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<td>Author(s)</td>
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Stress evolution of GaN/AlN heterostructure grown on 6H-SiC substrate by plasma assisted molecular beam epitaxy

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The stress evolution of GaN/AlN heterostructure grown on 6H-SiC substrate by plasma assisted molecular beam epitaxy (PA-MBE) has been studied. AlN nucleation layer and GaN layer were grown as a function of III/V ratio. GaN/AlN structure is found to form buried cracks when AlN is grown in the intermediate growth regime (III/V ~1) and GaN is grown under N-rich growth regime (III/V<1). The III/V ratio determines the growth mode of the layers that influences the lattice mismatch at the GaN/AlN interface. The lattice mismatch induced interfacial stress at the GaN/AlN interface relaxes by the formation of buried cracks in the structure. Additionally, the stress also relaxes by misorienting the AlN resulting in two misorientations with different tilts. Crack-free layers were obtained when AlN and GaN were grown in the N-rich growth regime (III/V<1) and metal rich growth regime (III/V≥1), respectively. AlGaN/GaN high electron mobility transistor (HEMT) heterostructure was demonstrated on 2-inch SiC that showed good two dimensional electron gas (2DEG) properties with a sheet resistance of 480 Ω/sq, mobility of 1280 cm²/Vs and sheet carrier density of 1×10¹⁳ cm⁻².

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I. INTRODUCTION

AlGaN/GaN high electron mobility transistor (HEMT) is an excellent candidate for high power, high frequency and high temperature device applications due to the superior properties of the GaN based material, such as wide bandgap energy, high breakdown field, high saturation velocity and high electron mobility. Due to the lack of bulk GaN substrates for the homoepitaxial growth, GaN based materials are grown heteroepitaxially on foreign substrates such as SiC, sapphire and Si. Among them, the growth of AlGaN/GaN HEMTs on SiC substrate is preferred because of its smaller lattice and thermal mismatch to GaN and higher thermal conductivity.1 The high thermal conductivity of SiC (4.9 Wcm⁻¹°C⁻¹) makes the device to operate at high power densities as it allows efficient heat dissipation compared to other foreign substrates such as Si (1.3 Wcm⁻¹°C⁻¹). This results in improved drain efficiencies and device performances by reducing channel temperatures that would result due to self-heating.2 With the wider commercial availability of SiC substrate and encouraging trend of the wafer price and size, SiC seems to be the best candidate for the growth of AlGaN/GaN HEMTs for high power and high frequency applications.

The lattice mismatch between GaN and SiC (3.4%) induces compressive stress during the growth while a thermal mismatch (20%) generates tensile stress upon cool down. The growth of GaN directly

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on SiC is found to exhibit three-dimensional (3D) growth mode and highly defective surface due to the large lattice mismatch between GaN and SiC. However, use of AlN nucleation layer for the growth of GaN on SiC ensures two-dimensional (2D) growth of GaN with gradual compressive stress relief. GaN is found to crack if this lattice mismatch induced compressive stress is unable to compensate the tensile stress generated due to the thermal mismatch. The growth of crack-free AlGaN/GaN HEMT on SiC is already reported, however, the interfacial stress generated at the GaN/AlN interface which leads to interfacial cracking is not reported. In this study, we investigate the effect of III/V ratio of both AlN and GaN on the stress evolution and cracking mechanism of GaN/AlN heterostructure grown on 6H-SiC substrate by plasma assisted molecular beam epitaxy (PA-MBE). This is followed by the demonstration of crack-free AlGaN/GaN HEMT heterostructure on 2-inch 6H-SiC substrate with good two-dimensional electron gas (2DEG) properties.

II. EXPERIMENTAL

The epilayer structures were grown on double side polished 6H-SiC (001) substrate using PA-MBE. The SiC substrate was subjected to ex-situ followed by in-situ cleaning for native oxide removal prior to the epitaxial growth. It first underwent organic cleaning and a deionized (DI) water rinse. Subsequently, it was subjected to an oxidation procedure by dipping in a 5:3:3 solution of HCl:H2O2:H2O at 60 °C, followed by a ~30s DI rinse. The resulting oxide layer was then removed by immersing the substrate into 10:1 solution of H2O2:HF for 20s. A 1 μm thick titanium film was deposited at the back side of the substrate to provide heat retention.

