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Impact of varying buffer thickness generated strain and threading dislocations on the formation of plasma assisted MBE grown ultra-thin AlGaN/GaN heterostructure on silicon

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Plasma-assisted molecular beam epitaxy (PAMBE) growth of ultra-thin Al0.2Ga0.8N/GaN heterostructures on Si(111) substrate with three buffer thickness (600 nm/400 nm/200 nm) have been reported. An unique growth process has been developed that supports lower temperature epitaxy of GaN buffer which minimizes thermally generated tensile strain through appropriate nitridation and AlN initiated epitaxy for achieving high quality GaN buffer which supports such ultra-thin heterostructures in the range of 10-15Å. It is followed by investigations of role of buffer thickness on formation of ultra-thin Al0.2Ga0.8N/GaN heterostructure, in terms of stress-strain and threading dislocation (TD). Structural characterization were performed by High-Resolution X-Ray Diffraction (HRXRD), room-temperature Photoluminescence (RT-PL), High Resolution Transmission Electron Microscopy (HRTEM) and Atomic Force Microscopy (AFM). Analysis revealed increasing biaxial tensile stress of 0.6918 ± 0.04, 1.1084, 1.1814 GPa in heterostructures with decreasing buffer thickness of 600, 400, 200 nm respectively which are summed up with residual tensile strain causing red-shift in RT-PL peak. Also, increasing buffer thickness drastically reduced TD density from the order 10^{10} cm^{-2} to 10^{8} cm^{-2}. Surface morphology through AFM leads to decrease of pits and root mean square value with increasing buffer thickness which are resulted due to reduction of combined effect of strain and TDs.

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I. INTRODUCTION

III-Nitride compound semiconductor materials are gaining huge attraction for high-power, high-frequency4 as well as quantum applications because of their advanced properties such as wide band gap, high breakdown field (10^9 V/cm), high electron mobility, high saturation velocity (10^7 cm/s), large bandgap discontinuity,2 and their ability to realize high electron density in two-dimensional electron gas (2DEG) at the AlGaN/GaN interface.3,4 However, strain minimized, lower defect-III-nitride based structures of high crystalline quality, especially ultra-thin heterostructures are desirable for many applications.

Ultra-thin barrier III-Nitride heterostructures, such as AlGaN/GaN heterostructures with barrier-well thickness in the range of 10-15Å provides improved performance for several type of quantum devices such as resonant tunneling diode (RTD)5 and resonant tunneling high electron mobility transistor (RTHEMT).6 Several approaches by previous researchers illustrated the growth of such thin heterostructures on different substrate such as sapphire or free standing/Lateral epitaxial overgrowth

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(LEO)/Kyma GaN.7,8 Till now, no significant research has been done for the growth of ultra-thin barrier-well-barrier AlGaN/GaN/AlGaN heterostructure on silicon substrate. Previous several literatures described the growth of GaN on various substrates such as, SiC or sapphire, where SiC has lower lattice mismatch (~3.3%) along [0001] with GaN,9 and sapphire has smaller lattice (~13%) and thermal (~25.5%) mismatch with GaN.10 But in view of cost, scalability, thermal conductivity, high resistivity, silicon is the best contender as a replacement of all other substrates for supporting such coveted heterostructures, though it is a challenging approach to grow such thin barrier heterostructure on silicon substrate because of its lattice mismatch (~17%) and thermal mismatch (~54%) with GaN.11 Overcoming these problems, use of silicon as a substrate for GaN growth is increasing12,13 but for the formation of such ultra-thin AlGaN/GaN barrier-well region on silicon, needs critically optimized GaN buffer on silicon which should be of high quality. Crucial growth steps along with critical optimization of buffer thickness can only allow to grow high quality GaN that supports the formation of ultra-thin Al_{0.2}Ga_{0.8}N/GaN/Al_{0.2}Ga_{0.8}N barrier-well-barrier heterostructure on it.

