Investigation of structural, optical, and electrical characteristics of an AlGaN/GaN high electron mobility transistor structure across a 200 mm Si(111) substrate

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Abstract

An AlGaN/GaN high electron mobility transistor (HEMT) structure is grown on a 200 mm Si(111) substrate. The AlGaN/GaN heterostructure atop, which forms the 2D electron gas, is studied via transmission electron microscopy (TEM), scanning tunneling microscopy, and TEM chemical analysis. To quantify the uniformity of structural, optical, and electrical properties of these AlGaN/GaN HEMT structures, scanning electron microscopy, optical microscopy, atomic-force microscopy, x-ray diffraction (\(\omega/2\theta\) scan and reciprocal space mapping) and Hall effect measurements are employed across the center, middle, and edge of the 200 mm wafer. Small thickness (<3%) and Al-content (<3%) variations in (Al)GaN layers across the wafer are recorded whereas a considerable change (28%) in the electron mobility is observed across the wafer that correlates with variations in surface roughness, defectivity, and layer stress. We attribute the higher mobility in the middle of the wafer to lower interface scattering, thanks to lower surface roughness and less edge-type dislocation density.

Additionally, argon (Ar) ion implantation is used as a means for planar electrical isolation, and a seven orders of magnitude decrease in leakage current is achieved when an optimum Ar dose of \(10^{13} \text{cm}^{-2}\) is used. The feasibility of scaling AlGaN/GaN HEMTs on a 200 mm Si(111) platform is discussed.

Keywords: AlGaN, high electron mobility transistor, silicon, x-ray diffraction, mobility, Hall effect, transmission electron microscopy

(Some figures may appear in colour only in the online journal)
1. Introduction

AlGaN/GaN high electron mobility transistors (HEMTs), thanks to their wide bandgap (~3.4 eV) and high critical electric field (~3 MV cm$^{-1}$) [1], have been explored for high power and high frequency applications in recent years. Conventionally, AlGaN/GaN HEMTs are grown on Al$_2$O$_3$ and SiC [2]. However, high substrate cost combined with limited substrate diameter fuels the research for GaN-on-Si technology where cheap and large diameter silicon substrates are employed for GaN epitaxy. Because the Si substrate is roughly 100 times more conductive than GaN and has a lower electrical breakdown field, thick, highly-resistive GaN buffers are needed to protect against buffer breakdown. Unfortunately, thicker GaN layers can increase wafer stress and curvature, yielding cracks that ruin device performance and decrease yield. Recently, however, growing thick (>2 µm), crack-free GaN epitaxial layers with low threading dislocation density on large Si substrates (200 mm diameter) has been achieved through careful considerations regarding layer stress and wafer curvature engineering [3–10]. When growing GaN on large diameter wafers, device performance uniformity is very important because one wants to fully utilize the entire wafer surface. Performance of AlGaN/GaN based HEMTs is directly related to the properties of the two-dimensional electron gas (2DEG), which forms at an AlGaN/GaN interface without doping thanks to conduction band offset and differences in polarization fields between AlGaN and GaN [11]. In particular, a high 2DEG mobility is desired to increase AlGaN/GaN HEMT high frequency performance [12], and a high 2DEG density is desired to increase power output. Furthermore, both high mobility and concentration reduce on-resistance, allowing for more energy efficient devices [13].

Here, we study an AlGaN/GaN HEMT structure grown on a 200 mm Si(1 1 1) substrate and report on the structural, optical, and electrical uniformity across the wafer. To study the properties and quantify uniformity of these AlGaN/GaN HEMT structures, scanning electron microscopy, optical microscopy, atomic-force microscopy, x-ray diffraction ($\omega/2\theta$ scan and RSM) and Hall effect measurements are employed across the center, middle, and edge of the 200 mm wafer.

