Investigation of annealed, thin (\(\sim 2.6\) nm)-\(\text{Al}_2\text{O}_3/\text{AlGaN}/\text{GaN}\) metal-insulator-semiconductor heterostructures on Si(111) via capacitance-voltage and current-voltage studies

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Abstract

Annealed, thin (\(\sim 2.6\) nm)-\(\text{Al}_2\text{O}_3/\text{AlGaN}/\text{GaN}\) metal-insulator-semiconductor (MIS) heterostructures on Si(111) are fabricated and studied via capacitance–voltage (C–V) measurements to quantify densities of fast and slow interface trap states and via current–voltage (I–V) measurements to investigate dominant gate current leakage mechanisms. Dual-sweep C–V measurements reveal small voltage hysteresis (\(\sim 1\) mV) around threshold voltage, indicating a low density of slow interface trap states of \(\sim 10^{10}\) cm\(^{-2}\). Frequency-dependent conductance measurements show fast interface trap state density ranging from \(8 \times 10^{12}\) to \(5 \times 10^{11}\) eV\(^{-1}\) cm\(^{-2}\) at energies from 0.275 to 0.408 eV below the GaN conduction band edge. Temperature-dependent I–V characterizations reveal that trap-assistant tunneling (TAT) dominates the reverse-bias carrier transport while the electric field across the \(\text{Al}_2\text{O}_3\) ranges from 3.69 to 4.34 MV cm\(^{-1}\), and the dominant \(\text{Al}_2\text{O}_3\) trap state energy responsible for such carrier transport is identified as 2.13 ± 0.02 eV below the \(\text{Al}_2\text{O}_3\) conduction band edge. X-ray photoelectron spectroscopy measurements on \(\text{Al}_2\text{O}_3\) before and after annealing suggest an annealing-enabled reaction between Al–O bonds and inherent H atoms. Overall, we report that annealed, thin-\(\text{Al}_2\text{O}_3\) dielectric is an effective (\(\text{AlGaN}\) surface passivation alternative when minimizing passivation-associated parasitic capacitance is required, yet non-ideal for significantly suppressing gate leakage current in MIS structures due to the governing TAT carrier transport mechanism.

1. Introduction

\(\text{AlGaN}/\text{GaN}\) high electron mobility transistor (HEMT) technology is the backbone of next-generation high power and frequency electronics thanks to the high thermal and chemical stability and high critical electric fields of III-nitrides [1]. Emerging GaN-on-Si(111) technology platform further promises high volume scalability of \(\text{AlGaN}/\text{GaN}\) HEMTs at low cost [2, 3]. Various dielectrics such as \(\text{Al}_2\text{O}_3\), \(\text{SiN}_x\), \(\text{SiO}_2\) and \(\text{HfO}_2\) are used as the insulator in metal-insulator-semiconductor (MIS) HEMTs or for \(\text{AlGaN}\) surface passivation in order to improve device performance. However, it is shown that the interface trap states at dielectric/(\(\text{AlGaN}\) interfaces cause frequency-dispersive charging (trapping) and discharging (de-trapping) effects, leading to compromised reliability of \(\text{AlGaN}/\text{GaN}\) HEMTs [4–11], therefore minimizing the density of interface trap states (\(D_{it}\)) is one of the most crucial tasks towards mature \(\text{AlGaN}/\text{GaN}\) HEMT technology. The density of interface trap states is sensitive to the choice of dielectric and how the dielectric was deposited. It has been reported that a high-quality dielectric/III–V interface can be achieved by \(\text{Al}_2\text{O}_3\) (a high-\(\kappa\) dielectric) prepared by atomic layer deposition (ALD) thanks to high deposition uniformity and low inherit defect density [12, 13]. Nevertheless, processing
challenges with AlGaN/GaN HEMTs, such as (Al)GaN surface treatment (prior to the dielectric deposition) and post-dielectric-deposition annealing (PDA) for ohmic contact formation, also profoundly affect $D_A$ [14].

The impact of PDA on $\text{Al}_2\text{O}_3$/AlGaN/GaN MIS HEMT characteristics is an active research area. Benefits of employing PDA have indeed been reported, including improving $\text{Al}_2\text{O}_3$ properties that leads to reduced oxide traps and threshold voltage hysteresis [15] as well as reducing average $D_A$ at the $\text{Al}_2\text{O}_3$/GaN interface [16]. Yet some studies report adverse effects [17, 18]. Further systematic work is therefore needed for better understanding the impacts of PDA on ALD $\text{Al}_2\text{O}_3$ properties and then correlating these effects on AlGaN/GaN HEMT performance.

