Novel High-k Dielectric Enhanced III-Nitride Devices

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy
in the Graduate School of The Ohio State University

By

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Graduate Program in Electrical and Computer Science

The Ohio State University

2015

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Abstract

This dissertation describes the design, fabrication and characterization of high-k dielectric enhanced Gallium Nitride (GaN)-based devices. Interface properties of atomic layer deposited (ALD) Aluminum Oxide (Al$_2$O$_3$) on GaN was initially investigated. The conduction band offset of Al$_2$O$_3$/GaN was experimentally found as 2.1 eV. High density of positive interface fixed charge (2.72x10$^{13}$ cm$^{-2}$) was observed in the Al$_2$O$_3$/GaN. These interface fixed charges can not only induce electrical field in the oxide which increases the reverse gate leakage, but shift the threshold voltage toward negative to prevent E-mode operation. A theoretical study using remote impurity scattering along with other scattering models showed that these interface fixed charges are able to degrade the electron mobility in the channel. From the calculation results, the impact of interface fixed charges in electron mobility became critical while the sheet charge density in the channel was below 5x10$^{12}$ cm$^2$, the interface fixed charge density was above 5x10$^{12}$ cm$^2$ and the fixed charges were close to the channel (less than 10 nm) which is essential in both power and high frequency applications. The Al$_2$O$_3$/III-Nitride interface fixed charges brought large effects in device characteristics. As a result, technologies need to be developed to improve the interface properties in Al$_2$O$_3$/III-Nitride.
Post-metallization-anneal (PMA) and oxygen plasma treatments were the techniques to achieve interface charge engineering. PMA treatment was conducted in Al₂O₃ on various polarities of GaN and was able to suppress the interface charges after annealing (up to 550°C). The reduction of reverse gate leakage after PMA was also observed. In the Al₂O₃/AlGaN interface, the combination of oxygen plasma and PMA treatments were applied. The Al₂O₃/AlGaN interface fixed charges were reduced to 2x10¹³ cm⁻² and electron mobility recovered after both treatments. E-mode MISHEMT with 1.5 V of threshold voltage was then demonstrated by interface charge engineering. The Al₂O₃/AlGaN interface property after oxygen plasma treatment was investigated by X-ray photoelectron spectrum (XPS). Stable Ga-O bonds were observed revealing that the fixed charges were passivated by oxidation. The MISHEMT characteristics such as C-V hysteresis interface fixed charge density and electron mobility were optimized by different post-deposition-anneal (PDA), PMA and oxygen plasma conditions. We found the best window for the device performance was in 400°C PMA, PDA below 500°C and with oxygen plasma. The idea of lateral energy band engineered E-mode MISHEMT was also demonstrated by patterning ALD Al₂O₃.

By applying similar techniques of Al₂O₃/GaN interface study, interface properties of ALD Al₂O₃ on InGaN, AlGaN and β-Ga₂O₃ were investigated. High quality and smooth 18% InGaN, which is promising as a channel material for high frequency device, was grown by molecular beam epitaxy (MBE). The Al₂O₃/In₀.18Ga₀.8₂N conduction band offset was found as 2.67 eV. For power devices, AlGaN and β-Ga₂O₃ are very attractive due to their wide bandgap characteristics. The conduction band offset Al₂O₃/Al₀.7Ga₀.3N
and Al$_2$O$_3$/β-Ga$_2$O$_3$ was found to be, 1 eV and 1.1 eV. The energy band alignment of these materials could be useful for the future MOS device design.
Dedication

Dedicated to my wife, Shiang-Yu
Acknowledgments

The journey of my PhD is full of joy, challenges and happiness. It is the most valuable and unforgettable part in my life. I am really grateful having so many people around to give me support. All of you make my life so meaningful.

First and foremost, I would like to thank my advisor, Siddharth for having me in his group. I have had valuable guidance on a variety of research aspects, including research experiments, theory and presentations. My device physics knowledge learned from him has given me profound impact. His attitude not only toward research but life and people has deeply inspired me. I really appreciate the opportunity to have Siddharth as my advisor.

I thank Prof. Ringel and Prof. Arehart for being on the committee. I appreciate the insights regarding semiconductor interface characterization from Prof. Ringel and valuable discussions in the DEFINE MURI project. It was also a great opportunity to collaborate with his group on defect characterization in Al$_2$O$_3$/III-Nitride. I thank Prof. Arehart for his experience in device characterization techniques which has always been very helpful. I thank Prof. Lu for his valuable suggestion to our research. The work on oxygen plasma treatment described in this thesis was inspired from the discussion with him. I thank Prof. T. P. Ma at Yale University for the collaboration in the DEFINE MURI project. We have more understanding in Al$_2$O$_3$/III-Nitride interface from his interface characterization techniques. I thank Prof. Mishra and Dr. Stacia Keller at UC Santa Barbara for providing the AlGaN/GaN substrates for the electron transport study. I also thank Prof. Jim Speck at UC Santa Barbara for the atom probe measurement in our Al$_2$O$_3$/GaN.

I thank Christine Jackson (Ringel group) for sharing the information about Al$_2$O$_3$/III-Nitride study, Mark Brenner for the help of low temperature Hall measurement and Zeng Zhang (Ringel group) for internal photoemission and C-V measurements. I thank Dr. Thomas Kent (Myers group) for help with PL measurements. I thank Jie Yang (Ma group at Yale) for the interface characterization in our MISHEMTs and Dr. Baishakhi Mazumder (Speck group at UCSB) for the atom probe measurement.

I have spent my best time in PhD working with Rajan group folks. We shared not only professional knowledge but everything in our life. Pil Sung, Diggi, Sriram, Michele
and Sanyam are the the coolest Rajan group old bones since we spent a lot of time together while this group was about to rise up. I thank Dr. Pil Sung Park, who is just like my big brother, for teaching me everything in the cleanroom. We were also the best coffee and bear partner. I appreciate all his support in my PhD journey. I would thank Prof. Digbijoy Nath (Diggi) for teaching me knowledge of measurement and analysis. I still remember my first conference with him in Nashville. I would also thank Dr. Sriram Krishnamoorthy, our mini-boss. He was my most-trusted MBE grower and coffee partner as well. I thank Dr. Michele Esposto as a mentor in my first year of PhD. I really appreciate his effort to initiate the DEFINE project. I thank Sanyam Bajaj for working in the same project together. He was very reliable on semiconductor process and gave me a lot of favor. I thank Fatih Akyol for his help with MBE growth. He also shared his insights regarding his LED research. I thank Edwin Lee for spending time talking about sports and history/politics. We have leaned a lot of American culture from him. I would like to thank Choonghee Lee for bring so many laughs here. It was great to have him in Rajan group to develop new technology in 2D materials. I thank Yuewei to work together in the lab. He is an ideal graduate student with his diligent character. I thank Santosh who worked here as a master student for his help of quasi-static C-V measurement. I also thank the other Rajan group members, Omor, Zhichao, and Craig, who helped a lot in AFM measurement when he was an undergrad researcher here. I also enjoyed working with our previous post-docs, Dr. Alessandro Giussani who shared the moment of my first OSU basketball game and Dr. Laskar who initiated the 2-D material growth. I would also thank Dr. Boucherit, and Dr. Di Lecce. I really enjoyed every moment working in Rajan group to make me experience different characters and cultures.

I thank all other fellows who worked in different groups at OSU; Zeng, Anup, Christine, Emre and Krishna who worked in Ringel group; Santino, Jing and Thomas in Myers group; Ye and Yuji in Lu group; Chung-Han in Brillson group.

I appreciate that I have a lot of good Taiwanese friends here in Columbus. We share a lot of precious mements no matter how good or bad, how happy or sorrow. Columbus is our second home, and we are family. We used to play guitar and have home-style karaoke every weekend. We enjoyed playing basketball game and working out every week. Hot pot parties were the most common events in cold and freezing winter. In Chinese New Year, we had big reunion to celebrate our traditional holiday. In summer, we had BBQ parties of course with beers. Football season was the most exciting season and all of us wore scarlet and gray to cheer for our buckeye team. So many sweet memories happened here with these friends. They will never, never be forgotten.

Last but not the least, I would like to thank my family. I thank my parents for raising and supporting me all my life. I can never pursue my dream without their endless love. Their love is more than words. Shiang-Yu, my dear wife, she is my soul and life inspiration. How lucky I am to meet her, fall in love with her, marry her and have our
adorable daughter, Olivia, here in Columbus. It was an amazing and unbelievable journey, and this journey keeps going on. We are writing our story, with all the blessing. One day I will tell my daughter that her father was so grateful and proud of being a buckeye.
Vita

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Publications

Journal


Conference Proceedings

1. Ting-Hsiang Hung, Lisa Hommel, Sanyam Bajaj, and Siddharth Rajan, "Interface Properties and Reliability Study of $\text{Al}_2\text{O}_3/\text{AlGaN}$ Interface with oxygen plasma treatment," EMC (Electronic Materials Conference) 2015, June 24-June 26, The Ohio State University, Columbus, OH, USA.


4. Ting-Hsiang Hung, Pil Sung Park, Sriram Krishnamoorthy, Digbijoy Neelim Nath, and Siddharth Rajan, "Interface Charge Engineering and Electron Transport in $\text{Al}_2\text{O}_3/\text{AlGaN}/\text{GaN},"" EMC (Electronic Materials Conference) 2014, June 25-June 27, University of California, Santa Barbara, CA, USA.

5. Ting-Hsiang Hung, Sriram Krishnamoorthy, Digbijoy Neelim Nath, Pil Sung Park and Siddharth Rajan, “Interface Charge Engineering in GaN-based MIS-HEMTs,” The 1st IEEE Workshop on Wide Bandgap Power Devices & Applications (WiPDA), October 27-29 2013, Columbus OH, USA.


