 40 nm for samples A, B, C, and D, respectively. For comparison, sample E was prepared by depositing $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ directly on GaN with no AlN IL. The surface of sample E shows a crack network.

A Bruker D8 Discover x-ray diffractometer with a monochromatic $\text{Cu } K\alpha_1$ x ray was used to perform reciprocal space mapping (RSM) measurements. The (0002) RSMs were obtained in a symmetric scan mode while the (10 $\bar{1}$ 5) RSMs in an asymmetric scan mode. A double-axis x-ray diffractometer at Beijing Synchrotron Radiation Facility was employed to measure x-ray rocking curves (XRCs) and get the Al composition of the thin ILs.

III. RESULTS AND DISCUSSION

Figure 1(a) is a (0002) RSM showing not only strong reciprocal lattice points (RLPs) for GaN and $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ but also two weak RLPs which are also observed in the (10 $\bar{1}$ 5) RSM [Fig. 1(b)] as well. According to the weak intensity and position of the two dispersed RLPs, they are assigned to the diffraction of the embedded HT-AlN ILs, which is consistent with their higher intensity in the (10 $\bar{1}$ 5) RSM of sample D with a thicker IL [Fig. 1(c)] and is also further confirmed by their absence in the RSM of sample E with no IL [Fig. 1(d)]. It is necessary to clarify that the two IL-related RLPs do not originate from any inhomogeneous incorporation of Ga/Al in the early stages of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ growth on the AlN IL. Otherwise, there would be a growth transition of

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FIG. 1. (Color online) (a) (0002) RSM of sample B and (1015) RSMs of samples (b) B, (c) D, and (d) E.

AlGaN from high Al composition to 25%. However, no diffraction pattern is observed between the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ and the distinct IL-related RLPs [Fig. 1(c)].

Meanwhile, it is noticed that although the GaN RLP stays at the same place in all the (1015) RSMs, the positions of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ and IL-related RLPs vary from sample to sample [Fig. 1(b)–1(d)]. The RLPs of the thick $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ layer and the ILs are displaced along the Q_x -axis with respect to the GaN RLP, showing that they are not coherently grown on the GaN pseudosubstrate. To get a panoramic view of the (1015) RSMs for all the five samples, we summarized the mean peak positions of AlGaN and IL-related RLPs in Fig. 2. As the HT-AlN IL thickness increases, the value of Q_x and Q_z of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ increases and decreases, respectively, indicating that $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ lattice cell shrinks laterally and expands vertically. Therefore, a thicker HT-AlN IL results in less tensile stress in the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overlayer. In contrast, the Q_x and Q_z values of the IL-related RLPs increase simultaneously as the HT-AlN IL gets thicker. The concurrent decrease in lattice constants a and c cannot be explained by an elastic distortion of the lattice cell due to strain. Instead, it indicates that the ILs sandwiched between $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ and GaN are not pure AlN but Al(Ga)N, and the AlN molar fraction x_{Al} in the thin ILs gradually increases from samples A to D. To estimate the x_{Al} in the thin ILs, x-ray skew symmetric

$\omega/2\theta$ scans were performed around (1012) since the (1012) plane spacing is not very sensitive to the strain status of AlGaN.¹¹ Due to a limited resolution, only an average x_{Al} is determined from a broad peak from the thin IL. As shown in Fig. 3, the x_{Al} of thin ILs spans a wide range, from 0.47 (sample A) to 0.88 (sample D), while the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overlayers within all the four samples have a nearly equal average x_{Al} (~ 0.25) of the two slightly different compositions due to the lateral phase separation.⁸ Reiher *et al.*⁴ reported a similar observation that a 10-nm-thick AlN IL grown at 1145 °C turns into an AlGaN IL with an x_{Al} of 0.4–0.5 after the AlGaN overgrowth.

FIG. 2. (Color online) The relative positions of (1015) reciprocal lattice points of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ layers and the transformed HT-Al(Ga)N ILs.

FIG. 3. (Color online) Al composition of the transformed HT-Al(Ga)N ILs and the thick $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ layers.

To identify the Ga source for the transformation of HT-AIN into AlGa_{0.25}N IL, a separate sample of 35 nm HT-AIN was grown on GaN with no subsequent $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overgrowth. The x-ray diffraction measurement shows that the as-grown AIN layer has an x_{Al} close to unity (~ 0.96), which indicates that the Ga content in the transformed Al(Ga)N ILs of the four investigated samples mainly comes from the subsequent $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ growth. In fact, the x_{Al} of transformed Al(Ga)N ILs is also a function of the x_{Al} of the subsequently grown AlGa_{0.25}N layer,⁴ which further confirms that the subsequent AlGa_{0.25}N overgrowth is the Ga source for the transformation of HT-AIN IL into Al(Ga)N IL.