This research reports the development of growth technology including minimization of thermally generated strain after strategically designed growth process involving adequately thin nitridation of silicon thus formation of SiN, followed by annealing before appropriate nucleation, subsequently transformation of SiN to AlN with optimized growth conditions, finally leading to expected quality of GaN buffer layer initiation resulting in high quality GaN on Si with lower tensile stress, all of which ultimately can support ultra-thin barrier AlGaN/GaN heterostructure in the range of 10-15Å.

The good quality heteroepitaxial GaN films on silicon are very attractive but strain and TDs due to mismatch limit structural formation of these heterostructures. Strain in GaN buffer layer strongly affects the formation of epitaxial layers, thus degrades devices electrical and optical properties.14–16 On the other hand, TDs also have impact on the formation of epitaxial layers on GaN buffer layer and compromise the device performance by reducing carrier mobility17–19 and increasing current leakage path in GaN devices.20,21 In fact, high electron mobility and low leakage current in GaN based devices are desirable to achieve high power performance at high frequency operations. Several attempts made by previous researchers to grow good quality heterostructures by choosing various intermediate layer in between GaN and Si, such as SiC,22 AlN,23,24 GaAs25 and different buffer layer such as GaN, AlGaN, graded AlGaN. However, critical optimization of epitaxial buffer layer with respect to its thickness and growth conditions is necessary to achieve good quality epitaxial layers. So, it is very important to study the strain and TDs in the buffer layer that can alter the structural formation as well as can change the device performance. Our critically evolved growth process involving pre-buffer nitridation and nucleation followed by buffer optimization is able to provide lower biaxial tensile stress in GaN buffer than the values already recorded in the literature.26,27

The critical thickness is inversely proportional to the Al content for GaN homoepitaxial growth.19 We have grown ultra-thin Al_{0.2}Ga_{0.8}N/GaN heterostructures where, barrier thickness is 1.5 nm which is less than the critical thickness (~1.8 nm). Thus, by employing low Al content (20%) in the barrier and keeping the barrier thickness less than the critical thickness, lattice relaxation via dislocation formation is prevented.28 This feature is essential for quantum devices where dislocations degrades its performance by causing leakage current.

In this work, first of all, we have successfully grown ultra-thin AlGaN/GaN heterostructures on Si(111) by PAMBE, after critical optimization of growth conditions. As buffer plays important role for the formation of epilayers, three samples of different buffer thickness have been grown to investigate the effect of strain and TDs of GaN buffer layer on the ultra-thin epitaxial heterostructures. The strain calculation has been performed by the results of HRXRD which is validated by RT-PL peak analysis. Clear images of HRTEM of all these samples helped us to find quantitative TD density values. Finally, AFM analysis indicates the overall surface morphology of these heterostructures.

II. EXPERIMENT

Three samples were grown on 2-inch Si (111) substrate using a PAMBE system, equipped with standard effusion cells for Ga, Al, and In. Activated nitrogen radicals were generated by
decomposing high-purity N$_2$ gas using an RF plasma cell. A 20-KeV RHEED system was used to monitor the growth process in real time. As shown in Fig. 1, three AlGaN/GaN samples are identical in structure except buffer thickness of 600 nm (sample 1), 400 nm (sample 2) and 200 nm (sample 3).

Outgassing the Si(111) substrate at around 510°C for almost 1 hour in the preparation chamber, it is transferred to the growth chamber, where, first of all, Si(111) substrates, for all the samples, were annealed at around 1000°C for 10 min to remove surface contamination. The clean Si(111)-(7x7) pattern in Fig. 2(a) indicates surface reconstruction where Kikuchi lines in Fig. 2(b) are slightly visible indicating clean, smooth surface with relatively free of oxides, other contaminations.

Absence of oxide from the substrate is confirmed through the RHEED pattern transformation from (7x7) to (1x1) at 830°C. In this process, intentional growth of very thin SiN layer over Si(111) substrate is done by exposing the substrate to RF plasma source for very small amount of time, which is confirmed by the (8x8)-like surface reconstruction (Fig. 2(c)). To maintain crystallinity of SiN layer, only 1 monolayer or less is grown, however; a single monolayer of Al is
sufficient in order to convert the crystalline SiN layer into AlN. This AlN formation transforms the (8x8) pattern to some other pattern, thus confirms the starting of AlN formation, shown in Fig. 2(d).