8. Ting-Hsiang Hung, Michele Esposto, Digbijoy Neelim Nath, Sriram Krishnamoorthy, Pil Sung Park and Siddharth Rajan, "Interface Charge Effects on Electron Transport in $\text{Al}_2\text{O}_3/\text{AlGaN}/\text{GaN},"" EMC (Electronic Materials Conference) 2013, June 26-June 28, University of Notre Dame, IN.


15. **Ting-Hsiang Hung**, Michele Esposto, Siddharth Rajan, *"A study of the interfacial charge effect on scaled AlGaN/GaN metal insulator semiconductor high electron mobility transistors by using remote charge scattering approximation"*, Sep 12-Sep 14, 2011, OSU Materials Week, Columbus, OH
Fields of Study

Major Field: Electrical and Computer Engineering
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Chapter 1
Introduction

The III-Nitride materials which include family of GaN, AlN, InN and their alloys with bandgap from 0.6 eV to 6.2 eV provide wide range of applications in electronic and optoelectronic devices. Substantial and rapid progress in epitaxy technology and device development has led to commercialization of GaN-based optoelectronic and electronic devices since the breakthrough of the growth of Mg-doping GaN by thermal annealing, [1][2][3][4][5] and the first demonstration of AlGaN/GaN high electron mobility transistors (HEMTs) [6] The wide band gap in GaN (3.4 eV) and AlN (6.2 eV) results in a high breakdown field [7] which is 3 MV in GaN and 11 MV/cm in AlN comparing to 0.3 MV/cm in Si (Table 1). Besides the high breakdown characteristic in GaN and AlN, high electron velocity (~ 2 x10^7 cm/s), high electron mobility of GaN (~ 1500 cm^2/V.s) and high carrier density in 2-dimentional electron gas (2DEG, ~10^{13} cm^-2) are able to provide high speed and high efficiency performances which are very attractive in power switching and RF power amplification applications [8][9][10][11].
<table>
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<td>0.3</td>
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<td>(0.4m_e)</td>
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</table>

Table 1 Materials properties comparison

The current market growth for GaN power semiconductor devices is mainly due to potential in the medium-voltage (300V to 1KV) power electronics market covering the major end-user verticals. Rising number of advanced -power applications of industrial, power, solar and wind sector make most of the market revenue. In the mean time, GaN transistors have been commercialized for communication technology [12][13]. Development of GaN technology has been focusing on replacing Si and GaAs counterparts in RF communication applications. GaN also has low sensitivity to ionizing radiation and better stability in some radiation environments[14][15][16][17][18]. Therefore, it is promising in solar cell arrays [19][20][21][22], satellites [23][24][25][26] and high-end power appliances in the military, defense and aerospace sector. GaN devices in automotive and transportation such as electric vehicles and hybrid electric vehicles have also attracted attention [27][28][29].
Extraordinary growth in power discrete, such as HEMTs, diodes, rectifiers and field-effect transistors (FETs), boosted the total revenue of the GaN power semiconductors market. GaN power ICs was another factor for revenue growth. Development of new power ICs such as MMICs[30][31][32][33][34][35][36] and RFICs [37][38] has been gained intensive attention by industry leading to rapid progress. Besides power semiconductors, GaN is predominantly used in optosemiconductors, such as LEDs and laser diodes[39][40][41][42][43][44].

In this thesis, technology to develop enhancement-mode(E-mode) GaN-based HEMT with low loss and high performance was investigated. Atomic layer deposited (ALD) High-k dielectric was used to enhancedevice characteristics in power application. High-k dielectric/III-Nitride interface properties were first investigated for device design. A comprehensive study of dielectric/III-Nitride interface optimization was demonstrated. E-mode metal-insulator-semiconductor high-electron-mobility-transistor (MISHEMT) and metal-oxide-semiconductor field-effect-transistor (MOSFET) were also shown. By applying similar techniques, interface properties of high-k dielectric on different III-Nitride materials, such as InGaN and AlGaN, and Ga$_2$O$_3$ were introduced.

1.1 Why high-k dielectric in III-Nitride device

As mentioned previously, III-Nitride material has superior electrical properties for both power switching and RF power applications. Atomic layer deposited (ALD) Al$_2$O$_3$
has advantages of conformal coverage, wide bandgap (~8.8 eV) and high dielectric constant (~9). In this section, we propose the motivation to integrate the ALD Al₂O₃ to GaN-based devices.

### 1.1.1. Enhancement-mode GaN HEMT for power switching

Enhancement mode (E-mode) devices are needed as they allow the fabrication of simpler power amplifier circuits by using a single-polarity voltage supply. Furthermore, a normally off device offers safer operation in high-power switching applications. To achieve E-mode GaN HEMT, one of the methods is to recess the AlGaN layer in the gate region. The mechanism of the normally-off GaN HEMT by gate recess is demonstrated as followed. Figure 1 shows the structure, charge, and energy band diagrams for Ni/Al₀.₁₅Ga₀.₈₅N/GaN, where Qₛ is the charges in gate metal, σₚₑ and σₛₚ the piezoelectric and spontaneous polarization charge density, A and G stand for Al₀.₁₅Ga₀.₈₅N and GaN, nₛ the 2DEG density, F₁ the electric field in Al₀.₁₅Ga₀.₈₅N, t₁ the thickness of Al₀.₁₅Ga₀.₈₅N, V₉ the gate bias, ϕₛ the barrier height of Ni/Al₀.₁₅Ga₀.₈₅N, and ΔEc the Al₀.₁₅Ga₀.₈₅N/GaN conduction band offset. Under the threshold condition, we assume the current level is 0.01 mA/mm and velocity of 2DEG is 6x10⁶ cm/s. Therefore, 

\[
n_s = \frac{I}{qV} \approx 10^8 \text{ cm}^{-2}
\]

which is negligible comparing to polarization charges at Al₀.₁₅Ga₀.₈₅N/GaN interface. So we can write the electric field F₁ in the AlGaN layer, and the threshold voltage Vth as

\[
F_1 = \frac{q(\sigma_{PE} + \sigma^A_{SP} - \sigma^G_{SP})}{\varepsilon}, \text{ and}
\]
Figure 1 The structure of 15% AlGaN/GaN HEMT (upper), electrostatic (middle) and energy band diagram.

\[ V_{th} = \frac{\phi_b}{q} - F_1 t_1 - \frac{\Delta E_C}{q}, \]

respectively.
To predict the threshold voltage value as a function of AlGaN thickness, we use $\varphi_b$ as 1.6 eV, $\Delta E_c$ as 0.53 eV, $\varphi_f$ as 0.6 eV, $\varepsilon$ as $9\varepsilon_0$ and net polarization charges at $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}/\text{GaN}$ interface as $8.4 \times 10^{12} \text{ cm}^{-2}$. All the calculation was processed by Mathematica. The calculation results are demonstrated as following.

![Figure 2 Threshold voltage versus 15% AlGaN thickness](image)

**Figure 2** Threshold voltage versus 15% AlGaN thickness

Fig.2 shows the threshold voltage ($V_{TH}$) of AlGaN/GaN HEMT as a function of $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$ thickness. The E-mode HEMT could be made by recessing the $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$ layer below 7 nm. Fig.3 shows the device structure of E-mode MISHEMT. The AlGaN cap layer is etched under the gate to eliminate the electron at zero gate bias while the 2DEG is maintained in the access region without any recess.

The main challenge in achieving normally off operation with such a structure is that the gate leakage would be high since the AlGaN layer is thin. This could be a critical issue for power switching devices. A solution to reduce the leakage while maintaining
normally off operation is to use a gate dielectric with a large band gap to efficiently suppress the gate leakage by blocking electron flow between the metal and semiconductor. Such a device structure is shown in Figure 3.

![Figure 3 The device structure of E-mode GaN MISHEMT](image)

1.1.2. High frequency devices

In scaled high frequency devices where the gate length is reduced below ~ 200 nm, a low gate-channel spacing is necessary to provide a good aspect ratio (to reduce short channel effects), high transconductance and high RF gain. For such scaled devices, the gate-channel barrier is required to be extremely thin (<10 nm) and a schottky barrier HEMT would have significantly high leakage. The use of non-epitaxial high-k dielectric such as Al₂O₃ with a band gap higher than AlGaN, can reduce the gate leakage but maintain the device performance.
1.2 Atomic layer deposited Al₂O₃

Atomic layer deposition (ALD) has emerged as an important technology for thin film growth in different applications. The development of ALD has been driven mainly by silicon semiconductor manufacturing where a conformal and uniform deposition method is needed to deposit ultra-thin gate dielectrics. Atomic layer deposition is a conformal technique, enabling uniform deposition on high aspect ratio structures. Furthermore, precise thickness control at the Ångstrom or monolayer level makes ALD an excellent process for precise nanometer-scale gate dielectrics. Since ALD is self-limiting, excellent control on the dielectric thickness can be achieved.