The substrate was further cleaned in-situ to remove oxide by exposing it to three cycles of Ga deposition and flash off. A (1×3) RHEED reconstruction pattern confirmed the clean SiC substrate. Subsequently, AlN nucleation layer with 100 nm thickness was grown at a substrate temperature of 740 °C followed by the growth of 500 nm thick GaN at 710 °C. As listed in Table I, two sets of samples set A and B were grown to investigate the effect of III/V ratio of both AlN and GaN on the stress evolution and cracking mechanism of GaN/AlN heterostructure. AlN nucleation layer was grown as a function of III/V ratio while the subsequent GaN layer was grown with a constant III/V ratio of 1.5 for the samples constituting set A. Set B comprises of samples grown with AlN layer at a fixed III/V ratio followed by GaN layer grown as a function of III/V ratio. All the layers were grown with a fixed RF power of 300 W and a nitrogen flow of 2 sccm. It should be noted that the III/V ratio is the beam equivalent pressure (BEP) ratio of group III element (N) and group V element (Al,Ga) during the growth of (Al,Ga)N.

The surface morphology of the samples was observed with the aid of an optical microscope and field emission scanning electron microscope (FE-SEM). The samples for the investigation of cracking were etched using inductive coupled plasma-reactive ion etching (ICP-RIE) method. The stress in the whole of the layers was determined from the Raman spectra obtained using a confocal micro-Raman spectrometer equipped with a wavelength of 532 nm. It was measured according to the stress-deviation relation from the measured Raman frequency shift of E2 phonon mode using a linear relation between the stress (σxx) and Raman shift (Δω) as shown in Eqn. 1

\[
\Delta \omega = K_x \sigma_{xx}
\]

Where \( K_x \) is the linear stress coefficient. High resolution X-Ray diffraction (HR-XRD) with a Cu Kα1 radiation source (λ = 1.5406 Å) was used to characterize the crystalline property of the layers.

<table>
<thead>
<tr>
<th>Set</th>
<th>III/V ratio</th>
<th>GaN</th>
<th>AlN</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>varied from 0.15 to 1</td>
<td>fixed at 1.5</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>fixed at 0.15</td>
<td>varied from 0.7 to 1.5</td>
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</table>

TABLE I. Two sets of samples, set A and B were grown to investigate the effect of III/V ratio of both AlN and GaN on the stress evolution and cracking mechanism of GaN/AlN heterostructure.
FIG. 1. RHEED reconstruction pattern during the growth of AlN grown with III/V = 1(a) and III/V < 1(b) along [2110] azimuths.

The full width at half maximum (FWHM) values were measured in an open detector configuration while the reciprocal space mapping (RSM) was performed using triple axis geometry.

III. RESULTS AND DISCUSSION

AlN nucleation layer for the samples in set A was grown on SiC substrate as a function of III/V ratio varying from the N-rich growth regime (III/V < 1) to the intermediate growth regime (III/V ~ 1) followed by Al rich growth regime (III/V > 1) similar to the studies performed on Si substrate.\(^{11}\) Fig. 1(a) and 1(b) show the reflection high energy electron diffraction (RHEED) reconstruction pattern during the growth of AlN grown with III/V ~ 1 and III/V < 1, respectively. Streaky RHEED pattern is obtained for AlN (III/V ~ 1) and spotty pattern is seen for AlN(III/V < 1) indicative of two-dimensional (2D) and three-dimensional (3D) growth modes, respectively. The subsequent GaN layer grown with constant III/V ratio of 1.5 showed streaky RHEED pattern suggestive of 2D growth mode.