As binding energy of Al-N (11.5 eV) is much stronger than Si-N (3.5 eV), AlN nucleation layer formation occurs at the expense of SiN interlayer when both RF plasma source and Al shutter are kept open. A sharp AlN-Si interlayer is formed after the Al exposure, as the SiN layer is very thin. Keeping the RF power at 600 W and N$_2$ flow of 3 sccm, through temperature ramping from 600°C to around 900°C, 50 nm thick AlN nucleation layer is grown, which transforms RHEED pattern to thicker (1x1) as shown in Fig. 2(e). Through critical optimization of growth conditions and observing the RHEED pattern, GaN buffer layer (600 nm/400 nm/200 nm) on the AlN nucleation layer for all three samples were grown around 720°C at a growth rate of 0.6μm/hour, keeping the RF power at 650 W and 4 sccm nitrogen flow. (1x1)-RHEED pattern in Fig. 2(f) indicates good surface reconstruction during growth of 600 nm thick GaN buffer layer. 500 nm thick bottom layer was grown just above the buffer layer, for all samples. It was followed by growth of ultra-thin active region that consists of 1.5 nm thick Al$_{0.20}$Ga$_{0.80}$N barrier, 1.25 nm thick GaN well, 1.5 nm thick Al$_{0.20}$Ga$_{0.80}$N barrier, surrounded by 2 nm thick spacer layer. 300 nm thick GaN top layer was grown for all. Growth temperature for ultra-thin region structure was around 720°C, as measured with pyrometer whose accuracy was estimated to be ±3°C. Pressure in the growth chamber during the epitaxial growth was set around 10$^{-5}$ Torr range.

Measurement of a- and c- lattice parameter, followed by in-plane, out-of-plane strain, biaxial, hydrostatic strain component as well as biaxial stress in GaN buffer layer for all have been carried out with the help of Omega-2Theta scan in HRXRD, at the vicinity of the symmetric and asymmetric plane. HRXRD measurement was performed using BEDE D1 (Jordan Valley) diffractometer equipped with CuK$\alpha_1$ (1.54056 Å) line and a Ge (004) channel-cut crystal. The symmetrical Omega-2Theta scan have been done in (00.1) plane (where l=2, 4, 6; l is in the order of reflection) and asymmetrical Omega-2Theta scan have been performed in glancing incidence (GI) and glancing exit (GE) mode for (hk.l) = (10.4), (10.5), (11.4) plane for all samples. PL measurements were carried out at room temperature by Accent RPM 2000 Photoluminescence, from Nanometrics. A Q-switched laser of 266 nm wavelength was used as the excitation source. We scanned a range from 330 nm to 410 nm for all the samples. TEM investigation was carried out on JEOL JEM-2100 (TEM) operated at 200 kV. Cross sectional samples were prepared by standard techniques of ultrasonic disc cutting, mechanical polishing, dimpling, and Ar$^+$ ion milling at 3 kV up to electron transparencies for bright field observations of dislocations. AFM imaging has been performed by Agilent Technologies 5500 AFM in tapping mode with a SiN tip.

III. RESULTS AND DISCUSSION

Double axis HRXRD scans of samples 1, 2 and 3, in accordance with the nominal structures illustrated in Fig. 1 are shown in Fig. 3. It shows two peaks of GaN and AlN in close proximity in (00.2) scan for all the samples where, no AlGaN peak is visible as these layers are very thin. Internal strain slightly shifts the GaN peak position towards left of the graph which is specified by the gray colored straight line in Fig. 3, whereas; no such shift of AlN peak position in these three samples can be observed as the AlN layer gets strain relaxed under thicker GaN buffer layer. Full Width Half Maximum (FWHM) values, obtained from the (00.2) x-ray rocking curves (RC) of GaN layers determines the crystalline quality of the samples. The respective values in sample 1, 2 and 3 are calculated as 372 arcsec, 403.2 arcsec, 417.6 arcsec and the smallest FWHM of the sample 1 (600 nm buffer thickness) confirms better crystal quality of the GaN epilayer.