Fig. 4 shows the process of ALD Al₂O₃ thin film growth. A substrate surface which is hydroxylated from exposure to air, oxygen or ozone is demonstrated in the fig. 4(a). The Pulsing TMA precursor is then introduced into the chamber and reacts with the OH groups on the surface at certain elevated temperature. TMA does not react with itself thus the TMA monolayer passivates the surface (fig. 4 b). Unreacted TMA molecules and CH₄, a gaseous by-product, are evacuated followed by nitrogen purge. Pulsing water (H₂O) is then introduced into the chamber and again followed by evacuation (fig. 4 c). Water reacts with TMA and creates a layer of Al-O-Al bridges. The top surface is terminated with Al-OH (fig. 4 d). Unreacted H₂O and CH₄ are purged with nitrogen carrier gas during pumping after the water pulse. Fig. 4 (a) to (d) show a full cycle of the growth of Al₂O₃ monolayer, and each cycle produces around 0.8 Å of Al₂O₃ layer at 300°C. Different temperature can lead to different growth rate and film quality. Water first growth with five water pulses at the beginning of the deposition is
used in our study. The higher quality of the first Al₂O₃ monolayer obtained by water first deposition gives better interface characteristics [45].
Figure 4 Schematics of ALD Al2O3 growth process.
Chapter 2

Interface Properties of Atomic Layer Deposited Al$_2$O$_3$ on GaN

2.1 Energy Band Line-up and Interface Charges at ALD Al$_2$O$_3$ on GaN

Insulators such as SiO$_2$, Si$_N_x$, Al$_2$O$_3$, and HfO$_2$ have been proposed as a means for gate current suppression and surface passivation of GaN metal insulator semiconductor high electron mobility transistors (MISHEMTs)[46][47][48][49][50][51][52][53][54][55]. Of these, Al$_2$O$_3$ has several desirable properties, including a large band gap, breakdown electric field, and ease of deposition. We report here a quantitative analysis of the interface barrier of Ni/Al$_2$O$_3$/GaN capacitors in terms of conduction band discontinuity, interface fixed charge, and Fermi-level pinning effect.

2.1.1 Experimental details

The samples used in this experiment, as shown in Fig. 5 (a), were grown using a Veeco RF-plasma molecular beam epitaxy system on semi-insulating GaN templates on sapphire from Lumilog, with threading dislocation density of $\sim 5 \times 10^8 \text{ cm}^{-2}$. The epilayer consisted of 200 nm unintentionally doped GaN on substrate followed by 100 nm silicon-doped GaN. The nominal doping density was $1 \times 10^{18} \text{ cm}^{-3}$. Fig. 5 (b) shows a scan of the
as-grown surface taken using atomic force microscope in tapping mode. The oxide layers were deposited in a Picosun atomic layer deposition (ALD) system, using trimethylaluminum (TMA) and H$_2$O as precursors.

Figure 5 (a) Schematic diagram of the MIS capacitors structure and (b) AFM image of the as grown surface.

After a HCl-based removal of the excess gallium droplets on the surface, three different thicknesses—i.e., nominal 6 nm, 12 nm, and 18 nm—of oxide were deposited at 300 °C with water precursor first process on three different pieces cleaved out of the same sample. The pre-deposition treatment of the surface consisted in a 10:1 HF-dip for 15 s. All three samples were then annealed at 700 °C in forming gas for 1 min. The post deposition annealing conditions here reported were chosen after a rigorous study on temperature and duration of the thermal treatment, while evaluating the hysteresis of the capacitance profiles. The gate pads were defined by optical contact lithography. Features of large contacts were also defined in the photo resist. Buffered oxide etch (BOE) 10:1
was used to remove locally the oxide layer in these large features in order to get ohmic contacts. A Ni/Au/Ni stack was e-beam evaporated, and a post metallization annealing was finally performed on all three samples at 400 °C in forming gas for 5 min.

The ohmic behavior of the large contacts was first checked and found to be good without any specific alloying. C-V measurements were performed using an Agilent B1500 semiconductor device analyzer equipped with medium power source/monitor units (MPSMUs) and multi frequency capacitance measurement unit (MFCMU). At equilibrium, the GaN was found to be depleted at the surface for 6 nm and 12 nm ALD samples, and in accumulation for the 18 nm thick ALD sample. Very low current densities below 10 nA/cm² over a wide voltage range were measured for all three samples, indicating that the Al₂O₃ layers have excellent insulation properties.

2.1.2 Energy Band Line-up and Interface Properties

The flat band voltage in the GaN for each of the structures was derived from the first derivative of capacitance voltage profiles (Fig. 6) and was found to be -0.2 V, -1.3 V, and -2.4 V for the 6 nm, 12 nm, and 18 nm thick oxides, respectively (inset of Fig. 6). The shift of the flat-band voltage as a function of oxide thickness is a clear indication of charges either at the interface or in the oxide. The experimental $V_{FB}$ vs. $t_{ox}$ data points plotted in the Fig. 7 (lower) shows a linear relationship with a high degree of correlation.
Figure 6 C-V characteristics of the MIS structures and (inset) The first derivative of the C-V profile to extract the flat band voltage in GaN from the peak values.

We use energy band diagram analysis to understand the physical properties of the interface. Figure 7 (upper) shows a qualitative conduction band diagram of the MIS capacitors with different oxide thicknesses at flat-band. $V_{f}$ is the flat-band gate bias for each thickness, $t_{ox}$, $\phi_{b}$ the barrier height at the Ni/Al$_2$O$_3$ interface, $F_{ox}$ the electric field in the oxide layer, $\Delta E_{c}$ the conduction band discontinuity between Al$_2$O$_3$ and GaN, and $\phi_{s}$ the energy separation of the conduction band from the Fermi level in the n$^+$ GaN layer. Assuming zero interfacial charge in the oxide, a simple analytical expression relating the applied flat band voltage to the interfacial parameters can be derived from Fig. 7 (upper) as
Here, \( V_g \) is the flat-band voltage for the given oxide thickness \( t_{ox} \). According to the analytical expression of the linear fit reported in the Fig. 7 (lower), the electric field dropping across the oxide at flat-band is 1.83 MV/cm and the \((\phi_b - \Delta E_c - \phi_s)\) band offset is 0.9 eV. Based on the doping density, the conduction band distance from the Fermi level \((\phi_s)\) is estimated to be 18 meV. Assuming a barrier height of 3 eV at the Ni/Al\(_2\)O\(_3\) interface[56], the conduction band offset between Al\(_2\)O\(_3\) and GaN is found to be 2.1 eV. This experimental value is in agreement with the theoretical prediction of 2.1 eV reported in Ref. [57]. The fixed Al\(_2\)O\(_3\)/GaN interface charge can be also estimated from the electric field in the oxide under semiconductor flat-band conditions. The non-zero field dropping across the oxide can be attributed to a net positive charge at the Al\(_2\)O\(_3\)/GaN interface, of approximately \(9.1 \times 10^{12} \text{ cm}^{-2}\).
Figure 7 (Upper) Schematic conduction band diagram of the MIS capacitors with different oxide thicknesses at flat-band and (Lower) extraction of the Ni/Al2O3/GaN conduction band alignment and the oxide electric field $F_{ox}$ from the VFB vs. tox plot.

We note that since the Fermi level is nearly at the GaN conduction band edge, the positive states causing this cannot be attributed to GaN mid-gap donor states which would have to be neutral under these conditions. The presence of net positive interface
charge can be explained by two possible scenarios. The first explanation (fig. 8 a) is based on the presence of interfacial _fixed_ charge, which we could attribute to energy states between the conduction band minima of $\text{Al}_2\text{O}_3$ and GaN. If we assume this, using the spontaneous GaN polarization charge ($\sigma_{\text{sp_GaN}}$) of $1.81 \times 10^{13} \text{cm}^{-2}$, we calculate the fixed interface charge ($\sigma_{\text{oxide}}$) density to be $2.72 \times 10^{13} \text{cm}^{-2}$. Under both positive and negative bias on the MIS structure, the Fermi level cannot modulate these states, and they will therefore behave like “fixed” charges. We note that they can, however, be modulated by optical excitation, and UV investigation of MIS structures should provide very useful information on these interface charges.

An alternative explanation (fig. 8 b) is based on the presence of Ga-O or Ga-Al bonds at the $\text{Al}_2\text{O}_3$/GaN interface, causing the inversion of the polarity of the surface. Such inversion of the polarity would result in the inversion of the polarization charge at the interface from negative to positive. Similar experimental observation is reported in Ref. [58], where an AlO$_x$ transition layer has been proven to be an effective mean for GaN polarity inversion. In such a case, we could explain the electrostatic of our system by assuming that a net positive spontaneous polarization charge of magnitude $9.1 \times 10^{12}$ terminates the surface. Further experiments to understand the origin of the electric field in the oxide will be discussed later.
Figure 8 Qualitative energy band diagrams and charge distribution, assuming either (a) ionized donor charge or (b) polarization-charge inversion at the Al2O3/GaN interface.

In conclusion, a quantitative analysis of the Al2O3/GaN interface barrier is presented. Ni/Al2O3/GaN MIS capacitors were fabricated on plasma assisted molecular beam epitaxy grown GaN using ALD for the dielectric deposition. Very low current densities were observed for all three samples, proving the good insulating properties of the Al2O3 layers. A linear relationship between flat-band voltage and oxide thickness has been experimentally observed pointing out the absence of any Fermi-level pinning at the Al2O3/GaN interface and the presence of interfacial charges. Assuming a Ni/Al2O3 barrier height of 3 eV, the conduction band offset between Al2O3 and GaN has been found to be 2.1 eV. This value well matches with the predicted value. A positive net Al2O3/GaN interface charge of $9.1 \times 10^{12} \text{cm}^{-2}$ was shown to exist, and we provide two hypotheses to explain the origin of these charges.
2.2 Interface charge effects on electron transport in III-Nitride MIS transistors

AlGaN/GaN high electron mobility transistors (HEMTs) are excellent candidates for high power [59][60] and high frequency [61] applications due to their superior material properties like high bandgap, high electron velocity and built-in and piezoelectric polarization. However, in order to improve the performance of AlGaN/GaN HEMTs at even higher frequencies, aggressive vertical and lateral scaling is required. As the gate to channel distance is reduced, gate leakage becomes a significant problem, to mitigate which, metal-insulator-semiconductor high electron mobility transistors (MIS-HEMTs) are used [48][62][63][54][64][55][49][65]. In such highly scaled devices, the insulator/AlGaN interface being very close to the 2DEG, can affect the mobility. In this work, we have investigated remote impurity scattering to analyze the effect of dielectric/AlGaN interface charges on 2DEG mobility.