2. Experiment

An AlGaN/GaN HEMT composed of 14 nm thick Al$_{0.25}$Ga$_{0.75}$N on unintentionally doped GaN was grown by metal-organic chemical-vapor deposition (MOCVD) using a 200 mm diameter, 1.5 mm thick Si(1 1 1) substrate. Figure 1(a) shows an illustration of the complete HEMT structure and buffer layers. The structure consists of an AlN nucleation layer to prevent Ga melt-back etching of Si [14] followed by a linearly step graded AlGaN buffer stack to control wafer curvature and establish the compressive strain necessary for crack-free GaN layers [15, 16]. The AlGaN buffer stack is then followed by thick GaN buffer layers. The first GaN layers and an AlN interlayer are used to further control wafer curvature and reduce dislocation density [17]. In these layers, carbon doping is used to compensate any unintentional doping caused by residual oxygen impurities added during crystal growth. Carbon doping lowers GaN’s conductivity to reduce leakage currents in AlGaN/GaN HEMTs, thus preventing premature buffer breakdown [18]. The AlN interlayer helps re-establish compressive stress to further reduce dislocation density in the upper GaN layer [19]. The top layers of the wafer form the HEMT structure, which contains an unintentionally doped (UID)-GaN layer (carbon content <5 × 10$^{16}$ cm$^{-3}$) followed by a 1 nm AlN spacer to increase the conduction band offset and better contain the 2DEG and a 14 nm Al$_{0.25}$Ga$_{0.75}$N layer to form the 2DEG. The last layer is a 2 nm UID-GaN cap to improve surface morphology and minimize electrical contact resistance [20]. Overall, the entire wafer had a bow of less than 30 µm, making it suitable for fabrication in a Si CMOS production line.

After growth, the wafer was cut and multiple pieces from the center, middle, and edge of the wafer were characterized by scanning electron microscopy, optical microscopy, atomic-force microscopy, x-ray diffraction ($\omega/2\theta$ scan and RSM) and Hall effect measurements to study the structural, optical, and electrical uniformity. Then, we investigated the effects of argon implantation as a means of device isolation without physical separation. Various doses of Ar implant samples were prepared and the resulting I–V characteristics were measured for leakage current comparison. Additionally, AFM was used to determine surface quality after implantation.

3. Result and discussion

3.1 Structural inspection

Figure 1(a) shows a cross-sectional sketch of the AlGaN/GaN HEMT structure, which was grown on a 200 mm diameter Si(1 1 1) substrate. TEM and STEM (figures 1(b) and (c)) of the top 80 nm of the structure clearly show the AlGaN barrier layer and a well-defined AlN layer, which is the visible dark band in figure 1(c). Energy-dispersive x-ray spectroscopy (EDS) (figure 1(d)) also shows a sharp increase in Al content at the surface (5 nm) and peak at 21 nm for the AlN interlayer. Past this, the Al content quickly decreases and the Ga content increases for the Al-free UID-GaN layer. TEM, STEM, and EDS show an AlGaN layer thickness of 14 nm.

Figure 2(a) shows a cross-sectional SEM image of the AlGaN/GaN HEMT structure where the AlN nucleation layer, AlGaN buffer stacks, and two GaN layers separated by an AlN interlayer are observed. The thicknesses of these layers are measured for the center, middle, and edge of the wafer and are plotted in figure 2(b) as a function of position. We see a small (~3%) increase in total structure thickness from the center towards the edge. The largest thickness variation comes from the last GaN layer, which is 3% smaller in the middle than the center and edge. For Al-containing compounds in the buffer, there is an approximately linear increase of about 10% from center to edge that together account for the 0.2 µm total thickness difference between the center and edge.
3.2. AFM and XRD defect and strain analysis

Figure 3 shows Nomarski interference contrast microscopy (NIC) and AFM images of the surfaces of samples from the center (figures 3(a) and (b)), middle (figures 3(c) and (d)), and edge (figures 3(e) and (f)). NIC images show a crack-free surface, indicating a high quality film. AFM was then used to calculate the density of threading dislocations visible on the surface of the samples using in-house software by counting the dark spots in the images. Table 2 summarizes the RMS roughness as well as defect density obtained from the AFM images. From this data, samples from the middle have the smoothest surface (0.266 ± 0.075 nm) with the fewest threading dislocations (0.89 ± 0.1 × 10⁹ cm⁻²), while samples from the center and edge positions are rougher (0.352 ± 0.145 nm and 0.322 ± 0.075 nm respectively) with more threading dislocations (1.00 ± 0.3 × 10⁹ cm⁻² and 1.09 ± 0.2 × 10⁹ cm⁻² respectively).

