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AlGaN/GaN two-dimensional-electron gas heterostructures on 200 mm diameter Si(111)

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This Letter reports on the epitaxial growth, characterization, and device characteristics of crack-free AlGaN/GaN heterostructures on a 200 mm diameter Si(111) substrate. The total nitride stack thickness of the sample grown by the metal-organic chemical vapor deposition technique is about $3.3 \pm 0.1 \mu\text{m}$. The structural and optical properties of these layers are studied by cross-sectional scanning transmission electron microscopy, high-resolution x-ray diffraction, photoluminescence, and micro-Raman spectroscopy techniques. The top AlGaN/GaN heterointerfaces reveal the formation of a two-dimensional electron gas with average Hall mobility values in the range of 1800 to 1900 cm^2/Vs across such 200 mm diameter GaN on Si(111) samples. The fabricated $1.5 \mu\text{m}$ -gate AlGaN/GaN high-electron-mobility transistors exhibited the drain current density of 660 mA/mm and extrinsic transconductance of 210 mS/mm . These experimental results show immense potential of 200-mm diameter GaN-on-silicon technology for electronic device applications. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4746751>]

Recently, gallium nitride (GaN)-based solid-state devices have shown exceptional capabilities for electronic devices operating at high power, high-frequency, and high-temperature. The fundamental properties of AlGaN/GaN material system also make it an ideal candidate for high-power microwave devices. However, a large scale deployment of GaN electronic devices in consumer market applications requires a substantially low cost. Due to the lack of commercially available large area GaN substrates, GaN heterostructures are currently grown primarily on sapphire, silicon carbide (SiC), and more recently on Si(111). For electronic applications, Si substrate is a very attractive alternative, being much cheaper than sapphire and SiC when substrate diameters are larger than 150 mm. There has been tremendous interest to grow III-nitride heterostructures on silicon substrates due to the huge market potential and possibly being able to be integrated with well-developed Si micro-electronic circuit technologies.^{1–3} However, the GaN epitaxial films grown on Si suffer from a significant mechanical strain that is caused by the lattice mismatch, a large difference in thermal expansion coefficients between substrate and epilayers, and the thermal gradients across the wafers. These result in a high density of misfit and threading dislocations (TDs) in the AlGaN/GaN heterostructures grown on Si substrates. Beside the tensile stress generated in GaN epitaxial

wafers on Si, the large diameter wafers show a pronounced bowing effect, leading to non-uniform electronic properties. To relieve the tensile stress and to achieve crack-free GaN heterostructures, a wide variety of buffer and inter layers such as low-temperature AlN,⁴ graded AlGaN buffers,⁵ and Al(Ga)N/GaN superlattices⁶ have been used. For integration with silicon process foundries based on complementary metal-oxide-semiconductor (CMOS) technologies, it is desirable to scale up GaN epitaxy to 200 mm on a 200 mm Si substrate. However, to date, there has been less success in achieving high quality AlGaN/GaN heterostructure on 200 mm Si substrates due to issues like epilayer cracking, wafer bowing, and high density of point and line defects when nitride stack thickness exceeds $3.0 \mu\text{m}$. To showcase high electron mobility transistors (HEMTs) on 200 mm Si platform with comparatively similar device performances levels as reported currently on Si substrate platform,^{7,8} it is necessary to grow thicker GaN buffer to minimize the buffer leakage and also to improve the layer crystalline quality.

In this Letter, we report crack-free AlGaN/GaN heterostructures grown on 200 mm diameter (111)-oriented silicon substrates and present an in-depth characterization study of epilayers grown by metal organic chemical vapor deposition (MOCVD). The GaN buffer thickness overgrown on AlGaN/AlN varies in the range of $\sim 2.4\text{--}2.5 \mu\text{m}$ (with a total nitride stack thickness of $3.3\text{--}3.4 \mu\text{m}$). The optical, electronic, and structural properties of the layers show their suitability for electronic device applications. In addition, we have demonstrated fabrication and device characteristics of HEMTs

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using such AlGaN/GaN heterostructures grown on a 200 mm diameter platform.