Quantitative and qualitative strain analyses in buffer of these samples have been performed through the calculation of lattice constant from HRXRD results. In-plane, out-of-plane strain, hydrostatic strain followed by biaxial strain and biaxial stress in GaN buffer layer were computed from the measurement of lattice constant. Growth of hexagonal crystallographic structure such as GaN, AlN on Si(111) causes plastic deformation in GaN and AlN along the parallel and perpendicular axes due to wide difference in thermal expansion coefficients of the materials. An isotropic behavior is also displayed by GaN with respect to hydrostatic pressure. The out-of-plane, $\varepsilon_c$, and
FIG. 3. Experimental diffraction curves Omega-2Theta (deg.) of symmetric (00.2) CuKα₁ reflection from the AlGaN/GaN heterostructures for sample 1, 2 and 3, respectively.

In-plane, $\varepsilon_a$, strain components for GaN buffer layer can be described by the relations given below:\textsuperscript{31}

$$\varepsilon_c = \frac{c_s - c_0}{c_0} \quad (1)$$

$$\varepsilon_a = \frac{a_s - a_0}{a_0} \quad (2)$$

where, $c_s$ and $a_s$ are strained lattice parameters and $c_0$ and $a_0$ are unstrained lattice parameters of GaN.

The real value of strained lattice parameter, $c_s$, is related to its experimental value, $c_{ex}$ through an angular parameter, $q_{ex}$ by the following relationship

$$c_{ex} = \frac{-Dc_s}{r} q_{ex} + c_s \quad (3)$$

where,

$$q_{ex} = \frac{\cos^2 \theta_e}{\sin \theta_e} \quad (4)$$

and $r$ ($\sim$460 mm) is the distance between the specimen to the detector. $D$ ($\sim$0.046°) represents the possible displacement of the specimen with respect to the goniometer axis in the equatorial plane. $c_s$ value can be determined from the plot of $(q_{ex}, c_{ex})$. Vegard’s law is used to find the $c_{ex}$ lattice parameter by using the Omega-2Theta scans of the (00.1) reflections for $l$=2, 4, 6

$$c_{ex} = \frac{l \lambda}{2 \sin \theta_e} \quad (5)$$

where, $\theta_e$ and $\lambda$ represents the peak position of reflection and wavelength of CuKα₁ reflection.

With the help of the symmetrical Omega-2Theta diffraction spectra and (3)-(5), strained lattice parameter, $c_s$ can be measured for all, which are displayed in Table I. The $a$-lattice parameter of the
TABLE I. The values of $c_s$ (measured for a certain azimuthal position of sample) and in GaN buffer layer of AlGaN/GaN samples.

| Sample | Diffraction peak position, $\theta_{hkl}$ (°), order of reflection in the degree unit | Measured c-lattice parameter $c(\text{Å})$ |
|--------|-------------------------------------------------------------------------------------|------------------------------------------|
|        | $h=2$                                                                 | $h=4$ | $h=6$ | $c_s$ | $\overline{c_s}$ |
| 1      | 17.310 ± 0.002                                                                   | 36.469 | 63.039 | 5.1836 ± 0.0002 | 5.1836 |
| 2      | 17.290                                                                         | 36.469 | 63.083 | 5.1827 | 5.1827 |
| 3      | 17.287                                                                         | 36.453 | 63.066 | 5.1823 | 5.1823 |

GaN layer is determined from the diffraction peaks of the asymmetrical reflections (hkl) which is given by

$$a_{(hkl)} = c d_{hkl} \sqrt{\frac{4/3(h^2 + k^2 + h k)}{c^2 - l^2 d_{hkl}^2}}$$

(6)

where, $c$ is equivalent to $\overline{c_s}$ calculated from four different azimuthal positions (by rotating the sample about the z-axis through 90°). Asymmetrical Omega-2Theta scan for sample 1, 2, and 3 in GI and GE mode are performed and diffraction peak positions are written in Table II. The strained a-lattice parameter for GaN is measured using values of Table II and (6), which is summarized in the last column of Table II. The out-of-plane strain component, $\varepsilon_c$ in GaN layer of AlGaN/GaN samples are calculated using (1), taking the average value of $c_s$, from Table I, considering the value of $c_0$ as 5.1855 ± 0.0002 Å. The $\varepsilon_c$ values for AlGaN/GaN samples are presented in second column of Table III.