2.2.1 Theoretical model of remote impurity scattering

In the AlGaAs/GaAs system, it has been shown that strong scattering at low temperature in the 2DEG system arises from defects or ionized charges which are separated from the 2DEG by a spacer [66]. In the Si-based system, the effect of remote charge scattering on electron mobility has been discussed as the gate oxide thickness becomes ultrathin [67][68][69]. In the doping-free AlGaN/GaN HEMT system, the above effect is not observed since the polarization dipoles that induce a 2DEG do not have as great an effect on mobility [70][71][72][70]. In MIS-HEMTs, as the dimensions of
devices scale down, the AlGaN layer becomes thinner and the 2DEG experiences increased scattering due to the fixed charge between dielectric and AlGaN layers. Figure 9 shows the schematic energy band diagrams and charge distribution for Ga-polar and N-polar MIS-HEMT structures used for our calculations.

The tensile strain caused by the growth of AlGaN on GaN results in a piezoelectric polarization charge $\sigma_{\text{PE}}$, which adds to the spontaneous polarization charge $\sigma_{\text{SP}}$, and gives positive net polarization charge at the AlGaN/GaN interface; $\sigma_{\text{PE}}$ and $\sigma_{\text{SP,AlGaN}}$ gives negative net polarization charge at the dielectric/AlGaN interface. In the case of Ga-polar structures (Fig. 9 a), there is a net negative polarization charge at the dielectric/semiconductor interface, which is compensated by positive (donor) charges [73]. The fixed charge density at the dielectric/AlGaN interface $n_{\text{fix}}$ can be expressed as

$$n_{\text{fix}} = n_{2D} + \Delta\sigma_{\text{SP,diff}} - \frac{Q_g}{q}$$  (1)

where $n_{2D}$ is 2DEG charge density, $\Delta\sigma_{\text{SP}}$ is the net spontaneous polarization charges at AlGaN/GaN interface, $\Delta\sigma_{\text{SP,diff}}$ is the difference of the net spontaneous polarization charges between AlGaN and GaN layers, and $Q_g$ is the charge in the metal gate.

In the N-polar case [74], the polarization charge at the semiconductor surface is actually positive, but the net charge is negative. This leads to a charge distribution shown in Fig 9 (b). The origin of these negatively charged states in the N-polar case is not known, but we can calculate the areal density by using a similar expression as (1)

$$n_{\text{fix}} = -n_{2D} + \sigma_{\text{polar}} - \frac{Q_g}{q} - F_{\text{AlGaN}}\varepsilon_{\text{AlGaN}} / q$$  (2)

where $\sigma_{\text{polar}}$ is the total polarization charge at the interface in the N-polar case; $F_{\text{AlGaN}}$ and $\varepsilon_{\text{AlGaN}}$ are the electric field and dielectric constant in the AlGaN layer.
The explanation of interfacial fixed charge could be attributed to energy states between the conduction band minima of dielectric and AlGaN. Under both positive and negative bias on the MIS structure, the Fermi level cannot modulate these states, and they will therefore behave like “fixed” charges [73]. The charge density at the dielectric/AlGaN interface $n_{\text{fix}}$ plays an important role especially in scaled MIS-HEMTs since it acts as fixed charge which would affect electron mobility under the gate. However, in the case of conventional Schottky gate, the charges are provided by electrons in the gate metal. Since these are not randomly distributed like interface or surface states, they do not cause significant scattering.

The expression for the remote scattering rate $1/\tau_{\text{tr}}$ using a self-consistent wave function can be derived from Fermi’s golden rule as
where \( m^* \) is the electron effective mass, \( k_F \) and \( q \) are Fermi wave factor and wave factor, respectively. \(^9\) \( V_{nm} \) is the two-dimensional Fourier transform of the scattering potential, which can be expressed as

\[
\frac{1}{A} \int u_n(z) u_m(z) \tilde{V}(q, z) \, dz
\]

\( \tilde{V}(q, z) = \left( \frac{e^2}{2\epsilon_0 \epsilon_r q} \right) e^{-q(z-d)} \)

The distance between 2DEG and dielectric/AlGaN interface is \( d \), \( u_n \) and \( u_m \) are the wave functions of initial and final subbands respectively, and \( \epsilon_b \) is the dielectric constant of GaN. The Thomas-Fermi screening effect term \( q_{TF} \) is expressed as

\[
\frac{m e^2}{2\pi \epsilon_0 \epsilon_r h^2}.\]

By applying the Fang-Howard approximation, the equation (3) can be written as

\[
\frac{1}{\tau} = n f \frac{m^*}{2\pi h^3 k_F^3} \int_0^{2k_F} \left| V_{nm}(q) \right|^2 \sqrt{1 - \left( \frac{q}{2k_F + q_{TF}} \right)^2} \, dq
\]

\( (3) \)

\[
\frac{1}{\tau} = n f \frac{m}{2\pi h^3 k_F^3} \left( \frac{e^2}{2\pi \epsilon_0 \epsilon_r h^2} \right)^2 \int_0^{2k_F} e^{-2qd} \left( \frac{b}{b+q} \right)^6 \sqrt{1 - \left( \frac{q}{2k_F} \right)^2} \, dq
\]

\( (4) \)

\[
b = \left( \frac{33 m e^2 n_{2D}}{8 h^2 \epsilon_0 \epsilon_r} \right)^{1/3}
\]

and

\[
G(q) = \frac{1}{8} \left[ 2 \left( \frac{b}{b+q} \right)^3 + 3 \left( \frac{b}{b+q} \right)^2 + 3 \left( \frac{b}{b+q} \right) \right].\]

The remote scattering mobility of 2DEG \( \mu_{\text{remote}} \) is \( \frac{e \tau_r}{m} \), where \( \tau_r \) is given by the equation (4). We also take into account phonon scattering limited mobility at room temperature[66]. The total mobility can be approximated as

\[
\frac{1}{\mu_{\text{total}}} = \frac{1}{\mu_{\text{remote}}} + \frac{1}{\mu_{\text{optical phonon}}} + \frac{1}{\mu_{\text{acoustic phonon}}},
\]

using Mattheisen’s rule. We have used the Fang-Howard approximation to calculate the
behavior of mobility as the difference in mobility between a full self-consistent wavefunction and the Fang-Howard wavefunction was not significant. From equation (4), the Fang-Howard wavefunction does not depend on the barrier composition, and our analysis makes the implicit assumption that there is no wavefunction extension into the barrier, and hence no alloy scattering effects. This approximation is very good for high composition AlGaN or AlN barriers, and when AlGaN/AlN interlayer/GaN structures are used. The details of barrier composition and thickness affect the *electrostatics* of the problem, and this is taken care of in our analysis from equation (1) by allowing $n_{\text{fix}}$ and $n_s$ to vary. Our analysis can therefore be applied to any structure if the interface charge and electron sheet charge density is known.

Figure 10 Remote-ionized impurity scattering-limited, (acoustic + optical) phonon limited- and total mobility as a function of the 2DEG density.
In Fig. 10, we show the electron mobility for an oxide/2.5 nm AlGaN/GaN structure combining remote scattering and phonon scattering rates (including contributions from both optical and acoustic phonons [66]), as a function of the 2DEG sheet charge density $n_{2D}$ assuming an impurity density of $10^{13}$ cm$^{-2}$ at the interface. At room temperature, phonon scattering dominates above the sheet carrier density of $\sim 5 \times 10^{12}$ cm$^{-2}$. The remote scattering becomes significant below this 2DEG density due to reduced screening.

![Figure 11 2DEG mobility as a function of the 2DEG density for various AlGaN cap thickness.](image)

**2.2.2 Impact of interface fixed charge in electron mobility**

To investigate the effect of scattering on 2DEG mobility in a scaled device, mobility is calculated as a function of 2DEG density for different AlGaN thickness with a
fixed charge density of $1 \times 10^{13}$ cm$^{-2}$ as shown in Fig. 11. The mobility of the 30 nm AlGaN structure is not significantly impacted by remote impurity scattering due to the larger distance from the charges. However, the mobility of MIS-HEMTs with thinner AlGaN cap layers is significantly impacted, with effective mobility dropping as the sheet charge density is reduced, in which case the screening becomes less effective and scattering due to interface charge dominates. We have investigated the effect of changing fixed charge density at dielectric/AlGaN interface on the 2DEG mobility for a highly scaled device with 2.5 nm AlGaN layer, in which the scattering effect plays a huge role. Figure 12 depicts the mobility calculation result using Fang-Howard approximation with various fixed charge densities at dielectric/AlGaN interface. It is clear that the mobility is lower at higher $n_{fix}$. As 2DEG density increases, electron mobility experiences less effect from dielectric/AlGaN interface charges as expected. In addition, the remote scattering-limited mobility becomes a dominant factor compared to phonon scattering when the interface charges increases.
Figure 12 The schematic of mobility versus dielectric/AlGaN interface charges density ($n_{fix}$) for various 2DEG densities. As the 2DEG density is reduced, the mobility drop is more substantial due to lack of screening.

The above calculations show how insulator/AlGaN interfacial charges in scaled structures affect the 2DEG mobility of MIS-HEMTs. Since remote scattering is the dominant effect at low $n_{2D}$, it may not impact access regions in a device where the surface to channel distance is larger, and the charge density is high. However, the impact is more significant below the gate where the 2DEG density is reduced. In this case, 2DEG mobility under the gate indirectly impacts $f_T$ or $f_{max}$ since the mobility affects the lateral electric field distribution and velocity. In most AlGaN/GaN HEMTs, the peak $f_T$ occurs close to the pinch-off where the typical carrier concentration is between $1$ to $3\times10^{12}$ cm$^{-2}$. Since this is the regime where the fixed remote charge has the greatest effect as shown in Fig. 11, we expect the scattering rate calculated here to have critical significance to
understanding and improvement of the high frequency performance of highly scaled devices.