The epitaxial growth of GaN on Si (111) substrates was carried out in a Veeco Turbodisc K465i high throughput MOCVD tool equipped with a DRT 210 *in-situ* process monitor. The starting 1.5 mm thick Si(111) substrate was heated to $\sim 1000^\circ\text{C}$ in H_2 atmosphere and annealed for about 3 min to remove native oxide from the surface. First, a high temperature (HT) AlN nucleation layer (thickness ~ 140 nm) was grown followed by three step-graded $\text{Al}_x\text{Ga}_{1-x}\text{N}$ buffer layers with an Al content of 75%, 50%, and 25%. About 2.4 to 2.5 μm thick GaN was overgrown on these buffers using a single strain-compensating low temperature (LT) AlN interlayer.⁴ The optimized buffer conditions of the HEMT layers used a growth temperature of about 1050°C for AlN nucleation layer and GaN at a pressure of about 75 and 200 Torr, respectively, while the three step-graded AlGaN buffers used a pressure of about 100 Torr. Using 1.5 mm thick Si(111) substrates, we could easily achieve crack-free epilayers with total nitride stack thickness $3.3 \pm 0.1 \mu\text{m}$, but with a significantly reduced wafer bowing $< 20 \mu\text{m}$. In order to make GaN semi-insulating for electronic applications, carbon auto-doping has been used. About 18 to 20 nm thick $\text{Al}_x\text{Ga}_{1-x}\text{N}$ (target Al content of 20%) barrier layer with a 2–3 nm thin GaN cap was grown to form a 2DEG interface. Furthermore, to improve the two-dimensional electron gas (2DEG) mobility, samples were grown with a thin AlN spacer (~ 1.0 nm) layer.

The layer thicknesses of the epilayers, the buffer, and interlayers, as well as the top $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier layers were determined using a Philips FEI CSM 300 transmission electron microscopy (TEM) set up. Figure 1 shows the typical cross sectional TEM micrographs of the AlGaN/GaN heterostructure grown on a 200 mm Si substrate. Two sets of measurements from center and edge of the epiwafers were performed to probe the total nitride stack thickness including the AlN starting buffer, step-graded multiple AlGaN buffer layers, the strain-compensating low-temperature (LT) AlN interlayers, and top AlGaN/GaN interfaces. An average thickness of about $\sim 3.35 \mu\text{m}$ nitride stack is confirmed from TEM data. The bright field TEM image in Fig. 1(a) shows the nature of three step-graded AlGaN buffers and the GaN epilayer. The thickness of LT-AlN interlayer is about 10–11 nm as probed by high-resolution (HR) TEM imaging. The HR-TEM imaging shown in Fig. 1(b) also reveals top $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier layer with a thin GaN cap. In order to probe AlGaN/GaN 2DEG interfaces and the nature of dislocation propagation, we have also explored imaging of high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM). The z-contrast HAADF-STEM images in Fig. 1(c) show the crystalline nature of the Al(Ga)N epilayers and accurate thickness profiles. The presence of a thin AlN spacer beneath the AlGaN barrier is also confirmed from the high-resolution HAADF-STEM image shown in Fig. 1(d). Deposition of AlN nucleation layer on Si(111) before GaN growth has often used to avoid the diffusion of Ga into the substrate. Furthermore, the thermal expansion coefficients of AlN is between those of GaN and Si, and hence, to control strain balance on the large area wafer, we have used three step-graded $\text{Al}_{1-x}\text{Ga}_x\text{N}$ buffer layers ($x = 75$ to 25%). The LT-AlN interlayer was grown at an in-

FIG. 1. Cross-sectional TEM images of the AlGaN/GaN heterostructures and full nitride stack on the HT-AlN nucleation layer on 1.5 mm thick Si(111) substrate. Images (a) and (b) represent bright-field XTEM of the layers and the top AlGaN/GaN interfaces. Micrographs (c) and (d) represent the HAADF-STEM z-contrast images of the sample 2, showing different interfaces and much accurate thickness profiles.

intermediate temperature range of 850 – 860°C . The LT-AlN interlayer offers in-plane compressive stress because of the $\sim 2.5\%$ lattice mismatch between the AlN and GaN, and usage of such an interlayer helps to partially offset the thermal tensile stress during temperature ramp-down.⁹ In addition, the compressive strain field in the interlayer also led to dislocation bending and annihilation of some screw dislocations as seen from TEM imaging. At the same time, some lattice mismatch induced misfit dislocations also appear at these interfaces, propagating to the top AlGaN barrier layer. In order to probe defect density in such 200 mm epiwafers, we have further explored the high resolution x-ray diffraction (HRXRD) and atomic force microscopy (AFM) measurements. The use of bottom AlGaN/AlN buffers and LT-AlN eventually led to realization of a crack-free 200 mm AlGaN/GaN heterostructure. The usage of a 1.5 mm thick Si(111) substrate reduced the post growth in-plane stress gradient and thus leading to a reduced wafer bowing. The micro-Raman, microscopic photoluminescence (PL), and Hall measurements were performed across the epiwafer to estimate variations in crystalline quality and electrical properties. To check the applicability of such AlGaN/GaN interfaces for HEMTs, Hall effect measurements were performed on the $1 \text{ cm} \times 1 \text{ cm}$ square shape diced pieces from 200 mm wafer center to edge.