The in-plane strain component of GaN buffer, $\varepsilon_a$ is computed using (2), and considering $a_0 = 3.1890 ± 0.0003$ Å which are summed up in third column of Table III. In all these samples, the strain component in the a- and c- directions change in compressive (negative strain) or tensile (positive strain) type exhibit a characteristic behavior depending on the thickness of GaN buffer on AlN. Strain in c-direction and a-direction of GaN buffer layer reveals compressive behavior and tensile behavior respectively. Table III shows a gradual increase in compressive strain along c-direction and tensile strain in a-direction of GaN layer. This case comes from the large lattice mismatch between a- and c- lattice parameter or the lattice mismatch between GaN-AlN buffer layer with silicon substrate.

$\varepsilon_{hy}$ is the hydrostatic strain which is given by the following expression

$$\varepsilon_{hy} = \frac{1 - \nu}{1 + \nu} \left( \varepsilon_c + \frac{2\nu}{1 - \nu} \varepsilon_a \right)$$

(7)

The behavior of GaN is described by one strain component which is determined from the elastic constants $c_{13}$ and $c_{33}$.

$\nu$ is known as Poisson’s ratio which is given by

$$\nu = \frac{c_{13}}{c_{13} + c_{33}}$$

(8)

TABLE II. The value of the a-lattice parameter in the GaN buffer layer of AlGaN/GaN heterostructures.

| Diffraction peak position, $\theta_{hkl}$ (°), Reflection (hk.l) | Sample | GI | GE | GI | GE | GI | GE | Measured a-lattice parameter $a(\text{Å})$ |
|---------------------------------------------------------------|--------|----|----|----|----|----|----|---------------------------------------------|
| (10.4)                                                        | 1      | 41.015 ± 0.002 | 41.029 | 52.485 | 52.516 | 49.981 | 49.983 | 3.1949 ± 0.0002 |
| (10.5)                                                        | 2      | 41.031 | 41.026 | 52.519 | 52.516 | 49.972 | 49.978 | 3.1986 |
| (11.4)                                                        | 3      | 41.056 | 41.018 | 52.494 | 52.527 | 50.008 | 49.961 | 3.1991 |
The sources of hydrostatic strain are the substitutional type point defects, interstitial point defects, and vacancies in AlN, GaN, AlGaN. Crystal lattice expansion and compression depend on these three factors. Poisson’s ratio of GaN (the values for the elastic constant for GaN, $c_{11}$ and $c_{33}$ are 106 GPa and 398 GPa respectively) is measured using (8).

Hydrostatic strain for sample 1, 2, and 3 are calculated using Poisson’s ratio and (7) which is written in the fourth column of Table III. Results demonstrate that $\varepsilon_{hy}$ of the GaN buffer of three samples exhibit tensile character in order of $10^{-4}$.

The $\varepsilon_c$ and $\varepsilon_a$ components in GaN buffer layer are superposition of biaxial and hydrostatic strains which are

$$\varepsilon_c = \varepsilon_c^b + \varepsilon_{hy}$$
$$\varepsilon_a = \varepsilon_a^b + \varepsilon_{hy}$$

where, $\varepsilon_c^b$ and $\varepsilon_a^b$ are the biaxial strain in the c- and a-direction, respectively. Biaxial strain in c- and a-direction of GaN buffer-bottom layer for these three samples were calculated using (9), (10) and hydrostatic strain values in Table III. Fifth column and sixth column of Table III show compressive and tensile character respectively for all these three samples.