In this work, annealed, thin (~2.6 nm)-$\text{Al}_2\text{O}_3$/AlGaN/GaN MIS HEMT capacitors on Si(111) are fabricated and studied via capacitance–voltage (C–V) and current–voltage (I–V) measurements (by Keithley 4200A-SCS Parameter Analyzer). In particular, employing a thin $\text{Al}_2\text{O}_3$ layer is advantageous for both gate insulator and (Al) GaN surface passivation in MIS HEMTs. For gate insulator, a thinner layer allows a larger capacitance to better couple the applied electric field for controlling the channel while suppressing the gate leakage current (compared to a Schottky gate configuration) [19]. In addition, it has been reported that in highly-scaled devices, fringing gate capacitance and drain-induced barrier lowering can be reduced with a thinner passivation, leading to a higher cutoff frequency and improved device performance [20]. Dual-sweep C–V and frequency-dependent conductance measurements are performed on the $\text{Al}_2\text{O}_3$/AlGaN/GaN MIS HEMT capacitors to quantify the densities of slow ($N_{\text{it,slow}}$) and fast interface trap states ($P_{\text{it,fast}}$), respectively. In addition, temperature-dependent I–V measurements are used to identify the dominant reverse-bias carrier transport across the thin $\text{Al}_2\text{O}_3$.

Finally, x-ray photoelectron spectroscopy (XPS) measurements are carried out in order to compare the chemical compositions of as-deposited and annealed $\text{Al}_2\text{O}_3$ films.

2. Device fabrication

By metal–organic chemical vapor deposition, the AlGaN/GaN HEMT structure is composed of AlGaN barrier layer (GaN capping layer/$\text{Al}_{0.23}\text{Ga}_{0.77}\text{N}$ barrier layer/AlN spacer layer, total thickness estimated as 13.7 nm by C–V measurements)/GaN channel layer, grown on a step-graded $\text{Al}_x\text{Ga}_{1-x}\text{N}$ buffer layer stack composed of 240-nm-thick $\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}$/210-nm-thick $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$/190-nm-thick $\text{Al}_{0.82}\text{Ga}_{0.18}\text{N}$/175-nm-thick AlN on a 200-nm-thick Si(111). Room temperature van der Pauw Hall measurements determined two-dimensional electron gas (2DEG) sheet concentration and mobility as 8.9 ± 0.1 $\times$ 10$^{12}$ cm$^{-2}$ and 1802 ± 102 cm$^{2}$ V$^{-1}$ s$^{-1}$, respectively.

Using this material stack, $\text{Al}_2\text{O}_3$/AlGaN/GaN MIS HEMT capacitors are fabricated. The fabrication starts with surface degreasing (with toluene, acetone, methanol, de-ionized water) and surface treatment using 6% HCl$_{aq}$ at room temperature for 1 min, 7% NH$_4$OH$_{aq}$ at room temperature for 1 min, and 5% (NH$_4$)$_2$S$_{aq}$ at 50 °C for 30 min to remove organic contaminants, alkali ions, and native oxide. Then, 10-nm-thick $\text{Al}_2\text{O}_3$ is deposited via ALD for 100 cycles using precursors of H$_2$O and trimethylaluminum at 250 °C to serve as GaN surface passivation layer as well as a protection layer for the next processing steps. Mesa isolation is performed via wet etching of $\text{Al}_2\text{O}_3$ (by buffered oxide etching (BOE)) followed by dry etching of (Al)GaN using Cl-based inductively coupled plasma reactive ion etching). Afterwards, ohmic contact window is opened by $\text{Al}_2\text{O}_3$ wet etching using BOE, followed by metal deposition (Ti(20 nm)/Al(120 nm)/Ni(55 nm)/Au(45 nm)) using electron beam evaporation. A three-step (450 °C for 3 min, 700 °C for 40 s, and 900 °C for 40 s) rapid thermal annealing (RTA) is carried out in N$_2$ ambient and a specific ohmic contact resistance of 4.04 $\times$ 10$^{-6}$ ohm-cm$^{-2}$ is achieved. The $\text{Al}_2\text{O}_3$ layer in the gate regions is then thinned by hot HCl$_{aq}$ for 1 min (remaining thickness estimated as 2.6 nm by C–V measurements), followed by the gate metal contact deposition (Ni(20 nm)/Au (200 nm)) using electron beam evaporation. Electrical measurements are then carried out. For comparison, AlGaN/GaN Schottky HEMT capacitors are also fabricated mostly in parallel with MIS ones except that $\text{Al}_2\text{O}_3$ in the gate regions is completely removed using BOE. Compared with the AlGaN/GaN Schottky HEMT capacitors, additional annealed 2.6-nm ALD $\text{Al}_2\text{O}_3$ in the MIS HEMT capacitors results in approximately two orders of magnitude reduction in reverse-bias current density (figure S1 is available online at stacks.iop.org/ MRX/6/105904/mmedia).