Dark field optical microscope image of GaN/AlN structure grown with AlN(III/V ~ 1) in set A shows crack free surface when focused on the surface while cracks (marked by arrows) can be clearly seen when focused into the GaN/AlN interface, as shown in Fig. 2(a) and (b), respectively. Moreover, Fig. 3 (a) and (b) show the FE-SEM images of the GaN surface and the surface obtained after etching down to 200 nm thickness of GaN, respectively. As can be seen, no cracks are seen on the GaN surface but micro-cracks appear when the GaN layer is etched down to 200 nm as indicated by the arrows. This was further confirmed by atomic force microscopy (AFM) technique (image not shown) that did not show any cracks on the GaN surface. It clearly indicates that the cracks are not on the surface but buried. However, the GaN/AlN structure grown with AlN (III/V < 1) in set A did not show any cracks.

Similar study was also performed for the samples grown in set B wherein, GaN was grown as a function of III/V ratio. The AlN nucleation layer for the samples in set B was grown with a fixed III/V ratio of 0.3. Streaky RHEED reconstruction pattern was obtained for GaN grown with III/V > 1 while spotty RHEED pattern was seen for III/V < 1 indicative of 2D and 3D growth modes, respectively. Streaky RHEED pattern with connecting dots was observed for GaN grown with III/V ~ 1 suggestive of a transition from 3D to 2D growth mode. The layers were found to be cracked for GaN(III/V < 1)

FIG. 2. Dark-field microscope images of GaN/AlN structure grown with AlN(III/V ~ 1) focused on the GaN surface (a) and into the GaN/AlN interface (b).
while crack free layers were obtained for GaN (III/V ≥ 1). Similar to the cracks in the sample grown with AlN (III/V ~ 1) in set A, the cracks were found to be not on the surface but buried.

In order to study the cracking mechanism in the GaN/AlN structure on SiC, the stress evolution and crystalline quality of both GaN and AlN layers of set A were investigated using micro-Raman spectroscopy and high resolution X-Ray diffraction (HR-XRD) techniques, respectively. Fig. 4 shows the stress in AlN and GaN as a function of III/V ratio of AlN determined using micro-Raman spectroscopy. As shown in Fig. 4(a), the stress in AlN is highly compressive for III/V ~ 1, and it gradually relaxes and becomes tensile with reducing III/V ratio except for the case of III/V = 0.15 that shows compressive stress in AlN. Fig. 4(b) shows that the stress in GaN is always compressive irrespective of the III/V ratio of AlN. However, it shows a sudden increase in stress with decreasing III/V ratio of AlN from III/V ~ 1 to III/V < 1. Thereafter, the stress is found to decrease systematically with further decreasing of the III/V ratio of AlN.

The lateral correlation length ($L_{\|}$) of AlN was calculated in order to understand the stress evolution in AlN as a function of III/V ratio. Fig. 5 shows the lateral correlation length of AlN as a function of III/V ratio. $L_{\|}$ was estimated using Eqn. 2

$$L_{\|} = \frac{0.9 \lambda}{\beta \left(0.017475 + 1.500484 \eta - 0.534156 \eta^3\right) \sin \theta}.$$  

(2)

![FIG. 4. The stress in AlN (a) and GaN (b) as a function of III/V ratio of AlN determined using micro-Raman spectroscopy.](image-url)
Where $\lambda$ is the X-ray wavelength, $2\theta$ is the scattering angle, $\eta$ is the parameter determined from the pseudo-Voigt function $P(x)$ by a least squares fit of diffraction intensity and $\beta_{22}$ is the integral width of the fit performed on (002) HR-XRD reflection. The Voigt function is a convolution of a Gaussian $G(x)$ and a Cauchy profile $C(x)$, which can be approximated by $P(x)$ as given in Eqn. 2, with $I_0$ as a scaling factor.

$$P(x) = I_0 \left[ \eta C(x) + (1-\eta) G(x) \right] \quad 0 \leq \eta \leq 1, \quad -\infty \leq x \leq \infty.$$  \hfill (3)

As can be seen, the lateral correlation length or the average grain size of AlN decreases with decreasing III/V ratio. The two data points at AlN (III/V = 0.15) correspond to the correlation lengths obtained by resolving the split peak of AlN along (002) caused due to misorientation in AlN. More details on the misorientation in AlN grown with III/V = 0.15 will be discussed later. Fig. 6 shows the FWHM of HR-XRD rocking curve scans along (102) plane of GaN and AlN as a function of III/V ratio of AlN. The FWHM shows degradation in mixed and pure edge dislocation density in AlN with decreasing III/V ratio. Moreover, the dislocation density in GaN increases and remains nearly the same with decreasing the III/V ratio of AlN from III/V ~ 1 to III/V < 1.