The in-plane biaxial stress in the GaN buffer can be expressed in terms of biaxial elastic modulus, $M_f$ as shown below

$$\sigma_{bs} = M_f\varepsilon_a^b$$

where, $M_f$ is expressed using the elastic constants $c_{ij}$ of GaN such as $c_{11}$, $c_{12}$, $c_{13}$, $c_{33}$.

$$M_f = c_{11} + c_{12} - 2\frac{c_{13}^2}{c_{33}}$$

Epilayer stress occurs in the film due to the mismatch of lattice constant and thermal expansion coefficients (TEC) between the substrate. In case of hexagonal GaN it is biaxial in nature. Measurement of in-plane biaxial stress in GaN buffer layer is performed using (11) and ((12)) which is displayed in the last column of Table III. Biaxial elastic modulus, $M_f$ in (12) can be calculated using the values of elastic constants $c_{11} = 390$ GPa, $c_{12} = 145$ GPa, $c_{13} = 106$ GPa and $c_{33} = 398$ GPa. Results show that biaxial stress in GaN buffer-bottom layer for all three samples is tensile type. Thicker GaN buffer-bottom layer provides minimum biaxial tensile stress compared to other two samples. Our evolved epitaxial buffer growth process leads to overall lower biaxial tensile stress in GaN buffer than the previously achieved values by other researchers, particularly with the lowest stress in the thickest buffer.

Both symmetric (00.2) and asymmetric (10.5) reciprocal space mapping (RSM) scans have been performed to validate the outcome of the strain calculation done by HRXRD results, that decreasing buffer thickness results degraded GaN quality. Symmetric and asymmetric both RSM images show the absence of (thin) Al$_{0.5}$Ga$_{0.5}$N layer. In asymmetric RSM, reciprocal lattice points of GaN is only visible, AlN layer is absent, which is probably because of higher peak separation between AlN and GaN layer in asymmetric scan. This is further worsened by the fact that AlN layer is buried deep under the upper epitaxial heterostructures, which is mostly GaN. Decreasing buffer thickness is confirmed with decreasing inclination angle of GaN RSM spectra. Thus, the increase in

| Sample | Measured strain in c-direction | Measured strain in a-direction | Hydrostatic strain | Biaxial strain in c-direction | Biaxial strain in a-direction | Biaxial stress $\sigma_{bs}$ (GPa) |
|--------|-------------------------------|-------------------------------|-------------------|-------------------------------|-------------------------------|----------------------------------|
| 1      | $-3.6641 \times 10^{-4}$      | $1.8495 \times 10^{-3}$       | $4.0370 \times 10^{-4}$ | $-7.7011 \times 10^{-4}$      | $1.4458 \times 10^{-3}$      | $0.6918 \pm 0.04$               |
| 2      | $-5.3997 \times 10^{-4}$      | $3.0104 \times 10^{-3}$       | $6.9391 \times 10^{-4}$ | $-1.2339 \times 10^{-3}$      | $2.3164 \times 10^{-3}$      | $1.1084$                        |
| 3      | $-6.1711 \times 10^{-4}$      | $3.1671 \times 10^{-3}$       | $6.9807 \times 10^{-4}$ | $-1.3152 \times 10^{-3}$      | $2.4691 \times 10^{-3}$      | $1.1814$                        |
broadening of diffraction spectra of GaN with decreasing buffer thickness concludes that the GaN quality degrades with decreasing buffer thickness, under similar growth conditions.

Room temperature PL spectrum of three samples of AlGaN/GaN heterostructures shown in Fig. 4(a) supports HRXRD results by indicating a slight red-shift of GaN peaks for sample 1 through 3. For sample 1, GaN peak is seen at 363.626 nm (E_g at 3.4101 eV) and for sample 2 and 3 peaks are observed at wavelength of 364.481 nm (3.405 eV) and 364.982 nm (3.3974 eV) respectively. This peak shift indicates the reduction of bandgap which is related to positional change of conduction band minimum (CBM) and valence band maximum (VBM) that occurs due to the biaxial stress. CBM shifts due to the kinetic energy effect and antibond state effect (interaction between cation-s and anion-s valence orbitals). Table II shows an increase of a- lattice parameter from sample 1 through sample 3 demonstrating that the kinetic energy between the cation and anion decreases and simultaneous reduction of energy due to the antibond state effect. As a result, CBM offsets to low energy. Shift in VBM arises due to kinetic energy effect and bond state effect (interaction between anion-p and cation-p valence orbitals) which partially cancel each other and results small VBM offset. As the VBM offset is smaller than CBM offset bandgap decreases with increase in the biaxial tensile stress which is achieved from the PL data.