3. Interface trap state characterization

Dual-sweep C–V measurements are first performed on the MIS HEMT capacitors to measure the hysteresis around the threshold voltages ($V_{T,MIS}$) in order to study $N_{\text{it,slow}}$ with time constant ($\tau_w$) of tens of seconds at the $\text{Al}_2\text{O}_3$/GaN interface [21]. Such measurement typically serves as the first approach to preliminarily comprehend how the capacitor responds to the AC signal within the DC bias range, and the resulted hysteresis is one indicative factor. It is understood that hysteresis is associated with charging of interface trap states, therefore it
offers a measure to quantify the density of these interface trap states. Depending on the AC signal frequency and the up/down voltage sweeping rate, density of a part of slow interface trap states could be estimated \[22\].

Electrical de-trapping is first performed by maintaining the gate voltage \( V_G \) at \(-4\) V for 2 min, followed by applying a slow ramping DC bias at a speed of \( 0.05 \text{ V s}^{-1} \) (first up-sweep and then down-sweep) superimposed with an AC signal at 100 kHz with 50 mV rms. The same measurements are also performed on Schottky HEMT capacitors in order to extract capacitance \( C_{\text{Schottky}} \) and threshold voltage \( V_{T,\text{Schottky}} \) to be later used as inputs for determining the \( \text{Al}_2\text{O}_3 \) capacitance \( C_{\text{ox}} \) and \( \text{Al}_2\text{O}_3 \) electric field \( E_{\text{ox}} \) in the MIS HEMT capacitor. As shown in figure 1(a), the MIS HEMT capacitor exhibits sharp transitions from depletion into accumulation, indicating decent interface qualities. The threshold voltages \( V_{T,\text{MIS}} \) and \( V_{T,\text{Schottky}} \) and \( C_{\text{ox}} \) are extracted as \(-1.58\) V and \(-0.89\) V, and \( 3088\) nF cm\(^{-2} \), respectively. During the dual sweep, when \( V_G \) is swept above \( V_{T,\text{MIS}} \) (MIS HEMT capacitor is then pushed into accumulation) and then back to \( V_{T,\text{MIS}} \), the energy of all the \( \text{AlGaN/GaN} \) interface trap states in the bandgap remain below the Fermi level, therefore no change of occupancy in these interface trap states is expected. However, the energy of some of the \( \text{Al}_2\text{O}_3/\text{GaN} \) interface trap states in the bandgap are first pushed below (when \( V_G \) is swept up) and then again pulled above (when \( V_G \) is swept down) the Fermi level, hence the possibility of changing the occupancy \[23\]. In addition, at the sweeping speed of \( 0.05 \text{ V s}^{-1} \), the time needed to first sweep above \( V_{T,\text{MIS}} \) and then back to \( V_{T,\text{MIS}} \) is around \( 100\) s, therefore only the \( \text{Al}_2\text{O}_3/\text{GaN} \) interface trap states with \( \tau_{it} \) longer than \( 100/2\pi \) s whose occupancy have also been altered during the measurement will contribute to the C–V hysteresis. According to the Shockley-Read-Hall (SRH) statistics

\[
\tau_{it} = \frac{1}{v_{th}\sigma_{th}N_C} \exp \left( \frac{E_C - E_T}{kT} \right),
\]