Figure 2(c) shows x-ray diffraction (XRD) 2θ-ω scans for the three wafer positions, which were used to determine (AlGaN) layer composition and strain. Using ω/2θ scans to probe the symmetrical lattice plan (0001), the aluminum content was computed for each layer with:
\[ x_{Al} = \frac{c_{AlN} - \frac{0}{c_{GaN}}}{c_{GaN} - \frac{0}{c_{AlN}}} \]  

(1)

where \( c_{AlGaN} \) is the average lattice parameter of the layer as determined by XRD, and \( c^0_{AlGaN} \) and \( c^0_{GaN} \) are the free-standing lattice parameters of GaN and AlGaN found using Vegard’s Law [21]. Analysis shows a consistent aluminum percentage for each layer. Full width at half maximum (FWHM) values for center, middle, and edge are 617, 376, 552 arcsec respectively. Because narrower FWHM values indicate more crystalline films, this again suggests that the middle position contains the highest crystalline quality material. Unfortunately, in addition to alloy composition, \( \omega/2\theta \) peaks positions are affected by epi-layer strain. Due to the lattice mismatch between layers, strain certainly exists and causes inaccurate composition measurements. To better estimate the layer compositions, we employ XRD RSM.

To more-accurately determine layer stress, XRD RSMs of the (0 0 0 2) and (1 0 1 5) planes were completed for the three wafer positions as shown in figures 4(a)–(c). Using the extracted \( d \)-spacing, we can compute the \( a \) and \( c \) lattice constants of the crystal with [22]:

\[
\left( \frac{l^2}{a^2} \right) = \frac{4}{3} \left( \frac{h^2 + 2hk + k^2}{a^2} \right) + \frac{l^2}{c^2}
\]  

(2)

where \( h, k, i, \) and \( l \) are the Miller indices of the scan planes \((h \ k \ i \ l)\), and \( a \) and \( c \) are the measured lattice constants of the material. From here, we can compute the alloy composition for a strained lattice by solving Poisson–Vegard’s law [22] with the addition of a bowing parameter:

\[
\begin{align*}
\text{Layer} & & \text{Center} & & \text{Middle} & & \text{Edge} \\
1\text{st AlGaN} & & A_l_{0.83}G_{0.17}N & & A_l_{0.82}G_{0.18}N & & A_l_{0.83}G_{0.17}N \\
2\text{nd AlGaN} & & A_l_{0.59}G_{0.41}N & & A_l_{0.59}G_{0.41}N & & A_l_{0.59}G_{0.41}N \\
3\text{rd AlGaN} & & A_l_{0.33}G_{0.67}N & & A_l_{0.32}G_{0.68}N & & A_l_{0.35}G_{0.65}N
\end{align*}
\]

(3.1)

where

\[
\begin{align*}
c_m(x) - c_0(x) & = -\frac{2\nu(x)}{1 - \nu(x)} \times \frac{a_m(x) - a_0(x)}{a_0(x)} \\
c_0(x) & = x_{GAiN} + (1 - x)c_{GaN} - b_x(1 - x) \\
a_0(x) & = x_{GAiN} + (1 - x)a_{GaN} - b_x(1 - x) \\
\nu(x) & = x_{GaN} + (1 - x)\nu_{GaN}
\end{align*}
\]  