Fig. 7 (a) and (b) show the reciprocal space mapping (RSM) plots for the GaN/AlN structure grown with AlN (III/V = 0.15) and AlN (III/V ~ 1) in set A, respectively. The inset shows the omega rocking curve for AlN. Both RSM and omega rocking curve scans were obtained along (002) plane using HR-XRD technique. As shown, the difference in the mosaic spread, particularly, for AlN is significant. The spread for the sample grown with AlN (III/V = 0.15) is $\Delta q_x \sim 50 \mu m^{-1}$. It shows two distinguishable centers at $q_x \sim -0$ and $6 \mu m^{-1}$, indicating two misorientations in AlN. Moreover, the split observed in the omega rocking curve for AlN along (002) plane confirms the presence of two
different misorientations in AIN. On the other hand, the mosaic spread for AIN grown with III/V ~ 1 is much smaller, with a value of $\Delta q_{\parallel} \sim 32 \mu m^{-1}$ centered along the SiC substrate. A single omega peak further confirms the presence of just one orientation in AIN.

The tilt in AIN for the GaN/AIN structure grown as a function of III/V ratio of AIN with a fixed III/V ratio of GaN (III/V = 1.5) is summarized in Table II. Please note that the misorientation of AIN with respect to SiC is referred to as tilt in AIN. Correspondingly, the tilts in AIN for the two different misorientations (split in the omega rocking curve) are denoted by Tilt 1 and Tilt 2. The relative tilt is given by the difference between these two tilts. The table shows that there is no tilt for the samples with III/V ratio of AIN ranging from 1 to 0.6, while there is an increase in both the tilt and relative tilt with reducing the III/V ratio from 0.6 to 0.15.

The lattice mismatch between GaN and AIN leads to the growth of compressively strained GaN on AIN. However, when grown on SiC substrate, AIN grows compressive, leading to the generation of additional compressive stress in GaN while AIN itself is under tensile stress relative to GaN. Thus, it is the tensile stress in the AIN layer or, in other words, the interfacial stress at the GaN/AIN interface of the structure grown with AIN (III/V ~ 1) leads to its cracking and subsequent relaxation. Bätzkom et al. have explained a similar mechanism during the growth of GaN on sapphire, where in the sapphire substrate is under tensile stress when the thickness of compressively strained GaN layer is no longer negligible compared to the sapphire substrate. On the other hand, the 3D growth of

<table>
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<th>Relative Tilt</th>
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<td></td>
<td></td>
<td>[Tilt 1 (%)]</td>
<td>[Tilt 2 (%)]</td>
</tr>
<tr>
<td>1</td>
<td>Crack</td>
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<td>*</td>
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<tr>
<td></td>
<td>0.85</td>
<td>0</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>0.60</td>
<td>0</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>0.30</td>
<td>Crack free</td>
<td>0.0371</td>
</tr>
<tr>
<td></td>
<td>0.15</td>
<td>0.0044</td>
<td>0.1148</td>
</tr>
<tr>
<td>AIN (fixed GaN III/V ratio = 1.5)</td>
<td>1.5</td>
<td>0</td>
<td>0.0371</td>
</tr>
<tr>
<td></td>
<td>1.20</td>
<td>Crack free</td>
<td>0.0760</td>
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<tr>
<td></td>
<td>1.0</td>
<td>0.0124</td>
<td>0.1250</td>
</tr>
<tr>
<td></td>
<td>0.66</td>
<td>Crack free</td>
<td>0.0013</td>
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*There is no second misorientation or tilt in AIN.
AIN (III/V < 1) is associated with island growth. The reduction in the average grain size of AIN with decreasing III/V ratio in Fig. 5 indicates that there is an increase in the number of initial nucleated grains during the onset of AIN growth on the SiC substrate with reducing III/V ratio of AIN.