interface trap states with \( \tau_{it} > 100/2\pi \) s correspond to energy levels with respect to the conduction band edge \( (E_C-E_T) > 0.81 \text{ eV} \) at room temperature, where \( v_{th} \) (average thermal velocity of an electron), \( \sigma_{th} \) (trap state capture cross section) and \( N_C \) (effective density of states in the conduction band) are taken as \( 2 \times 10^7 \text{ cm s}^{-1} \), \( 1 \times 10^{-14} \text{ cm}^2 \), and \( 4.3 \times 10^{14} \times T^{3/2} \text{ cm}^{-3} \), respectively \[8, 18, 21, 24\]. Given the voltage hysteresis (\( \Delta V \)) extracted from the MIS HEMT capacitor (1 mV), the \( N_{it,\text{slow}} \) with \( E_C - E_T > 0.81 \text{ eV} \) that have also altered occupancy in response to the dual sweeping is estimated as \( 3.33 \times 10^9 \text{ cm}^{-2} \) via

![Figure 1.](image-url)
where \( C_{\text{MIS}} \) is the total capacitance of the MIS HEMT capacitor in accumulation and \( q \) is elementary charge \((1.6 \times 10^{-19} \text{ C})\).

It has also been reported that the hysteresis of a second capacitance increasing step in the forward bias region, associated with electrons in MIS HEMT capacitors out-spilling from the 2DEG channel and then accumulating at the \( \text{Al}_2\text{O}_3/\text{AlGaN} \) barrier interface, can be used for analyzing \( D_{\text{it,fast}} \) [8], however, such method is not always feasible for MIS HEMT capacitors with thin insulator where the high forward bias leakage current can prohibit the appearance of such capacitance increase at elevated AC signal frequencies. The inset in figure 1(a) shows the C–V characteristics of the MIS HEMT capacitor measured at 1 kHz where the reduced capacitive admittance allows the appearance of the capacitance increase that is otherwise non-observable at 100 kHz. Even so, the capacitance still drops rapidly before reaching a constant value that corresponds to \( C_{\text{ox}} \), negating the feasibility of reliably measuring the hysteresis for further \( D_{\text{it,fast}} \) analysis. Therefore, other methods for probing \( D_{\text{it,fast}} \) is required, such as frequency-dependent conductance method.

On the other hand, apparent carrier density in the two capacitors as a function of depth is extracted from the 100 kHz C–V characteristics, as shown in figure 1(b). The peak positions approximately correspond to the 2DEG positions, and the shift between the two peaks indicates the thickness of the \( \text{Al}_2\text{O}_3 \) \((d_{\text{Al2O3}})\) in the MIS HEMT capacitor being approximately 2.6 nm [8, 25]. Integrating the apparent carrier density distribution over depth gives 2DEG sheet concentration of the MIS and Schottky HEMT capacitors being 5.25 \( \times 10^{12} \text{ cm}^{-2} \) and 2.6 nm, respectively. In addition, the small frequency dispersion of 2DEG sheet concentration in the MIS HEMT capacitor (shown in supplementary material) indicates a minor effect of series resistance in the structure [26].

Frequency-dependent conductance method was originally developed for analyzing \( D_{\text{it}} \) in conventional MOSFETs [27], and it has also been widely adapted for GaN-based MIS HEMT interface analysis [5, 6, 23, 28–32]. This method measures the equivalent parallel conductance \( (G_p) \) that represents the power loss due to interface trap states capturing and emitting carriers as a function of \( V_G \), DC biasing and AC signal frequency \( (\omega) \). Using this method, density of fast interface trap states with \( \tau_{\text{it}} \) being around 0.1 to 100 \( \mu \text{s} \) is highlighted in this work. During the measurements, the MIS HEMT capacitor is biased above \( V_{\text{T,MIS}} \) in order to have uncharged occupancy of the \( \text{AlGaN/GaN} \) interface trap states in the bandgap [23]. The Equivalent parallel conductance can be extracted using the measured parallel capacitance \( (C_{\text{p,meas}}) \), parallel conductance \( (G_{\text{p,meas}}) \), \( C_{\text{ox}} \) and \( \omega \) via the equation derived from MIS capacitor equivalent circuit model [5, 33]

\[
G_p = \frac{\omega^2 C_{\text{ox}}^2 G_{\text{p,meas}}}{G_{\text{p,meas}}^2 + \omega^2 (C_{\text{ox}} - C_{\text{p,meas}})^2}.
\]

(3)

Then, \( D_{\text{it,fast}} \) is extracted via fitting the normalized conductance \( G_p/\omega \) as a function of \( \omega \) at a given \( V_G \), as shown figure 2, using equation [27]

\[
\frac{G_p}{\omega} = \frac{q D_{\text{it,fast}}}{2\omega \tau_{\text{it}}} \ln [1 + (\omega \tau_{\text{it}})^2],
\]