To analyze the crystalline quality of the as-grown layer structure, HRXRD measurements were performed with a PANalytical X'Pert PRO diffractometer using a 4-bounce hybrid mirror monochromatized $\text{Cu K}\alpha 1$ radiation ($\lambda = 1.5406 \text{ \AA}$). The full-width at half-maximum (FWHM) of x-ray rocking curves of various symmetrical and asymmetrical Bragg reflections was studied, and a quantitative

evaluation of dislocation densities was also performed for a wide variety of HEMT epilayers grown on 200 mm diameter Si(111) substrates. In such samples, the threading dislocation density was further confirmed by the etch pit densities of samples evaluated by performing hot phosphoric acid etching followed by AFM topography imaging. Figure 2(a) shows a post-growth picture of the crack-free 200 mm AlGaIn/GaN HEMT structure on 1.5 mm thick Si(111) substrate. Figure 2(b) represents a typical HRXRD ω -2 θ scan of (0002) diffraction plane of such AlGaIn/GaN structures on 200 mm Si. The spectrum shows clear satellite peaks at lower Bragg angle side representing good crystalline quality interfaces. The dominant peak is from the thick GaN layer, while the peaks at higher Bragg angles originate from the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and AlN layers. The inset shows the rocking curves of (002) and (102) diffraction planes of GaN from this sample. We have observed an average (002) and (102) rocking curve FWHM of 418–420 and 612–625 arcsecs, respectively,

FIG. 2. (a) Picture of the 200 mm GaN-on-Si HEMT wafer after epitaxial growth. (b) HRXRD ω -2 θ scan of (0002) diffraction plane of AlGaIn/GaN heterostructures on 200 mm Si(111). The inset shows the HRXRD rocking curves of (002) and (102) planes giving a measure of tilt and twist in such large area epiwafer. The sample uniformity is probed by such measurements of rocking curves at wafer center and wafer edges.

at the epiwafer center areas. However, at the edge of the wafer, the (002) rocking curve linewidth increased to 460 arcsecs while (102) FWHM of about 612 arcsecs shows no significant change. The (105) diffraction plane rocking curve shows an FWHM of about 504 arcsecs. These values are indicative of high crystalline quality device grade GaN on 200 mm Si. The screw and edge dislocation densities can be calculated from the analysis of symmetrical and asymmetrical reflections, respectively.¹⁰ From our study on this 200 mm diameter HEMT epitaxial wafer with a much lower wafer bowing, we estimated an average screw dislocation density of $3.9 \times 10^8 \text{ cm}^{-2}$ and $4.1 \times 10^8 \text{ cm}^{-2}$, at wafer center and wafer edges, respectively. Furthermore, the average edge dislocation density at the wafer center and wafer edges was estimated to be about $9.8 \times 10^8 \text{ cm}^{-2}$ and $1.0 \times 10^9 \text{ cm}^{-2}$, respectively. To further probe the dislocation density at the top 2DEG interfaces, we have carried out an estimation of etch pit density. The AFM imaging gives a root mean square roughness of about 0.2 nm ($5.0 \mu\text{m} \times 5.0 \mu\text{m}$ scans) on the as-grown HEMT wafer surface. From the AFM images of the as-grown and etched samples, the etch pits are mostly found at the step terminations. Hence, we consider the average etch pit densities to be mostly screw/mixed type TDs and are estimated to be about $1.0 \times 10^9 \text{ cm}^{-2}$ in these samples, agreeing closely with the TD density calculations from the HRXRD asymmetrical reflections.