Results of this analysis can be used to select device design structures that could mitigate the effect of remote impurity scattering. While the vertical scaling necessary for high frequency transistors necessitates small gate to channel distances, tailoring the interface charge density by varying dielectric and deposition conditions could improve the mobility. Our work indicates that low interfacial fixed charge densities could greatly improve the performance of device, especially in highly vertically scaled devices.

2.3 Summary

High density of interface fixed charge ($2.72 \times 10^{13}$ cm$^{-2}$) was observed in the Al$_2$O$_3$/GaN. These interface fixed charges can not only induce the electrical field in the oxide but also substantially decrease the electron mobility especially in highly scaled devices. Furthermore, the positive fixed charges push the threshold voltage toward negative direction which prevents normally-off operation. As a result, it is essential to find techniques to efficiently mitigate these interface fixed charges. In the next chapter, techniques of engineering interface charges will be introduced. Device characteristics such as I-V, C-V and electron mobility impacted by interface charge engineering will be discussed.
Chapter 3
Interface Charge Engineering at ALD Al₂O₃/III-Nitride Interfaces

3.1 Introduction

III-nitride-based high electron mobility transistors (HEMTs) are outstanding systems for applications of high power switching [75][76][77][78][79][10] and high frequency devices[80] due to the combination of large band gap and good electronic transport properties. Dielectric layers inserted between the gate and the semiconductor can suppress gate leakage power switching devices, and in scaled high frequency devices. Metal-insulator-semiconductor HEMTs (MISHEMTs) [46][48][49][50][51][64][52][54] structures can efficiently suppress gate leakage in transistors scaled to achieve higher frequency operation, and could also be used for applications in GaN power switching [75][77].

The interface trap density and related dispersion in atomic layer deposited (ALD) dielectric/III-nitride interfaces is significantly lower than in III-As semiconductors [82][83], but our previous work has shown that a high density of fixed charges of the order of 1 μC/cm² is induced at ALD-grown Al₂O₃/GaN and Al₂O₃/AlN structures [73][84][85], an effect that is unique among previously investigated semiconductor
material systems. While this charge is not modulated by gate voltage and does not lead to hysteresis under normal device operation, it does significantly modify the electrostatics in the system. The high interfacial fixed charges may degrade the mobility of the 2-dimensional electron gas (2DEG) [86], and induce electric fields in the oxide leading to increased tunneling-related leakage currents. This fixed-charge-induced electric field also causes leakage through gate dielectrics in N-polar III-Nitride HEMTs [74].

3.2 Interface charge engineering by post metallization anneal (PMA)

Following previous work on post-metallization annealing (PMA) to passivate interface states in silicon technology [87][88], in this work, we investigated the effect of post-metallization anneal on AlO3/GaN interface charge density for different polarities of GaN.

3.2.1 Experimental details

Ga-polar GaN samples were grown using a Veeco GEN 930 plasma molecular beam epitaxy system (PAMBE), on Fe-doped semi-insulating GaN/sapphire templates [89]. The N-polar samples were grown by PAMBE on n-doped free standing GaN template [89]. The epitaxial layer consisted of 200 nm unintentionally doped GaN followed by 100 nm silicon-doped GaN ([Si] ~ 1x10^{18} cm\(^3\)). As-received bulk m-plane GaN samples ([Si] ~6x10^{16} cm\(^3\)) were used [90]. A 29 nm Al\(_{0.3}\)Ga\(_{0.7}\)N/1 nm AlN/GaN HEMT[91] sample on Si substrate with 2DEG sheet carrier density of 1.1x10^{13} cm\(^2\) (as-received) was used in the study. The Al\(_{0.3}\)Ga\(_{0.7}\)N layer was then recessed to 9 nm. Three
Al₂O₃ layers of nominal thickness 6 nm, 12 nm, and 18 nm were deposited by atomic layer deposition (ALD) on each Ga-polar, N-polar GaN, and m-plane GaN sample at 300°C, using trimethylaluminum (TMA) and H₂O as precursors. For the case of Al₂O₃ on AlGaN, 17nm Al₂O₃ was deposited by ALD. Six H₂O pulses (0.1 sec for each) were used at the beginning of deposition, and then followed by TMA precursor. The difference between estimated and measured Al₂O₃ thickness was less than 0.3 nm as confirmed by ellipsometry. Post-deposition anneal (PDA) consisted of 700°C in forming gas for 1 minute. Gate patterns were defined by optical contact aligner, and a Ni/Au/Ni (30/200/30 nm) stack was deposited using an e-beam evaporator. Large contacts for ohmic contact were patterned using contact lithography, and buffered oxide etch (BOE) 10:1 was used to locally remove the oxide layer for large features in order to get ohmic contacts. After gate metallization, PMA was carried out in the forming gas (5% H₂, 95%N₂) in a rapid thermal annealing system at temperatures varying from 400°C, to 550°C.

3.2.2 Electrical characterization of Al₂O₃ on different polarities of GaN

A quantitative analysis of the Ni/Al₂O₃/GaN capacitors was done to determine conduction band discontinuity, electric field in the dielectric layer, and interface fixed charge for each polarity. C-V measurements were performed using an Agilent B1500 semiconductor device analyzer equipped with medium power source/monitor units (MPSMUs) and multi frequency capacitance measurement unit (MFCMU). Fig. 13 (a) shows the C-V measurement result for three different thicknesses of Al₂O₃ on Ga-polar GaN before PMA treatment. The flat band voltage (V_{FB}) was derived from capacitance
voltage profiles, and was found to be -2.8 V, -1.7 V, and -0.5 V for 18 nm, 12 nm and 6 nm Al₂O₃/GaN, respectively. The conduction band diagram of Ni/Al₂O₃/GaN MIS structure is shown in the inset of fig. 13 (a).

Figure 13 (a) C-V characteristics for Al₂O₃/Ga-polar GaN before PMA. (b) Flat-band voltage versus oxide thickness for the Ga-polar GaN for different PMA temperatures.

A simple analytical expression relating the applied flat band gate voltage to the interfacial parameters can be derived as

\[ qV_{gi} = (\phi_b - \Delta E_c - \phi_s) - qF_{ox}t_{oxi} \]  \hspace{1cm} (1)

where \( \phi_b \) is the Ni/Al₂O₃ conduction band barrier height, \( F_{ox} \) the electric field in the oxide, \( \phi_s \) is the energy difference between conduction band and Fermi level in GaN, \( \Delta E_c \) is the conduction band offset between Al₂O₃ and GaN, and \( V_{gi} \) is the flat band gate bias for Al₂O₃ thickness \( t_{oxi} \).
From C-V measurements, the $V_{FB}$ extracted was found to vary linearly with oxide thickness, confirming the validity of equation 1 (Figure 13 b) and indicating that the charge was distributed as a sheet, rather than throughout the oxide. Since the flat band voltage dependence on $\text{Al}_2\text{O}_3$ thickness is linear, the electric field in the oxide can be assumed to be independent of the oxide thickness, indicating the absence of a significant density of bulk oxide charges. From equation 1, the slope of this curve gives the oxide field, while the intercept can be used to determine the conduction band offset. $\varphi_s$ is estimated as 18 meV using doping density in GaN, and the Ni/$\text{Al}_2\text{O}_3$ conduction band barrier height $\varphi_b$ was estimated to be 3 eV from internal photoemission measurements[92]. Using the slope and intercept of the fitted line, $F_{ox}$ was determined to be 1.92 MV/cm before PMA. Using $F_{ox}$ at the $\text{Al}_2\text{O}_3$/GaN interface, we estimate a net sheet charge density of $+9.5 \times 10^{12}$ cm$^{-2}$. The total interface fixed charge ($\sigma_{fix}$), derived by adding the interface net charge ($\sigma_{net}$) and GaN spontaneous polarization charge ($\sigma_{sp\_GaN} = 1.81 \times 10^{13}$ cm$^{-2}$) in the Ga-polar case, is $2.7 \times 10^{13}$ cm$^{-2}$. Figure 13 (b) shows the flat band voltage ($V_{FB}$) vs. oxide thickness curves for 5-minute post-metallization anneals at 400°C, 450°C, and 500°C. The slope of the curve in the figure 13 (b) decreases as the PMA temperature is increased, indicating a reduction in the electric field and the net interface charge density, as shown in Table 2. After 500°C PMA, the interface net positive charges were reduced to $1.1 \times 10^{12}$ cm$^{-2}$, almost 95% lower than the pre-anneal charge density, and the total $\sigma_{fix}$ was reduced to $1.9 \times 10^{13}$ cm$^{-2}$. The intercept of the curves was used to determine the conduction band offset, which was found to be 2.1 eV.
before PMA. After PMA, $\Delta E_c$ was found to approximately the same (2.3 eV), showing that the annealing does not the band line-ups significantly.

While the N-polar samples have opposite surface termination and spontaneous polarization to the Ga-polar samples, our results indicated that the electrostatics of the ALD/GaN interface is similar to the Ga-polar surface. After ALD deposition, a net positive charge density was found at the N-polar GaN surface. Figure 14 (a) shows the C-V measurement results of the Al₂O₃/N-polar GaN after different PMA treatments. We extracted flat band voltage from C-V results, and the relation between $V_{FB}$ and oxide thickness for N-polar case is shown in Figure 14 (b). The conduction band offset for the N-polar case was found to be 2.1 eV. The electric field in the oxide was found to reduce from 1.7 MV/cm to 0.2 MV/cm, indicating that the interface net charges were reduced to $9.0 \times 10^{11}$ cm$^{-2}$ as the PMA temperature was increased from 400°C to 550°C. This indicates that, in N-polar case, positive GaN spontaneous polarization charges were neutralized after higher temperature of PMA. The oxide field $F_{ox}$ and net interface charge density $\sigma_{net}$ are listed in Table 2.
Figure 14. (a) C-V profile for Al$_2$O$_3$/N-polar GaN after 400°C PMA. (b) Flat-band voltage versus oxide thickness for Al$_2$O$_3$/N-polar GaN at different temperature anneals.
Table 2 Electric field in the oxide and interface charge density for different polarities of GaN after PMA.