(4)

where \( \tau_{\text{it}} \) further yields \( E_c - E_F \) via equation (1). Note that the measured \( G_p/\omega \) increases towards lower frequencies, which necessitates an employment of a two-trap fitting model to better extract \( D_{\text{it,fast}} \) [34]. As shown in figure 3, the extracted \( D_{\text{it,fast}} \) as a function of \( E_c - E_F \) of the MIS HEMT capacitor is plotted along with the

![Figure 2](image-url)
results from selected literatures \[21, 28, 35\]. The highlighted $E_{\text{C}} - E_T$ ranging from 0.275 to 0.408 eV corresponds to $D_{\text{it,fast}}$ ranging from $8 \times 10^{12}$ to $5 \times 10^{11}$ eV$^{-1}$ cm$^{-2}$, in line with the literature. In the literature, an order of magnitude lower $D_{\text{it,fast}}$ at the ALD Al$_2$O$_3$/GaN interface \[28\] compared to ours was reported (figure 3), suggesting room for improvement in reducing $D_{\text{it,fast}}$ through Al$_2$O$_3$ ALD or RTA conditioning studies.

Though the frequency-dependent conductance method is widely used for extracting $D_{\text{it,fast}}$ in MIS HEMT structures \[5, 6, 23, 28–32\], it has also been suggested that using such method could render the $D_{\text{it,fast}}$ analysis in MIS HEMT structures inaccurate \[36, 37\]. Unlike in conventional MOSFETs, in MIS HEMT structures the dielectric/barrier interface trap states and the carriers in the channel are spatially separated by the barrier that has a gate-bias-dependent resistance \[36\]. The presence of this resistive and capacitive barrier might post an artificial peak as large as $C_{\text{Schottky}}/q$ in the $G_p/\omega$ versus $\omega$ plot thereby producing a false $D_{\text{it,fast}}$ under certain conditions \[37\]. For instance, when the barrier is highly resistive, the main peak in the $G_p/\omega$ versus $\omega$ plot that corresponds to the interface trap states may be pushed beyond the measurement frequency range, leaving the artificial peak misinterpreted as the main peak \[37\]. In this work, due to the relatively thin (13.7 nm) and thus low resistive barrier, $C_{\text{Schottky}}/q$ is around $4.0 \times 10^{12}$ eV$^{-1}$ cm$^{-2}$ whereas the extracted $D_{\text{it,fast}}$ corresponding to the peaks in the $G_p/\omega$ versus $\omega$ plot mainly ranges from $10^{12}$ to $10^{13}$ eV$^{-1}$ cm$^{-2}$. This suggests that in our work $D_{\text{it,fast}}$ is not being capped by the detection upper limit.

4. Estimation of Al$_2$O$_3$ electric field and analysis of reverse-bias carrier transport

Gate leakage current analysis is used to study carrier transport mechanisms across insulators and thus evaluate the material quality. Common carrier transport mechanisms include trap-assisted tunneling (TAT), Poole-Frenkel (PF) emission, and Fowler-Nordheim (FN) tunneling \[38–41\]. To distinguish the governing carrier transport mechanism, electric field across the insulator, in this work Al$_2$O$_3$ ($E_{\text{ox}}$), needs to be estimated first. Methods that involve different levels of complexity have been proposed to estimate $E_{\text{ox}}$. It is reported that the electric fields in the Al$_2$O$_3$ and the AlGaN barrier layers are considered identical and was estimated by using the concentrations of 2DEG and the sum of the polarization charges \[39\]. On the other hand, it was also proposed to consider the two electric fields separately and then estimate $E_{\text{ox}}$ by comparing the characteristics of Al$_2$O$_3$/AlGaN/GaN MIS HEMT capacitors and AlGaN/GaN Schottky HEMT capacitors \[41, 42\]. In this work,
The oxide as a function of \( V \) is estimated via

\[
E_{\text{ox}} = \frac{Q}{\varepsilon_{\text{ox}} \varepsilon_0} = \frac{n_{2\text{DEG}}}{q} - \frac{\Delta E_C}{q} C_{\text{Schottky}} - V_{\text{T,MIS}} \tag{5}
\]