(3.2)

\[
\begin{align*}
\begin{align*}
\begin{array}{l}
\text{Layer} \\
1\text{st AlGaN} & & A_l_{0.83}G_{0.17}N & & A_l_{0.82}G_{0.18}N & & A_l_{0.83}G_{0.17}N \\
2\text{nd AlGaN} & & A_l_{0.59}G_{0.41}N & & A_l_{0.59}G_{0.41}N & & A_l_{0.59}G_{0.41}N \\
3\text{rd AlGaN} & & A_l_{0.33}G_{0.67}N & & A_l_{0.32}G_{0.68}N & & A_l_{0.35}G_{0.65}N
\end{array}
\end{align*}
\]

In these equations, \( c_m(x) \) and \( a_m(x) \) are the measured \( c \)-axis and \( a \)-axis lattice parameters and \( c_0(x) \) and \( a_0(x) \) are the relaxed lattice parameters for the Al content percentage, \( x \). For accurate lattice constant determination, we use the \( a \) and \( c \)-axis bowing parameters, \( b_a \) and \( b_c \) for the \( Al_{1-x}Ga_xN \) lattice constants where \( b_a = 0.018 \) and \( b_c = -0.036 \) along with Poisson ratios \( \nu_{GaN} = 0.272 \) and \( \nu_{GaN} = 0.183 \) [22, 23]. Solving these equations, we obtain the alloy compositions listed in table 1.

With the determined lattice constants, we can also determine in-plane (\( \varepsilon_{xx} \)) and out-of-plane strain (\( \varepsilon_{yy} \)) using:

\[
\varepsilon_{xx} = \frac{a_m(x) - a_0(x)}{a_0(x)}
\]  

(4.1)
The results of the strain measurements for each layer are shown in figure 4(d). Layers with positive in-plane strain are under tensile stress while layers with negative in-plane strain are under compressive stress. These results agree with other stress measurements reported elsewhere which show AlN being grown in tension, followed by increasing additional compressive stress as the AlGaN buffer stacks are added and then returned tensile stress as the thick GaN layers continue to grow [15].

Other works suggest that in-plane layer stress plays an important role in 2DEG mobility, where lower stress corresponds to higher mobility due to less strain induced relaxation mechanisms [17]. Furthermore, having more compressive stress in the GaN layer will reduce the tensile stress in the top AlGaN barrier layer, which can improve surface morphology and increase mobility. These samples are relatively close in layer stress, so we believe layer stress is not a dominating mechanism in changing the 2DEG mobility within our samples.

Additionally, we can use the symmetric (0002) and asymmetric (1015) ω scans to determine the densities of screw-type and edge-type threading dislocations, which have Burgers vectors of $b_{screw} = 0.5185 \text{ nm}$ and $b_{edge} = 0.3189 \text{ nm}$. Using the FWHM of the (0002) ($\beta_{(0002)}$) and (1015) ($\beta_{(1015)}$) scans, we can approximate the threading dislocations (D) using the Dunn and Kock equations [22, 24]:

$$D_{screw} = \frac{\beta_{(0002)}}{4.35b_{screw}^2}, \quad (5.1)$$

$$D_{edge} = \frac{\beta_{(1015)}}{4.35b_{edge}^2}. \quad (5.2)$$

Calculating these values for the GaN layers, we get $D_{screw} = 4.17 \times 10^8$, $3.83 \times 10^8$, and $4.45 \times 10^8 \text{ cm}^{-2}$ for center, middle, and edge respectively, and $D_{edge} = 9.00 \times 10^8$, $8.38 \times 10^8$, and $9.67 \times 10^8 \text{ cm}^{-2}$, again for the center, middle, and edge respectively. While this method of defect density determination tends to overestimate the actual values [24], this XRD analysis suggests that the middle position has the lowest edge and screw type threading dislocation densities when compared to the center and edge. In terms of relative defect density, these values match the trend seen from our AFM analysis where the middle contains the fewest defects.

3.3. 2DEG Characterization via Hall measurement

Hall measurements for electrical characterization were also performed using the Van der Pauw configuration at room temperature (RT, 300 K) and low temperature (LT, 77 K). Samples were prepared via electron-beam evaporation to deposit a 200 nm thick Ti and 200 nm thick Ni metal stack. The contacts were then annealed at 750 °C for 45 s in a nitrogen environment. To isolate the samples, the surface was coated in a thick, protective resist layer and diced into 4 mm × 4 mm squares. The sheet resistance, 2DEG concentration, and electron mobility from the measurements can be seen in table 2 for the three sample locations.