To determine the effects of polarization on the interfacial properties, a series of PMA experiments were done on non-polar surfaces using Al₂O₃/m-plane GaN structures. Before Figure 15 (a) and 15 (b) shows the C-V measurement and $V_{FB}$ verses oxide thickness plot for such a structure. Before PMA, positive interface fixed charges ($7.8 \times 10^{12}$ cm$^{-2}$) were found to exist at the Al₂O₃/m-plane GaN interface, causing an electric field in the oxide under flat band conditions in the GaN. The conduction band offset as determined from the measurements was 2.1 eV. PMA was found to remove the interface charges completely, similar to the Ga- and N-polar samples.
3.2.3 Electrical characterization of Al₂O₃ on AlGaN

The case of Al₂O₃ on AlGaN is of special technological interest for AlGaN/GaN HEMTs. Figure 16 shows C-V profile before and after PMA treatment at different temperatures for Al₂O₃/AlGaN structures. We found that there was a higher positive charge at the Al₂O₃/AlGaN interface than at the Al₂O₃/GaN interface, as predicted from previous work [85]. The flat band voltage shifted in the positive direction after higher temperature PMA, similar to the case of Al₂O₃ on GaN, showing that the positive charge density has been reduced. However, there were still a large number of positive fixed charges existing at the Al₂O₃/AlGaN interface since the flat band voltage is at -14 V after 500°C PMA. The theoretical flat band voltage for zero interface fixed charge in this case was around -9 V. Therefore, other technology needs be applied in the Al₂O₃/AlGaN interface to efficiently suppress the fixed charges.
Based on the energy band diagrams, the bare n-type GaN surface and the AlGaN surface without ALD dielectric has net negative surface charges (equal to the positive depletion layer charge). Our results show that after ALD deposition, net positive charges are induced at the ALD/GaN interface for all polarities, showing that $\sigma_{\text{net}}$ changes from negative to positive after depositing ALD Al$_2$O$_3$. We also find that PMA treatment can efficiently reduce the interface positive net charges in Al$_2$O$_3$ on Ga-polar, N-polar, m-plane GaN and AlGaN. The origin of this net positive charge is not known - it could be attributed to either the increase of positive interface fixed charges, or a reduction in the number of previously existent negative surface states after Al$_2$O$_3$ deposition. The

Figure 16 C-V profile for Al$_2$O$_3$/ Al$_{0.3}$Ga$_{0.7}$N/AlN/ GaN before and after 400°C, 450°C, 500°C PMA.
polarity-independent result indicates that the source of the \( \text{Al}_2\text{O}_3/\text{III-Nitride} \) interface fixed charge do not originate from intrinsic polarization-charge inversion [73], but rather may be due to defects at the surface [93]. We hypothesize that the gate metal assists the absorption of forming gas at the \( \text{Al}_2\text{O}_3/\text{III-Nitride} \) interface, and compensate the spontaneous polarization charge. The absorption of hydrogen atoms becomes more efficient when we increased the PMA temperature, and the interface net charge is reduced substantially.

The use of PMA to control the \( \text{Al}_2\text{O}_3/\text{III-Nitride} \) in interface net charges is important for design of AlGaN/GaN HEMTs for various applications. The positive interface charge also affects the dielectric leakage characteristics significantly. In Figure 17, the gate leakage current for the \( \text{Al}_2\text{O}_3/\text{Ga-polar GaN} \) structures discussed earlier in this letter are shown. As expected, the decrease in the electric field in oxide reduces the leakage currents by suppressing field-assisted tunneling mechanisms (Fowler-Nordheim tunneling). The high interface fixed can act as remote scattering centers and decrease electron mobility especially when gate oxide thickness is scaled [86], and the channel is close (several nm) from the fixed charges. The results described here provide a method to reduce the interface charge density, thereby eliminating mobility degradation due to remote ionized impurity scattering. Perhaps unique to the III-nitride system, the ability to tune high dielectric/semiconductor charge densities (of the order of \( 10^{13} \)) can provide a new way to engineer lateral band structures and charge density in semiconductor devices. For example, selective patterning of metals can be used to create different band profiles
in different regions of a device, giving unprecedented flexibility in lateral band structure design.

Figure 17 Gate leakage current in Al₂O₃/Ga-polar GaN after different PMA temperatures showing suppression of leakage with increased PMA.

In conclusion, that post metallization anneal in a hydrogen containing ambient can effectively reduce the Al₂O₃/III-Nitride interface net charges in Ga-polar, N-polar, non-polar GaN and AlGaN cases. The investigation gives further insight of the origin of the interface fixed charges at oxide/III-nitride interface, and provides a method to engineer interface charge density. The suppression of the interface charges using PMA is shown to reduce the gate leakage in reverse bias and could be critical for mitigating remote ionized impurity scattering in GaN-based MISFETs.

3.3 Interface charge engineering by oxygen plasma treatment

The previous study showed the interface fixed charge was able to be reduced by
post metallization anneal (PMA) in the case of ALD Al₂O₃ on different polarities of GaN, which implied the origin of interface fixed charge may be due to the surface defects [94]. However, PMA has limited effect in the dielectric/AlGaN (or AlN) interface which directly affects the design of normally-off device. Oxidizing the AlGaN (AlN) surface to form a native oxide layer is one of the efficient methods to passivate the surface. In this section, we used the combination of oxygen plasma and PMA treatments to engineer the Al₂O₃/AlGaN (AlN) interface fixed charges. Both experimental and theoretical electron mobility characteristics were investigated. A normally-off MISHEMT was also demonstrated.

3.3.1 Experimental details

A MOCVD-grown 29 nm Al₀.₃Ga₀.₇N / 1 nm AlN / GaN HEMT sample on Si substrate with 2DEG sheet carrier density of 1.1x10¹³ cm⁻² (as-received) was used in the study [NTT-AT Co.]. Device fabrication was started from Ti/Al/Ni/Au ohmic contact annealed at 850°C in N₂ ambient and followed by mesa isolation. For vertically scaled devices, the Al₀.₃Ga₀.₇N layer thickness in the active device region was varied by inductively coupled plasma reactive ion etching (ICP-RIE) using a Cl₂/BCl₃ gas mixture. After photoresist removal, the samples were exposed to oxygen RIE plasma (20 W, 30 sccm, 5 mTorr) (Plasma Therm SLR770) ex-situ before the Al₂O₃ deposition. A 20 nm Al₂O₃ gate dielectric was deposited by ALD with TMA and water as precursors at 300°C. A Ni/Au/Ni metal stack was then deposited as gate. Five-minute post metallization anneal (PMA) under 5% H₂ / 95% N₂ ambient was conducted to further reduce the
positive interface fixed charges. The AlGaN etching depth was confirmed by both C-V and AFM measurements. The process flow of the MISHEMT is shown in Fig. 18.

![Figure 18 Process flow of the MISHEMT](image)

Mobility measurements were done using gated transmission line measurement (gated TLM) combined with C-V characterization by Agilent B1500 semiconductor device analyzer equipped with medium power source/monitor units (MPSMUs) and multi frequency capacitance measurement unit (MFCMU). Frequency of 1 MHz was used for C-V measurement. The gated TLM-measured mobility eliminates the effect of contact
resistance and can be repeated after different PMA treatments on the same device. The gate recessed length ($L_g$) varied from 2 um to 20 um and gate metal overhang length was 0.4 um in each side (Fig. 19 a). The AlGaN/AlN thickness after recess was determined by the C-V measurement. The theoretical mobility calculation was based on our previous study [86] and further includes other scattering mechanisms such as dislocation scattering, dislocation strain field scattering and interface roughness scattering [94]. A surface roughness of 0.49 nm and a dislocation density of $2 \times 10^9$ cm$^{-2}$ were used for calculations. The interface fixed charge density was varied from $2 \times 10^{13}$ cm$^{-2}$ to $8 \times 10^{12}$ cm$^{-2}$ to match the measured density after different oxygen plasma and PMA conditions. Fig. 20 shows mobility versus 2DEG density profiles of different mechanisms with 9 nm AlGaN cap layer and $1 \times 10^{13}$ cm$^{-2}$ of interface fixed charges.
3.3.2 Electrical characterization

Fig. 21 (a) shows the experimental C-V characteristics of a non-recessed MISHEMT with no treatment (circle), O<sub>2</sub> plasma (triangle) and O<sub>2</sub> plasma/PMA (diamond), together with theoretical C-V curves. The threshold voltage ($V_{th}$) shifted from -16 V to -12 V after O<sub>2</sub> plasma/PMA treatments and the C-V hysteresis characteristics were also improved. We found a significant reduction of the interface fixed charges from $3.2\times10^{13}$ cm<sup>-2</sup> to $2.2\times10^{13}$ cm<sup>-2</sup> after O<sub>2</sub> plasma treatment (simulated by Poisson-Schrodinger solver [96]). The polarization charge density of 30% AlGaN was assumed as $3.1\times10^{13}$ cm<sup>-2</sup>. Thus, the interface net charge density changed from $+1\times10^{12}$ cm<sup>-2</sup> to -
9x10^{12} \text{ cm}^{-2}. Energy band diagram with different positive interface fixed charges (fig. 21 b) shows a remarkable change after O_2 plasma. The Al_2O_3/AlGaN positive fixed charges became less than the negative polarization charge, which leads to negative net interface charges. This enables an efficient approach to engineer Al_2O_3/AlGaN interface fixed charges, and could be used to design normally-off MISHEMTs with high threshold voltage.