where \( n_{2\text{DEG}} \) is 2DEG sheet concentration as a function of \( V \) obtained from the MIS HEMT capacitor \( C - V \) measurement. \( \varepsilon_{\text{ox}}, \varepsilon_0, \frac{\Delta E_C}{q} \) are relative permittivity of \( Al_2O_3 \), vacuum permittivity, Ni/\( Al_2O_3 \) barrier height, Ni/GaN Schottky barrier height, and \( Al_2O_3/GaN \) conduction band offset, respectively. \( V_{\text{T,MIS}} \) and \( V_{\text{T, Schottky}} \) are 644 nF cm\(^{-2}\), 3088 nF cm\(^{-2}\), \(-1.58 \) V, and \(-0.89 \) V, respectively.

Reverse-bias carrier transport in the \( Al_2O_3/AlGaN/GaN \) MIS HEMT capacitors is then analyzed using temperature-dependent I–V characteristics, as shown in figure 4(a), as well as the estimated \( E_{\text{ox}} \). In this bias region, carriers (electrons) are sent from the gate metal and then directly encounter the \( Al_2O_3 \), hence allowing a direct measure of the electrical property of the \( Al_2O_3 \) layer. Figure 5 schematically depicts electron transport across the \( Al_2O_3 \) via TAT, and the TAT current density \( J_{\text{TAT}} \) can be modeled as

\[
J_{\text{TAT}} \propto \exp \left( -\frac{8\pi \sqrt{2qm_{\text{ox}}^*}}{3hE_{\text{ox}}} \phi_T^{3/2} \right) \tag{8}
\]

where \( h, m_{\text{ox}}^* \) and \( q/\phi_T \) are Planck’s constant, \( Al_2O_3 \) effective electron mass, and the trap energy relative to the conduction band edge, respectively. Slopes in \( \ln(J_{\text{TAT}}) \) versus \( 1/E_{\text{ox}} \) plot, as shown in figure 4(b), yield \( q/\phi_T \) as 2.13 ± 0.02 eV that exhibits a weak temperature dependence. In addition, the highlighted voltage region in figure 4(a) that fits the TAT model corresponds to \( E_{\text{ox}} \) ranging from 3.69 to 4.34 MV cm\(^{-1}\), which is lower than the breakdown field of \( Al_2O_3 \) reported (5 to 10 MV cm\(^{-1}\)). Note that the
increase in the reverse-bias current as a function of temperature can be explained by phonon-assisted TAT \[46\]. Other than TAT, PF emission is also a trap-related carrier transport mechanism where thermal fluctuation randomly promotes the trapped electrons in the insulator to the conduction band. These electrons will then momentarily propagate in the layer following the electric field before falling into another trap state. The current density \(J_{PFE}\) of such emission can be modeled as \[38\]

\[
J_{PFE} \propto E_{ox} \times \exp \left[ -\frac{q}{kT} \left( \phi_T - \frac{qE_{ox}}{\pi \sigma_{ox}} \right) \right],
\]

and slopes in \(\ln(J_{PFE}/E_{ox})\) versus \(E_{ox}^{0.5}\) plot (not shown here) yield \(q\phi_T\) as 0.17 eV. The barrier height for electrons to overcome is therefore 3.33 eV (\(q\phi_T - q\phi_B\)); such a high barrier indicates that PF emission should not be a dominant reverse-bias carrier transport mechanism \[38\]. On the other hand, Fowler-Nordheim tunneling typically occurs at high electric fields where the barrier is in a triangular shape. The FN tunneling current density \(J_{FNT}\) can be modeled as \[38\]

\[
J_{FNT} \propto E_{ox}^2 \times \exp \left[ -\frac{8}{3} \frac{\pi \sqrt{2m_{ox}^* (q\phi_B)^3/2}}{qh E_{ox}} \right],
\]

and the slopes in \(\ln(J_{FNT}/E_{ox})\) versus 1/\(E_{ox}\) plot (not shown here) yield \(q\phi_B\) (Ni/\(\text{Al}_2\text{O}_3\) barrier height) as 2.0 eV that is however much smaller than the reported value 3.5 eV \[43\]. It is therefore considered that FN tunneling is not a dominant reverse-bias carrier transport mechanism either in the selected bias range at temperatures above 30 °C.