It can be noted that for all the samples the buffer thickness is much higher than critical thickness of GaN grown on AlN layer, so GaN buffer layer of all the samples are relaxed. As the lattice constant of GaN (3.186 Å) is higher than lattice constant of AlN (3.114 Å), after growth, initially, a compressive strain occurs in thin GaN layer. If the thickness of GaN increases, after cooling, due to the difference in thermal expansion coefficient between AlN (4.6 x 10^{-6} K^{-1} at 300K) and GaN (5.6 x 10^{-6} K^{-1} at 300K), a residual in-plane tensile strain occurs in GaN layer of all samples which is not dependent on the AlN layer thickness. In this condition when AlGaN is grown on GaN, a natural tensile strain (due to lattice mismatch) appears which simply adds up with the existing residual tensile strain in GaN. As the thin buffer AlGaN/GaN heterostructure is more strained, its PL peak is more red-shifted as shown in Fig. 4a. Fig. 4(b) summarizes whole analysis by concluding that with the increase of thickness of GaN buffer layer biaxial tensile stress increases by reducing the band gap of GaN layer.

Structural qualities such as threading dislocations for the samples were investigated by TEM analysis. To determine the dislocation types g (diffraction vector) and b (Burgers vector) were used. Notably, most of the dislocations were projected and visible with g = 11-20, thus designating edge type (pure a-type or mixed a + c- type) with b = 1/3(11−20) for majority of dislocation. Using these dislocation visibility (g,b) criteria, density of dislocation was determined.
Large lattice mismatch between AlN and Si (19%) induced high dislocation density in AlN layer for all samples, but just above the AlN/GaN interface, this density is lower as some TDs originating from the AlN layer ended up in this layer and did not start threading into the GaN buffer layer (This situation is same for all the three samples). Though, some of the TDs originating from AlN layer continued to threading up towards GaN buffer layer, in fact, some reached to GaN bottom layer depending on buffer thickness for these three samples. TEM image of sample 1 observed in Fig. 5(a) shows very dense TDs visible in ~200 nm of GaN buffer above the AlN layer, whereas; annihilation or bending of TDs originating from AlN or from AlN/GaN interface was reduced more than half if we move ~100 nm more in GaN buffer layer in sample 1. Though some of the TDs are ended up near the GaN buffer-GaN bottom layer interface (Fig. 5(a)), but, the remaining TDs of the GaN bottom layer were nearly parallel to the growth direction. These TDs were disturbing the formation of the ultra-thin $\text{Al}_0.2\text{Ga}_{0.8}\text{N}$/GaN heterostructure for these samples. The TD density can be recorded through trace analysis from several regions of sample 1 as $\sim 8 \times 10^{10}$ cm$^{-2}$ near AlN-GaN buffer layer interface, and $\sim 5 \times 10^9$ cm$^{-2}$ in GaN top layer near GaN buffer-GaN bottom layer interface. Thin region shows a dislocation count of $\sim 4 \times 10^9$ cm$^{-2}$.

Thus, in sample 1, the thick buffer (600 nm) was capable to stop the propagation of TDs towards the ultra-thin $\text{Al}_0.2\text{Ga}_{0.8}\text{N}$/GaN layers by almost 95%, only few TDs were affecting the formation of this thin barrier-well layer in some regions as shown in Fig. 5(a). Two zoomed versions of this in Fig. 5(b) and Fig. 5(c) indicate how nicely ultra-thin 1.5 nm $\text{Al}_0.2\text{Ga}_{0.8}\text{N}$–1.25 nm GaN–1.5 nm $\text{Al}_0.2\text{Ga}_{0.8}\text{N}$ layers were formed in sample 1. Effect of buffer thickness on the formation of thin region plays significant role due to the origination of TD in the sample. While comparing the quality of this thin region, it is clearly observed that with the reduction of buffer thickness quality as well visibility of thin AlGaN/GaN region is becoming poor compared to sample 1 as shown in Fig. 5(d), Fig. 5(e). TD density varies from $\sim 10^{10}$ cm$^{-2}$ – $\sim 8 \times 10^9$ cm$^{-2}$ in between AlN/GaN interface to thin region for sample 2, whereas, sample 3 shows TD density in the order of $10^{10}$ cm$^{-2}$ throughout, validating the fact that thin buffered heterostructure is heavily affected by the TDs originated from the lower layers. TEM image for sample 3 in Fig. 5(e) indicates that the formation of continuous thin region is interrupted by TDs and in some region (as shown in circle in Fig. 5(e)) due to the accumulation of TDs no such region could be formed.
FIG. 6. Atomic force microscopy images of 20 x 20 µm² area AlGaN/GaN based heterostructures (a) sample 1, (b) sample 2, and (c) sample 3.