Figure 21 (a) Experimental (symbols) and theoretical (lines) (b) Energy band diagram with different positive oxide/AlGaN interface fixed charge density

After finding the significant impact of O_2 plasma and PMA, we investigated the effect on electron mobility for vertically scaled MISHEMTs. The schematic of AlGaN-recessed MISHEMT structure is shown in fig. 19 (a). Surface morphology and roughness of AlGaN before and after ICP-RIE etching were confirmed by atomic force microscope (AFM). Fig. 19 (b) and (c) shows the AFM images before and after 20 nm AlGaN
etching. There is no significant difference in morphology and roughness (0.40 nm and 0.49 nm) of the surface which indicates that the chlorine-based dry etching did not cause significant physical damage on the AlGaN surface. Fig 22 (a) shows the experimental (symbols) and theoretical (solid line) C-V characteristics of recessed (8 nm AlGaN/1 nm AlN) MISHEMTs before and after 400°C PMA with O₂ plasma treatment. The $V_{th}$ shifted from -7V to -4V and the interface fixed charges were substantially reduced to $2 \times 10^{13}$ cm$^{-2}$ (-1.1x$10^{13}$ cm$^{-2}$ for net charge density) after both O₂ plasma and PMA treatments. In the absence of plasma treatment and PMA, MISHEMTS with 20 nm Al₂O₃/AlGaN/GaN cap were found to have high interface fixed charges (> $3 \times 10^{13}$ cm$^{-2}$). In the case of thin AlGaN cap, this led to significant mobility degradation (< 400 cm$^2$V$^{-1}$s$^{-1}$ for 6 nm AlGaN cap), directly demonstrating the impact of remote interface charge scattering on the electron mobility.
Figure 22 (a) The experimental (symbols) and theoretical (lines) C-V characteristics with and without PMA after oxygen plasma of 9 nm AlGaN/AlN MISHEMT. (b) Mobility profiles of 9 nm AlGaN/AlN MISHEMT with and without PMA after oxygen plasma treatment.

Fig. 22 (b) shows the experimental and theoretical electron mobility profile before and after 400°C PMA with O₂ plasma treatment. We find that the mobility increases, especially in the lower 2DEG density regime, after 400 °C PMA. This suggests that while the effect of remote impurity scattering can be observed experimentally, there is still some disagreement between theoretical and experimental curves. It is possible that in addition to the net interface fixed charges, trapped states may also need to be considered since they can also act as scattering centers. However, our results confirm that the combination of oxygen plasma and PMA leads to an improvement of electron mobility in recessed MISHEMTs, and that there is a correlation between interface fixed charges and
electron mobility, as predicted earlier [86].

Since the existence of Al$_2$O$_3$/AlGaN or Al$_2$O$_3$/AlN [85] positive interface fixed charges can bring the threshold to negative direction, fabrication of normally-off MISHEMTs becomes a challenge. The ability to reduce the interface fixed charge is important. Fig 23 (a) demonstrates the device structure of normally-off MISHEMT. The active region recess length is 2 um and source-to-drain distance is 6 um. A thin AlN layer was present after dry recess etching, based on comparison of the drain current level to a MISFET where the channel was etched by an additional 3 nm (dotted line in fig. 23 b). Using the recipe developed above, native oxide was formed by O$_2$ plasma and 400 °C PMA treatment for 5 minutes in forming gas ambient was done. Figure 23 (b) shows the transfer characteristics of the normally-off device at $V_{ds}=7$V. The drain current density was more than seven times larger than 3 nm over etched MISFET and the transconductance ($g_m$) was 43 mS/mm. Fig. 23 (c) shows the transfer characteristics in log scale. Here we define the threshold voltage at $I_{ds}=10$ μA/mm, which gives us $V_{th}=1.5$ V. The gate current density is at the order of $10^{-8}$ A/mm from $V_g=0$ V to 7 V. The C-V characteristics for the transistor and MIS diode (18 nm Al$_2$O$_3$/n+ GaN, no oxidation/PMA)[94] are shown in the inset of fig 23 (c). The hysteresis $\Delta V$ for the transistor is 0.8V, and the threshold voltage from C-V matches well with the transconductance curve for the transistor. The positive threshold voltage shift in the MIS diode (from -2.8 V to +1.5 V) due to the oxidation/PMA step could be useful for achieving high positive threshold voltage in enhancement mode devices. The $I_{ds}$-$V_{ds}$ characteristic is shown in fig. 23 (d). Gate bias ($V_{gs}$) was applied from 0 V to 10 V and
more than 140 mA/mm drain current density was achieved at $V_{ds}=7V$. The on-resistance is $20 \, \Omega \cdot \text{mm}$. Further improvement of off-state current needs to be achieved by optimizing device isolation. We analyzed the device characteristics to extract the field effect mobility in the channel. Based on these estimates, the field effect mobility ($100 \, \text{cm}^2\text{V}^{-1}\text{s}^{-1}$) is relatively low. We believe this may be due to etch damage. Therefore, reducing the gate recess etch damage may provide a pathway to higher mobility and current. Nevertheless, the device demonstration shown here confirms that the combination of O$_2$ plasma treatment and post-metallization annealing can be used to eliminate fixed positive charges, and achieve normally off transistors.
A comprehensive study of interface fixed charge engineering approaches and E-mode MISHEMT is reported. The impact of remote impurity scattering on scaled MISHEMT was demonstrated experimentally. The combination of oxygen plasma and PMA treatments can efficiently reduce positive interface fixed charges and improve the...
electron mobility, and enable the demonstration of normally-off devices. An E-mode MISHEMT with $V_{th}=1.5$ V was shown in this study, but with optimized device design, the charge engineering approach demonstrated here could lead to devices with significantly higher threshold.

3.4 X-ray photoelectron spectroscopy and reliability analysis of Al$_2$O$_3$/AlGaN Interface

In the previous section we have shown that oxidizing nitride surface by oxygen plasma before ALD enabled the removal of the interface fixed charges to achieve E-mode MISHEMTs. To understand the dielectric/III-Nitride interface properties and stability after oxygen plasma treatment, further interface and reliability characterizations need to be done. In this section, we used X-ray photoelectron spectroscopy (XPS), which is an interface analysis tool [97][98][99][100][101][102] and electrical measurements to understand the effects of oxygen plasma treatment on Al$_2$O$_3$/AlGaN interface properties. We investigate the long-term stability of the interface after oxygen plasma treatment.

3.4.1 XPS analysis of Al2O3/AlGaN interface

A commercially obtained HEMT (22 nm Al$_{0.23}$Ga$_{0.77}$N/GaN) grown on Si substrate was used in this study. Fig. 24 shows the MISHEMT structure for XPS measurement. 20W oxygen plasma was applied. 4 nm ALD Al$_2$O$_3$ was deposited at 300ºC with TMA and water as precursors. Both Mg and Al K$_\alpha$ sources were used in the XPS measurement and calibrated by C 1s peak (284.8 eV).
Ga 3d peaks from both samples with and without (control sample) oxygen plasma treatment were analyzed. In the control sample, a Ga 3d peak was observed at 19.6 eV [103][104](Ga-N bond) from both Mg (fig. 25 a) and Al (fig. 25 b) sources. The O 2s signal is mainly from the Al$_2$O$_3$ film which we can ignore in the case of interface analysis. Therefore, only Ga-N signal was observed in the control sample. Fig. 26 (a) and (b) show the Ga 3d signal of oxygen plasma sample from Mg and Al sources including an additional peak at 20.5 eV (Ga-O bond) [103][104]. The XPS measurement qualitatively shows that AlGaN surface was oxidized by oxygen plasma.
Figure 25 XPS measurement of non-treatment sample in (a) Mg and (b) Al sources
To correlate the oxidation of the nitride surface to the reduction of the interface fixed charges, we propose a hypothesis based on the XPS measurement. Before any oxygen plasma treatment, N vacancies leads to Ga dangling bonds which form donor states at Al$_2$O$_3$/AlGaN interface (fig. 27 a). This donor states act as positive fixed charges (fig. 27 b). After oxygen plasma treatment, oxygen provides electrons which neutralize the donor states created by Ga dangling bonds, and reduces the interface fixed charges (fig. 28).
Figure 27 (a) The schematic of Al$_2$O$_3$/AlGaN interface without oxygen plasma (b) Electron statistic chart of MISHEMT
Figure 28 (a) The schematic of Al₂O₃/AlGaN interface after oxygen plasma (b) Electron statistic chart of MISHEMT

3.4.2 Reliability analysis of oxygen plasma treatment

Fig. 29 (a) and (b) show the XPS results three weeks from the first measurement in Mg and Al sources respectively. Both signals of Ga-N and Ga-O bonds can be observed. One week later, thermal anneal (400°C in N₂ ambient) for 10 minutes was treated to simulate long term characteristics. The Ga-O XPS signal in both X-ray sources (fig. 29 c and d) remained relatively unchanged, revealing the stability of the oxidation treatment.
Figure 29 XPS measurement of oxygen plasma treatment sample after three weeks in (a) Mg and (b) Al sources and after four weeks under thermal stress in (c) Mg and (d) Al sources
To further understand the reliability of device performance after oxidation treatment, the transfer characteristics of oxygen plasma treated MISHEMTs were measured (fig. 30). The $V_{th}$ did not change after the one week delay and temperature stress, indicating that the $O_2$ plasma could be used to create stable E-mode transistors. However, increase of hysteresis indicates that more interface traps were created after certain time. For the details of the impact to the interface traps by oxygen plasma treatment, further study needs to be done.

![Figure 30](image.png)

Figure 30 The transfer characteristics of recessed MISHEMT with oxygen plasma treatment
In conclusion, a comprehensive time-dependent XPS study shows that surface oxidation of AlGaN by oxygen plasma could be correlated with the reduction in the positive fixed interface charge at dielectric III-Nitride interfaces. The $V_{th}$ stability in MISHEMTs shows that the method can be used to make stable E-mode devices. This study provides informative details of oxygen plasma treatment and reliability toward device performance.