According to the Nix and Clemens\textsuperscript{14} analysis, the average tensile stress (σ) generated by coalescence is related to their grain size (d) by Eqn. 4

\[
\langle \sigma \rangle = \left[ \left( \frac{1}{1 - v} \right) E \frac{2 \gamma_{sv} - 2 \gamma_{sb}}{d} \right].
\]

Where \( E \) is the elastic modulus, \( v \) is the Poisson’s ratio, and \( \gamma_{sv} \) and \( \gamma_{sb} \) are the surface and grain boundary energies, respectively. Eqn. 4 shows that the tensile stress (\( \sigma \)) is inversely proportional to the grain size (\( d \)). Thus, it can be contemplated from Fig. 5 and Eqn. 4 that there is an increase in the overall tensile stress of AIN with reducing III/V ratio. The grains tend to coalesce as the growth progresses resulting in the generation of tensile stress.\textsuperscript{15,16} The increase in the tensile stress, or in other words, the reduction in the compressive stress in AIN with reducing III/V ratio from III/V ~ 1 to III/V < 1 reduces the lattice mismatch between GaN and AIN. Consequently, the lattice mismatch induced interfacial stress reduces at the GaN/AIN interface, thereby preventing the formation of buried cracks at the GaN/AIN interface. This possible mechanism potentially explains why GaN/AIN structure grown with AIN (III/V < 1) is crack free while cracks occur when grown with AIN (III/V ~ 1).

Generally, the stress in a layer relaxes via generating dislocations (i.e. tilt or twist) and/or by the formation of cracks.\textsuperscript{17} As discussed, the interfacial stress is found to relax by cracking of GaN/AIN structure grown with AIN (III/V ~ 1). Furthermore, the relaxation also occurs by inducing tilt in AIN lattice as listed in Table II. The interfacial stress may be sufficient enough to crack the structure for the AIN layer grown with III/V ~ 1. However, with reducing III/V ratio to less than 1, the stress may be insufficient to cause cracking. For III/V < 0.6, although the interfacial stress is minimal, the poor quality of AIN as shown in Fig. 6 might have allowed the developed stress to relax by misorienting the AIN and resulting in two misorientations with different tilts. Moreover, the tilt for III/V = 0.15 is so large that it might have caused the complete relaxation of interfacial stress leading to compressive stress in AIN as shown in Fig. 4(a).

As shown in Fig. 6, the dislocation density for both AIN and GaN is found to be comparable for the sample grown with AIN(III/V ~ 1). It can be understood that the high lattice mismatch induced compressive stress at GaN/AIN interface got relaxed by the formation of cracks without generating any dislocations in GaN. Thus, there is no change observed in the dislocation density in GaN for this sample. However, the dislocation density in AIN was found to increase while it remained nearly constant in GaN with reducing III/V ratio of AIN. The increase in the number of nucleated grains of AIN and their subsequent coalescence with reducing III/V ratio not only increased the tensile stress in AIN but also resulted in the generation of dislocations\textsuperscript{18} in addition to the AIN/SiC lattice mismatch induced dislocations. Moreover, the lattice mismatch between GaN and AIN could potentially favor the generation of new dislocations in GaN. As discussed by Sahonta et. al.\textsuperscript{19} the presence of compressive stress at the GaN/AIN interface would have guided these dislocations to bend and loop leading to their annihilation and relaxation of the compressive stress in GaN. Thus, a reduction in the compressive stress (Fig. 4(b)) and nearly the same dislocation density is observed in GaN with reducing III/V ratio of AIN. This explanation of the evolution of stress and dislocations in GaN is a speculation and additional characterization by transmission electron microscopy (TEM) will be required to support the same.

The stress evolution and crystalline quality of GaN and AIN were also investigated for the samples in set B. Fig. 8 shows the stress in GaN and AIN as a function of III/V ratio during GaN growth determined using micro-Raman spectroscopy. The AIN was grown with a fixed III/V ratio of 0.3. In addition to assisting in obtaining crack-free layers, the growth of AIN(III/V < 1) has also shown to result in lower buffer leakage current.\textsuperscript{8} Moreover, the chosen III/V ratio of AIN is also well within the suggested range in order to suppress the silicon carry-over from the SiC substrate to the layers grown subsequently.\textsuperscript{7,20,21} As shown in Fig. 8 (a), the stress in AIN is tensile for all the samples except for AIN with III/V ~ 1 that shows compressive stress. On the other hand, the stress in GaN is always compressive at room temperature irrespective of the III/V ratio of GaN, as
illustrated in Fig. 8 (b). The stress is nearly the same with reducing III/V ratio from GaN (III/V>1) to GaN(III/V ~1). However, it is found to relax when grown in III/V<1.