In order to address the optical properties of the 2DEG hetero-interfaces, we have carried out micro-PL and micro-Raman measurements. Variable temperature PL measurements were performed to probe the optical quality of the 2DEG at the top surface. The emission from top AlGaIn barrier is studied using ultraviolet (UV) PL spectra excited using the 266 nm laser. The multiple peak spectral deconvolutions gave rise to peaks originating from the top AlGaIn barrier and underlying GaN 2DEG channel. A much broader and weaker room-temperature PL peak from AlGaIn barrier appears at 3.545 eV, whereas the stronger PL peak centered around 3.405 eV appears from the underlying GaN layer. PL peak from GaN using both 266 and 325 nm laser excitations show a variation from 3.404 to 3.408 eV across the 200 mm wafer and such a small variation is due to the flat GaN wafer with a reduced bow. Figure 3(a) shows the variable temperature PL spectra recorded close to the wafer center from sample 2. At 77 K, the strong PL peak at 3.456 eV corresponds to a near-band-edge free exciton transition from GaN while the broader peak located at 3.588 eV corresponds to the emission from the top thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier layer. The emission peaks show monotonic bandgap shrinkage with increasing temperature and the line width of PL peaks increases as a function of temperature due to increased lattice vibrations and thermal damping. The PL line scan across the 200 mm wafer using 325 nm excitation shows a very uniform spectral intensity distribution of GaN band-edge PL peak (inset of Fig. 3(a)) and much weaker deep level luminescence bands, thus representing good crystalline quality at the 2DEG GaN channel region. To complement optical quality of the HEMT epilayers across the 200 mm wafers, the electrical properties of the 2DEG structures were further probed by Hall effect measurement system. Figure 3(b) shows the experimental data from Hall measurements

FIG. 3. (a) Variable temperature micro-PL spectra from AlGaIn/GaN heterostructure on Si(111) recorded under 266 nm laser line excitation. The broader PL at higher energy side appears from the top thin AlGaIn barrier. The inset shows PL spectra excited under 325 nm laser line from regions marked across a full wafer. Much uniform GaN luminescence profiles across the 200 mm wafers representing high quality GaN growth. (b) Hall measurements data depicting typical center to edge variation of electrical properties of a 200 mm HEMT epiwafer. The schematic describes measurement locations.

performed on the diced samples taken from wafer center to edge. Such epitaxy of AlGaIn/AlN/GaN 2DEG heterostructures in a series of samples resulted in an average mobility of 1800–1900 $\text{cm}^2/\text{V.s}$ with the center to wafer edge variation being reduced to 7 to 9%. The sheet resistivity in such a case has shown a variation of about 10 to 12% when Hall measurements were done across wafer center to edge locations. Despite a low wafer bowing, such a variation is expected due to a slight variation of Al content in the AlGaIn top barrier and a small thickness variation expected in AlN/AlGaIn/GaN top layers.

The characteristics of optical phonons originating from such 2DEG AlGaIn/GaN interfaces were probed by variable temperature UV micro-Raman measurements using a Jobin Yvon LABRAM-HR setup. The 325 nm UV Raman near-resonantly excites the top $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interfaces. Figure 4(a) shows the typical Raman spectra recorded from the 200 mm AlGaIn/GaN epiwafer under $z(x, \_)z$ polarization geometry. The Raman spectra are excited with a low laser power to avoid thermal red shift. Beside the typical GaN E_2 -high mode, the Raman spectra are dominated by peaks at 600–602, 725–727, and 770–772 cm^{-1} . The Raman measurements are carried out from wafer one edge to other edge to

FIG. 4. (a) Room temperature micro-Raman spectra from AlGaIn/GaN heterostructure on Si(111) with a thin AlN spacer recorded under 325 nm laser line excitation from various positions across the wafer as labeled in the inset. (b) Variable temperature Raman spectra excited under 325 nm showing the presence of disorder activated (DA) mode, interface modes IF1 and IF2, and AlGaIn alloy A_1 -like LO mode from the same sample. The inset shows peak fitting representing different optical phonons at 2DEG interfaces. The quasi-LO (Q-LO) phonon of GaN appears at low temperature and the peak position of this mode lies in between A_1 -LO and E_1 -LO phonon peak of GaN.