Our high-resolution transmission electron microscopy (HRTEM) study of the samples revealed the existence of V trenches in the IL, filled up during the subsequent $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ growth.⁸ The commonly observed feature of mesalike islands separated by V trenches in a HT-AIN layer grown on GaN has been reported by various research groups.^{7,10,12,13} The formation of V trenches in HT-AIN, with a thickness beyond 6 nm or so, partly relaxes the tensile stress within the AIN layer.⁷ V trenches have inclined faceted sidewalls and hence are different from cracks.⁷ By virtue of the strain field in the vicinity of V trench apexes, misfit dislocations prefer nucleating at the bottom of V trenches⁷ and then glide into the mesalike islands for their strain relaxation.^{7,13} During the subsequent $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ growth, the V trenches in the HT-AIN IL are filled up with AlGa_{0.25}N, which is the process that brings the Ga into the HT-AIN IL. Reier *et al.*⁴ observed a strong dependence of the AIN IL transformation on its growth temperature. In contrast to HT-AIN ILs, a 10-nm-thick LT-AIN IL grown at 600 °C still holds a high Al composition of $\sim 85\%$ after AlGa_{0.25}N overgrowth.⁴ Thus, it is reasonable to assert that the effective transformation of AIN into AlGa_{0.25}N IL hinges on the presence of V trenches in the AIN IL. The filling up of V trenches turns the AIN IL into a AlGa_{0.25}N-like IL consisting of many closely packed small AIN/AlGa_{0.25}N domains. It is possible that among the adjacent small domains, the strain field facilitates the interdiffusion of Ga and Al atoms¹⁴ through the original V trench boundaries between $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ -filled V trench domains and mesalike AIN domains, which can further help the strain relaxation of mesalike domains. The difference in x_{Al} between the V trench domains and the mesalike domains

FIG. 4. (Color online) Skew symmetric (1012) XRC linewidths of $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ layer, transformed HT-Al(Ga)N IL, and GaN template as a function of HT-AIN IL thickness.

might correspond to the two dispersed IL-related RLPs in the (1015) RSMs. A more detailed HRTEM study is needed to verify this conjecture.

It has been reported that when a HT-AIN IL reaches a certain thickness (~ 15 nm), V trenches are fully developed in depth with their apexes reaching the AIN/GaN interface, and a further growth of AIN will not significantly change the depth of V trenches but lead to a nearly equal advancement of their sidewalls along the growth direction.⁷ In other words, the total volume of all the V trenches in thick HT-AIN ILs does not vary significantly with the AIN IL thickness. Therefore, the total Ga content getting into the HT-AIN ILs after the filling up of V trenches should be similar from sample to sample. A rough estimate of the total Ga content (the product of the IL thickness and its Ga composition) in the ILs of samples B, C, and D based on Fig. 3 gives a small relative variation of less than 20%, which is another supportive evidence for the identification of the filling up of V trenches by the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overgrowth as the Ga source for the HT-AIN IL transformation.

During the advancement of V trenches via a sustained HT-AIN growth and/or their filling up by $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overgrowth, many *a*-type dislocations with threading arms are generated in the IL (Ref. 7) and get propagated into the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overlayer.¹⁰ Figure 4 shows that the density of *a*-type threading dislocations (TDs) in $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ and Al(Ga)N IL increases dramatically with the HT-AIN IL thickness. It has been observed and reported that the inclined *a*-type TDs in GaN grown on a HT-AIN IL, having projection segments in the basal plane, facilitate the compressive strain relaxation in the overgrown GaN.¹⁵ The higher the density of the inclined *a*-type TDs, the more relaxed the compressive strain of the overgrown GaN.¹⁰ In sample A, the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ layer is almost coherently grown on the Al(Ga)N IL (Fig. 2). However, as the IL thickness increases, the Q_x distance between the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ and the IL-related RLPs also increases, meaning that the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overlayer has an enhanced relaxation with respect to the IL, which can be well accounted for by the increased density of the inclined *a*-type TDs (Fig. 4).

It is necessary to point out the marked differences between the dynamic transformation of HT-AIN IL into AlGa_{0.25}N IL and a direct insertion of HT-AlGa_{0.25}N IL between GaN and AlGa_{0.25}N thick layers. For the growth of HT-AlGa_{0.25}N IL with an

x_{Al} below 70% on GaN, the critical thickness for the strain relaxation via V trench formation is much larger than that of HT-AlN IL, and the V trenches never reach the interface.⁷ Furthermore, the V trenches are not connected to each other because of the low density.^{7,13} Therefore, the primary slip system for dislocation gliding is disabled and the HT-AlGaIn IL remains highly strained on GaN, a further growth of which will trigger crack formation.^{7,13}

IV. CONCLUSIONS

In summary, the V trenches formed in HT-AlN IL not only relieve the tensile stress but also make it possible for AlN IL to transform into AlGaIn IL through their being filled up by the subsequent $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ growth, which partially reduces the lattice mismatch between $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ and the IL. During the filling up, a -type dislocations are generated and get propagated into the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ overlayer, which greatly contribute to the strain relaxation of the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ layer. The effect of the dynamic transformation of HT-AlN IL is very different from that of a direct insertion of HT-AlGaIn IL through which the tensile stress cannot be effectively relieved.

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