In set B samples, the crystal quality doesn’t play any important role in determining the stresses and the tilting in the structure as the growth condition for AlN is kept fixed and only GaN condition is varied. The variation in the III/V ratio of GaN does not show a very significant change except a slight reduction in the overall dislocation density for the structure grown with GaN (III/V <1).

The cracks are observed in the GaN/AlN structure grown with GaN (III/V<1) in set B even when the III/V ratio of AlN was kept less than 1 (III/V = 0.3) while no cracks were observed when GaN was grown with III/V≥1. The 3D growth of GaN (III/V<1) tends to generate tensile stress in GaN due to island coalescence. The increase in the III/V ratio (III/V≥ 1) or in other words, increase in Ga metal promotes 2D growth of GaN. The lattice mismatch between AlN and GaN layer increases during the 3D growth of GaN leading to the cracking of GaN/AlN interface. The lattice mismatch tends to reduce when increasing the III/V ratio of GaN from III/V<1 to III/V≥ 1 resulting in a crack free GaN/AlN structure. Consequently, the stress is nearly the same with reducing III/V ratio from III/V>1 to III/V ~1. However, it is found to relax due to cracking when grown with III/V<1.

It is interesting to note that the stress in AlN is found to be varying for a fixed AlN growth condition when III/V ratio of GaN is varied from III/V>1 to III/V ~1. Thus, it can be inferred that the growth conditions of GaN are clearly influencing the stress states in both GaN as well as AlN.

Fig. 9(a) and (b) show RSM plot for the GaN/AlN structure grown with GaN(III/V ~ 1) and GaN(III/V = 1.5) in set B, respectively. The inset shows the omega rocking curve for AlN along (002) plane. Similar to set A, both RSM and omega rocking curve scans were obtained along (002) plane using HR-XRD technique and the corresponding mosaic spread for AlN nucleation layer was analyzed. As shown in Fig. 9(a), the mosaic spread for the AlN layer for the sample grown with GaN III/V ~ 1 is Δω~60 μm⁻¹. It shows two distinguishable centers at q~6.7 and 0.67 μm⁻¹, indicating two misorientations in AlN. The presence of two misorientations is further indicated by a split in the AlN (002) omega rocking curve. However, as shown in Fig. 9 (b), the AlN mosaic spread for the sample grown with GaN(III/V = 1.5) is much smaller Δω~40 μm⁻¹ and is centered at 0.07 μm⁻¹. A single omega peak further confirms the presence of just one orientation of AlN. The tilt in AlN for the set B samples is included in Table II. As can be seen, Tilt 1 and Tilt 2 as well as the relative tilt in AlN are found to increase with reducing III/V ratio of GaN with a maximum relative tilt for GaN (III/V ~1). Similar to set A, the interfacial stress at the GaN/AlN interface relaxes by either cracking or misorienting of the AlN.
The lattice mismatch induced compressive stress in GaN reduces due to the transition of growth mode from 2D to 3D when reducing its III/V ratio. It can be observed from Fig. 8 that the compression in GaN reduces while AlN becomes more tensile when reducing the III/V ratio from 1.5 to 1.2. For GaN grown with III/V ~ 1, the increase in the interfacial stress leads to misorientation of AlN in the form of tilting. This leads to compressive stress in AlN similar to the sample with III/V = 0.15 in set A. On the other hand, the excess interfacial stress causes the formation of buried cracks for III/V<1.