5. Chemical characterization

Before the ALD \(\text{Al}_2\text{O}_3\) in the MIS HEMT capacitors is thinned by hot HCl(aq), it also went through the high-temperature PDA with a maximum temperature at 900 °C for 40 s known to alter the film property presumably due to microcrystallization \[47\]. Dielectric constants of as-deposited and annealed ALD \(\text{Al}_2\text{O}_3\) are extracted from additionally fabricated Si-based metal-oxide (\(\text{Al}_2\text{O}_3\))-semiconductor capacitors as around 8 and 9 (∼12.5% increase), respectively. During fabrication, the same three-step RTA condition is used. Determined by ellipsometry, the thickness of the \(\text{Al}_2\text{O}_3\) film decreases by approximately 8.4% due to the RTA, in line with the previously reported trends \[47\]. Using the dielectric constant value of 9 and \(C_{ox}\) value of 3088 nF cm⁻², \(\text{Al}_2\text{O}_3\) thickness in the \(\text{Al}_2\text{O}_3/\text{AlGaN/GaN}\) MIS HEMT is determined as 2.6 nm, agreeing with our earlier result in figure 1(b). Furthermore, other effects associated with PDA-enabled microcrystallization could include defect generation in the film and thus increased conductivity. To investigate the effect of high-temperature PDA on the ALD \(\text{Al}_2\text{O}_3\) chemical composition, XPS measurements are further performed on as-deposited and annealed ALD \(\text{Al}_2\text{O}_3\) with monochromatized Al Kα line (1486.61 eV) x-ray source. The obtained spectra are calibrated with respect to adventitious C 1s peak (284.8 eV) and then fitted with Gaussian—Lorentzian function where the full width at half maximum is restrained within 1.7 eV. As shown in figure 6, the O 1s peaks in the two cases both reside at 531.1 eV, which correspond to the chemical state of \(\text{Al}_2\text{O}_3\). The rather broad Al 2p peaks are then deconvoluted into two components that correspond to Al-O-H (74.1 eV) and \(\text{Al}_2\text{O}_3\) (74.6 eV) chemical states \[48\]. The shown escalated Al-O-H component in the Al 2p peak after the PDA could be attributed to the PDA-enabled reaction between the Al-O bonds and the adjacent unbonded H residues/defects that inherently present in the ALD \(\text{Al}_2\text{O}_3\) film, possibly coming from the chemical by-products of H₂O precursor and organic sources \[49, 50\]. Since it was reported that the conductivity of ALD \(\text{Al}_2\text{O}_3\) is decreased upon dehydration that removes O-H \[51\], we suspect that the escalated Al-O-H component contributes to the dominating TAT carrier transport across the annealed \(\text{Al}_2\text{O}_3\).
6. Conclusion

Annealed, thin (∼2.6 nm)-Al2O3/AlGaN/GaN MIS HEMT capacitors on a Si(111) substrate are fabricated and studied via C–V and I–V measurements to characterize $N_{it,slow}$, $D_{it,fast}$, and the dominant leakage mechanism associated with the annealed thin Al2O3. The small voltage hysteresis from the dual-sweep C–V measurement indicates low density of mobile ions and low $N_{it,slow}$ in the MIS HEMT capacitors, upholding the effectiveness of the GaN surface degreasing and treatment methods. The frequency-dependent conductance measurement shows that from 0.275 to 0.408 eV below the GaN conduction band edge, $D_{it,fast}$ at the Al2O3/GaN interface ranges from $8 \times 10^{12}$ to $5 \times 10^{11}$ eV$^{-1}$ cm$^{-2}$, comparable with the literature results. Temperature-dependent I–V characterization reveals that TAT dominates the reverse-bias carrier transport across the annealed thin Al2O3 while $E_{ox}$ ranges from 3.69 to 4.34 MV cm$^{-1}$, and the energy of the Al2O3 trap states responsible is extracted as 2.13 ± 0.02 eV below the Al2O3 conduction band edge. In addition, XPS suggests a PDA-enabled reaction between the Al–O bonds and the adjacent unbonded H residues/defects that inherently present in the Al2O3 film due to the chemical by-products of H2O precursor and organic sources. Such reaction is suspected to assist TAT in dominating the carrier transport across the annealed Al2O3. This work suggests that it is feasible to employ annealed thin ALD Al2O3 for effective (Al)GaN surface passivation, in order to reduce passivation-associated add-on parasitic capacitance, but not ideal for gate insulator for significantly suppressing leakage current due to the governing TAT carrier transport mechanism.

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