study the variation of optical phonon peak energies across the epiwafers. A variation of in-plane interfacial stress at the top AlGaIn/(AlN)/GaN layers leads to a change in the GaN E_2 -high phonon peak position and the softening of this phonon mode with respect to strain-free peak value (567.5 cm^{-1} recorded from a freestanding GaN substrate) reveals the presence of a biaxial tensile stress when a very thin AlN spacer layer was used. Using the relationship between in-plane stress and E_2 -high peak shift, the UV Raman data across various 200 mm HEMT wafers show an average stress values in the range of 0.68 to 0.46 GPa induced at the 2DEG interfaces.¹¹ Such interfacial strain at top barrier/spacer layers also influences electronic properties due to a change in optical phonon dispersion. Figure 4(b) presents the variable temperature Raman spectra from such an AlGaIn/GaN HEMT structure. The low-temperature spectra could clearly distinguish all Raman active modes. The weak feature around 701 cm^{-1} can be attributed to a disorder-activated mode related to lattice defects at the AlGaIn/GaN interfaces.¹² The other two modes at 600 and 727 cm^{-1} are the

FIG. 5. (a) I_{DS} - V_{DS} and (b) dc transfer characteristics of 1.5 μm -gate AlGaIn/GaN HEMTs fabricated using 200 mm diameter GaN-on-Si(111) sample.

interface modes from AlGaIn/GaN system.¹⁰ The interface mode at 727 cm^{-1} appears at the expense of the A_1 -longitudinal optical (LO) phonon of GaN and represents the 2DEG nature of the hetero-interface. The temperature-induced shifts of the two interface modes are opposite (from sample temperature variation of 77 K to 350 K) as such modes show an anti-symmetric potential and interact more strongly with free carriers. Furthermore, spectrum at 77 K clearly show the $A_1(\text{LO})$ -like phonon peak at 775 cm^{-1} originating from the thin AlGaIn barrier. The LO-phonon from the AlGaIn barrier in such 2DEG interfaces shows anomalous temperature behavior with and without the thin AlN spacer and is the subject of a further study with respect to transistor device characteristics from such samples. At low-temperature, the quasi-LO phonon from GaN also appears due to the top thin GaN cap interface inhomogeneity. The room-temperature deconvoluted $A_1(\text{LO})$ alloy peak of AlGaIn has been used to estimate the Al content using the relationship reported in Ref. 13 for samples with low Al content range when excited close to resonance. Using the experimental data and the relationship of AlGaIn alloy LO phonon peak vs Al content:¹³ $\omega_{\text{LO}}(x) = 734 + 356.8x - 814.7x^2$; average Al compositions of $17 \pm 2\%$ are obtained in top $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barriers in a series of HEMT samples. The micro-Raman method addresses such local inhomogeneities across the full 200 mm epiwafers, and such variations could be easily correlated to the electrical characteristics of 2DEG interfaces.

The fabrication of 1.5 μm -gate-length AlGaIn/GaN HEMTs was performed on samples diced from 200 mm epiwafer. The device mesa was formed using the Cl_2 -based dry

plasma etching technique. The source/drain ohmic contacts were formed with electron beam evaporated Ti/Al/Ni/Au layers and lift-off processed followed by annealing at 825°C for 60 s. The gate electrodes were created by contact photolithography with evaporated Ni/Au metal stack and a lift-off process. Figure 5 shows the I_{DS} - V_{DS} and transfer characteristics of 1.5 μm -gate-length transistors fabricated from such AlGaIn/GaN 2DEG heterostructures grown on 1.5 mm thick 200 mm diameter Si(111) substrate. The fabricated devices exhibited a maximum drain current density ($I_{D\text{max}}$) of 660 mA/mm (at $V_{gs} = 2\text{ V}$ and $V_{DS} = 6\text{ V}$) and a maximum extrinsic transconductance ($g_{m\text{max}}$) of 210 mS/mm. We have also fabricated HEMTs with recess-etched ohmic source/drain from such 8-in. AlGaIn/GaN layers with improved pinch-off characteristics (supplementary materials).¹⁴ These observations show good crystalline quality GaN on 200 mm Si platform for application in power electronic devices.

In summary, we report on the 200 mm AlGaIn/GaN epiwafer development on a Si substrate platform. An in-depth characterization study is presented to check the applicability of such MOCVD grown material system for high-voltage electronics. The transistors fabricated from such epilayers exhibited good electrical characteristics with an $I_{D\text{max}}$ of 660 mA/mm and $g_{m\text{max}}$ of 210 mS/mm. The structural and optical characterization shows tremendous potential of such device grade GaN layers on silicon.

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¹⁴See supplementary material at <http://dx.doi.org/10.1063/1.4746751> for electrical properties of transistors and structural characterization of layers.