From this study, it can be concluded that crack free GaN/AlN structure was obtained when the growth of AlN was performed under N-rich growth condition while metal rich growth condition was used for the growth of GaN. AlGaN/GaN HEMT heterostructure was then grown using the optimized conditions on 2-inch 6H-SiC substrate. The AlN and GaN layer were grown at an optimized III/V ratio of 0.3 and 1.5, respectively. GaN was grown with systematic growth interruptions to desorb excess Ga at the growth temperature. Both Ga and N shutters were closed at regular intervals to avoid the formation of heavy Ga droplets due to the accumulation of excess Ga on the surface. The poor surface below the droplets has been found to degrade the bulk properties of GaN. Thus, “modulated growth” was performed in order to obtain atomically smooth surfaces without droplet formation. The barrier and cap layers were grown with no growth interruption at a constant Ga flux.

**FIG. 9.** The reciprocal space mapping of the GaN/AlN structure grown with GaN(III/V ~ 1) (a) and (III/V = 1.5) (b) in set B. The inset shows the omega rocking curve for AlN respective sample. Both RSM and omega rocking curve scans were obtained along (002) plane using HR-XRD technique.

**FIG. 10.** ω-2θ scan along symmetric reflection of (002) for estimating the AlGaN barrier layer composition and thickness.
The AlGaN/GaN HEMT structure consists of AlN nucleation layer (100 nm), GaN layer (1000 nm), an Al_{0.25}Ga_{0.75}N (25.5 nm) barrier layer, and a GaN (2 nm) cap layer. The Al composition and thickness of the AlGaN barrier layer were measured using HR-XRD symmetric (002) ω-2θ scan as shown in Fig. 10. The measured data were simulated in order to estimate the barrier layer composition and thickness based on peak separation and broadening, respectively.

Fig. 11 shows the $2 \times 2 \mu m^2$ AFM image of the surface of the optimized AlGaN/GaN HEMT heterostructure exhibiting smooth surface morphology and low RMS roughness of 0.75 nm. As can be seen, the monolayer steps and spiral hillocks are clearly visible on the surface.

Hall measurements were performed on 2-inch AlGaN/GaN HEMT wafer to determine the electrical properties. The room temperature Hall measurements showed an average sheet resistance of 480 Ω/sq and 2DEG mobility and sheet carrier density values of 1280 cm$^2$/Vs and $1 \times 10^{13}$ cm$^{-2}$, respectively. Mercury probe CV measurement was done to confirm the presence of 2DEG at AlGaN/GaN interface as shown in Fig. 12. A very high carrier density is obtained at the interface between AlGaN barrier and GaN channel. The charge carriers deplete throughout GaN resulting in a low background carrier density of $\sim 10^{14}$ cm$^{-3}$. Inset shows the temperature dependent hall...
measurements done to obtain the 2DEG electrical properties from 90 to 400K. As shown, the carrier density remains constant irrespective of the operating temperature while the mobility increased to 2800 cm²/V·s at 90K. This further confirms the presence of 2DEG at the AlGaN/GaN interface.

IV. CONCLUSION

The stress evolution in GaN/AlN structure grown on 6H-SiC by PA-MBE is studied as a function of III/V ratio of GaN and AlN. The lattice mismatch between GaN and AlN was found to generate interfacial stress at the GaN/AlN interface. The interfacial stress was relaxed either by the formation of buried cracks in the structure or by misorienting the AlN layer in the form of two tilts. Crack free GaN/AlN structure was obtained when the growth of AlN was performed in the N-rich growth condition (III/V<1) while metal rich growth condition (III/V ≥ 1) was used for the growth of GaN. The 3D growth of AlN (III/V<1) relaxed the interfacial stress by generation of tensile stress due to grain coalescence and prevented cracking. On the other hand, increase in Ga metal promoted 2D growth of GaN (III/V ≥ 1) thereby preventing the relaxation of the GaN layer and subsequent cracking of the interface. It was also found that the growth conditions of GaN influenced the stress states in AlN.

Finally, crack free AlGaN/GaN HEMT heterostructure was grown on 2-inch SiC substrate using optimized growth conditions. An average sheet resistance, 2DEG mobility and sheet carrier density of 480 Ω/sq, 1280 cm²/V·sec and 1 × 10¹⁵ cm⁻² were achieved, respectively. A low background carrier density of ∼ 10¹⁴ cm⁻² indicated the growth of highly resistive GaN buffer layer.