Typical surface morphology of the three samples characterized by AFM which are presented in Fig. 6. Fig. 6(a)-6(c) are 20 x 20 µm² AFM images of these three AlGaN/GaN based heterostructure. Pits of different sizes correspond to different type of dislocation as the largest pits are formed on screw, intermediate size pits on mixed- and the smallest ones on edge type dislocation.39 Analysis of stress-strain explains the presence of tensile strain in AlGaN/GaN samples which increases from sample 1 through sample 3 producing dislocation in the sample which are clearly displayed as pit in the AFM images. The pit is minimum in sample 1 of AlGaN/GaN heterostructure as shown in Fig. 6(a) which increases abruptly from sample 2 to sample 3 as shown in Fig. 6(b) and Fig. 6(c) respectively. It indicates the increase of dislocation density from sample 1 through sample 3 of AlGaN/GaN heterostructures. However, no such large size pits are visible in these figures, only the pits of median and smaller sizes are observed.

Surface roughness is measured by root mean square (RMS) values which are 2.37 nm, 2.71 nm, and 2.81 nm for sample 1, 2 and 3 respectively, indicating better surface quality for sample 1 compared to other two samples of AlGaN/GaN heterostructures. The growth process has been further optimized to achieve nominal AFM-RMS values around 1 nm reproducibly.

IV. CONCLUSIONS

This paper presents a critically optimized growth regime for growing high quality GaN on silicon substrate by following unique steps such as adequately thin nitridation, appropriate nucleation and initiation of high quality GaN buffer with comparable lower strain, that supports the formation of ultra-thin 1.5 nm AlₐGa₀₋ₐN–1.25 nm GaN–1.5 nm AlₐGa₀₋ₐN heterostructure. The impact of buffer thickness on the development of ultra-thin AlₐGa₀₋ₐN/GaN heterostructures has been investigated by HRXRD, PL, TEM and AFM. Studies showed that the stress-strain, peak-shift, dislocations and surface morphology are all interdependent. The most striking features of the study is the observation of reduction of red-shift of GaN PL peak with increasing buffer thickness, which is resulted due to the cumulative decrease in internal tensile strain (due to lattice mismatch) and residual tensile strain (due to thermal mismatch) in the GaN buffer layer. In addition, TEM results reveal reduction of dislocation density in the thick-most buffer (600 nm GaN buffer) structure in the order of 10⁸ cm⁻² from 10¹⁰ cm⁻² in the thin 200 nm GaN buffer. It can be concluded from the present analysis that tensile strain and TDs combined affecting the formation of thin 1.5 nm AlₐGa₀₋ₐN–1.25 nm GaN–1.5 nm AlₐGa₀₋ₐN heterostructure on Si(111). So, the thick buffer-structure (600 nm GaN buffer) with biaxial tensile stress of 0.6918 ± 0.04 GPa and TD density in the order of 10⁸ cm⁻² is able to provide best thin AlGaN/GaN heterostructure compared to other two samples with lower buffer thickness (400 nm and 200 nm GaN buffer). Surface morphology through AFM analysis also supports our study by indicating decrease of pits and RMS value with increasing buffer thickness which are resulted due to the decreasing strain and TD density. It is expected that this research output will catalyze realistic implementation of quantum devices empowered by ultra-thin barrier-well heterostructures, which will further lead to III-N based high frequency applications on much coveted silicon substrate along with possibility of integration with main stream silicon based electronics.
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