For the center, middle, and edge positions, the 2DEG concentration is approximately the same (<2% variation), but we see a 28% increase in room temperature electron mobility from the center to the middle position and an 18% increase from the center to the edge. A similar increase in electron mobility is also observed at 77 K. We believe that this is due to reduced interface scattering from the smoother surface and lower edge-type dislocation density present in the middle position. From the AFM surface study and XRD defect analysis, we can see that the middle wafer position has the lowest RMS surface roughness (0.266 ± 0.075 nm) and defect density (0.89 ± 0.1 × 10⁹ cm⁻²), while the center position has the highest RMS roughness (0.352 ± 0.145 nm) and the edge has the highest defect density (1.09 ± 0.2 × 10⁹ cm⁻²). Edge-type defects are also considered to have the greatest effect on mobility because they are negatively charged and act as scattering sites [25] Therefore, the lower edge-type dislocation density in the middle position (8.38 × 10⁸ cm⁻²) and higher edge-type dislocation density from the center and edge (9.00 × 10⁸ and 9.67 × 10⁸ cm⁻² respectively) may explain why the middle has the highest mobility while the center and edge mobilities are lower. Moreover, the in-plane strain measurements reveal that the middle sample with the highest mobility and smoothest surface contains the GaN layer with the most strain. This is attributed to relaxation in the AlGaN barrier layers of the center and edge that reduces their strain and increases edge-type defectivity. Hence, we believe the higher mobility of the middle position is caused by reduced interface scattering thanks to the lower edge-type dislocation density and a smoother surface.

3.4. Isolation study

Device isolation is an important requirement in integrated circuits. For AlGaN/GaN HEMTs, plasma mesa etching is typically used to create device isolation. However, mesa etching
Figure 4. (a)–(c) XRD reciprocal space mapping of the center, middle, and edge respectively with calculated Al content percentage. (d) The in-plane strain is calculated for each layer and plotted in the order of growth.
results in non-planar devices with the possibility of the gate metal contacting the 2DEG, both of which decrease yield. Alternatively, ion implantation can be used to achieve planar device isolation by selectively creating highly resistive regions on the wafer [26]. Argon implantations with doses of $10^{12}$, $10^{13}$, $10^{14}$, and $10^{15}$ cm$^{-2}$, were performed at 100 keV to study its effects on electrical isolation. Figure 5(a) presents $I$–$V$ curves for the sample before and after implantation with the optimum dose of $10^{13}$ cm$^{-2}$, which corresponds to the lowest leakage current. As the inset to figure 5(a) shows, electrical isolation is effective to at least 40 V. (b) AFM images after implantation show minimal surface damage.

4. Conclusion
Thick (>5 μm), crack-free GaN layers has been successfully grown by MOCVD on 200 mm Si (1 1 1) substrate. The uniformity of the structural, optical, and electrical properties of the AlGaN/GaN HEMT structure were examined with respect to the center, middle, and edge positions on the wafer. Our results reveal that when compared to the center and edge of the wafer, the middle position contains the smoothest surface (0.266 ± 0.075 nm) with the fewest defects ($0.89 \pm 0.1 \times 10^{9}$ cm$^{-2}$) leading to higher mobility ($1447 \pm 54$ cm$^2$ V$^{-1}$ s$^{-1}$) and lower sheet resistance (360 ± 16 Ω/sq.), which we show is due to reduced interface scattering and fewer edge-type defects ($8.38 \times 10^{8}$ cm$^{-2}$). Argon ion implantation was also shown to effectively isolate AlGaN/GaN HEMT structures. Using a dose of $10^{13}$ cm$^{-2}$, leakage current was reduced by seven orders of magnitude and provided effective isolation up to 40 V. By increasing the dose past this value, however, leakage current increased.

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