3.5 Device optimization by interface charge engineering

In the previous section, we introduced PMA and oxygen plasma treatments to efficiently reduce the Al$_2$O$_3$/III-Nitride interface fixed charges. Not only threshold voltage shifted back toward positive but lower gate current was observed. We also both theoretically and experimentally demonstrated the impact of interface charge engineering in the electron mobility. In this section, we will discuss the optimization for the device characterizations including C-V hysteresis, threshold voltage and electron mobility in both D-mode and E-mode MISHEMTs (fig. 31). The effect of photoresist (PR) will also be discussed.
3.5.1 Experiment design and characterization methods

A commercially obtained HEMT (2 nm GaN/18 nm Al\textsubscript{0.26}Ga\textsubscript{0.74}N/GaN) grown on Si substrate was used in this study. For the non-recessed samples, 5 nm of ALD Al\textsubscript{2}O\textsubscript{3} sacrificial layer with TMA and water as precursors at 300°C was initially deposited to avoid contamination followed by Ti/Al/Ni/Au anneal ohmic contacts (20/120/30/50 nm at 850 °C under N\textsubscript{2} ambient). The sacrificial layer was then removed by BOE 10:1 dip for 30 seconds. Before the 10 nm Al\textsubscript{2}O\textsubscript{3} gate dielectric which was deposited by ALD with TMA and water as precursors at 300°C, three different treatments were conducted. Fig. 32 shows the process flow for the experiment. The samples with clean surfaces were prepared by the standard solvent clean (acetine/IPA/DI water for 5 minutes each). 20W oxygen plasma treatment in the ICP-RIE chamber for 2 minutes was done before the ALD. To understand the effect of photoresist (PR), the top GaN surface was spin-coated with SPR-950 with spin rate of 5000 rpm for 40 seconds and removed by acetine/IPA/DI.

Figure 31 The schematic of D-mode and E-mode MISHEMTs in the same substrate.
water for 5 minutes each before the gate dielectric deposition. Post deposition anneal (PDA), which is a common method to condense the dielectric film [105][106], was treated after the ALD Al₂O₃ deposition in the forming gas (5% H₂ and 95 % N₂) for 5 minutes. Ni/Au/Ni gate metal stacks with 30/100/30 nm thickness were deposited by e-beam evaporator. PMA was done after the gate metallization.

![Diagram of the process flow](image)

Figure 32 The process flow of the non-recessed MISHEMT optimization experiment.

For E-mode MISHEMTs, gate recess needs to be done before the deposition of dielectric. Fig. 33 shows the schematic of the process flow of recessed MISHEMTs. 5 nm of Al₂O₃ sacrificial layer was also deposited to protect the III-Nitride surface. After ohmic contact fabrication and removal of sacrificial layer, smooth etched surface after ICP-RIE dry etching was obtained and both 4 nm and 1 nm of AlGaN cap layers were
used in this study. 10 nm of ALD Al₂O₃ was deposited at the temperature of 300ºC with TMA and water as precursors. Treatments of oxygen plasma, PDA and PMA were done for the optimization study.

Figure 33 Process flow of the recessed MISHEMT optimization experiment.
To characterize both the non-recessed and recessed MISHEMTs, we focused on the analysis of the interface fixed charge density, C-V hysteresis and electron mobility. The interface fixed charge density was extracted from the C-V measurement swept from minus to +4 V. The C-V characterization was measured by Agilent B1500 semiconductor device analyzer equipped with multi frequency capacitance measurement unit (MFCMU). Frequency of 1 MHz was used for C-V measurement. The theoretical C-V curve was simulated by Bandeng with Poisson/Schrodinger solver. Fixed charges can be inserted into the desired interface therefore the interface charge density can be obtained by fitting the simulated C-V curve to the experimental data (fig. 34).

![Theoretical and experimental C-V for interface fixed charge extraction.](image)

Figure 34 The theoretical and experimental C-V for interface fixed charge extraction.

The C-V hysteresis ($\Delta V$) analysis was also swept from minus to +4 V and then back to the start point. The measurement was conducted in 1 second per step and no wait at +4 V. Hysteresis is estimated as the maximum voltage difference at a constant
capacitance (fig. 35). Detail of electron mobility characterization was similar to our previous study. Gated TLM combined with C-V characterization by Agilent B1500 semiconductor device analyzer equipped with medium power source/monitor units (MPSMUs) and MFCMU. Frequency of 1 MHz was used for C-V measurement.

![Figure 35 Extraction of C-V hysteresis (ΔV).](image)

3.5.2 Effect of photoresist in the Al₂O₃/III-Nitride interface face property

It is essential to use photoresist in the photolithography process. However, since the sensitive surface of III-Nitride materials due to their polarization property, it is important to understand the effect of PR to the Al₂O₃/III-nitride interface.

Fig. 36 shows C-V hysteresis (ΔV) versus PDA temperature for both cases of with and without PR exposure. The insignificant difference between these two cases reveals that PR has limited effect in the C-V hysteresis cross temperatures. However, the interface fixed charge density shows the sensitivity to the PR. Fig. 37 (a) shows the
interface fixed charge density versus PDA temperature. We can obviously observe higher density of interface fixed charge in the sample exposed to PR and even more at higher PDA temperature (up to $6.5 \times 10^{13}$ cm$^{-2}$). The energy band structure also shows significant difference between these two cases (fig. 37 b). It implies that PR needs to be prevented to expose to Al$_2$O$_3$/III-nitride interface thus a sacrificial layer is necessary in the device fabrication.

![Graph showing C-V hysteresis versus PDA temperature for samples with and without PR exposure.](image)

Figure 36 The C-V hysteresis verses PDA temperature for samples with and without PR exposure.
3.5.3 Optimization of interface fixed charge and hysteresis

As mentioned in the previous chapter, positive interface fixed charges are able to shift the threshold toward negative thus prevent the normally-off operation. C-V hysteresis due to the interface traps is also an issue especially in E-mode MISHEMT since electron can always travel to the dielectric/III-Nitride interface and be captured by the interface traps because of the energy barrier under positive gate bias operation. This large hysteresis can lead to unstable threshold voltage during operation. In this section, we find out the best window of oxygen plasma, PDA and PMA treatments for optimal fixed charge density and hysteresis characteristics in both non-recessed and recessed MISHEMTs.
All the samples in this study deposited sacrificial layer initially to prevent PR contamination. Fig. 38 (a) shows the hysteresis versus PDA temperature with different conditions of PMA and oxygen plasma treatments. Before PMA, oxygen plasma increased the hysteresis. However, after higher temperature of PMA, $\Delta V$ was substantially reduced to 0.2 V. PDA is also helpful for the reduction of $\Delta V$. On the other hand, figure 38 (b) shows interface fixed charge density versus PDA temperature. The interface fixed charge density was greatly suppressed by the combination of oxygen plasma and PMA down to $2 \times 10^{12}$ cm$^{-2}$ before PDA, similar to the study presented in the previous section. However, higher temperature of PDA can increase the fixed charge density. Therefore, by comparing both the hysteresis and interface fixed charge density characteristics, the best window we found in non-recessed MISHEMT was treatments with oxygen plasma, PDA temperature below 500°C PDA and 400°C PMA.
Figure 38 Characterizations of (a) hysteresis and (b) interface fixed charge density versus PDA temperature with different PMA and oxygen plasma conditions in non-recessed MISHEMTs.

For the case of recessed MISHEMT, similar experiment was also done before PMA treatment. Fig 39 (a) demonstrates the hysteresis versus PDA temperature of different thickness of AlGaN cap layer. Similar to the non-recessed case, larger $\Delta V$ was observed after oxygen plasma treatment in both cases of 4 nm and 1 nm AlGaN cap thickness. Oxygen plasma treatment reduced the interface fixed charge density in the scaled MISHEMTs, and PDA made it higher which is similar to the non-recessed case (fig. 39 b). The measurement result indicates that the importance of PMA treatment in the recessed MISHEMT which will be discussed in the next section along with the electron mobility analysis.
3.5.3 Mobility study in highly scaled MISHEMT

Impact of oxygen plasma and PMA in electron mobility was discussed in the section 3.3. Remote impurity scattering was proposed to explain the mobility degradation by the interface fixed charges. Combination of PDA, PMA and oxygen plasma treatments are the methods for the interface charge engineering. More details regarding oxygen plasma, PMA and PDA in electron mobility optimization are introduced in this section.

The MISHEMT with 10 nm Al$_2$O$_3$ and 4 nm AlGaN was used in this study. Fig. 40 (a) shows the interface charge engineering by PMA and oxygen plasma treatments. Similar to the previous result in the non-recessed MISHEMT, treatments with oxygen plasma and 400°C PMA gave the lowest interface charge density. Profile of electron
mobility versus 2DEG density is shown in fig. 40 (b). Before PMA, MISHEMTs with and without oxygen plasma treatment show very low mobility (below 300 cm\(^2\)V\(^{-1}\)s\(^{-1}\)). However, electron mobility was recovered up to 500 cm\(^2\)V\(^{-1}\)s\(^{-1}\) after PMA. It implies the PMA treatment can not only suppress the interface fixed charges but efficiently recover the electron mobility.

Fig. 41 (a) demonstrates the interface fixed charge density versus PDA temperature. Similar to the case in non-recessed sample, fixed charge density was increased to 4x10\(^{13}\) cm\(^{-2}\) after 600 °C PDA even with 400 °C PMA. The mobility versus 2DEG density profile after different temperatures of PDA (fig. 41 b) shows that the case with 600 °C PDA has the higher mobility (peak at 600 cm\(^2\)V\(^{-1}\)s\(^{-1}\)). This result is opposite to our prediction since the sample with 600 °C PDA has highest interface fixed charge density creating more remote scattering centers to reduce the electron mobility. The possible explanation regarding this is deep traps at Al\(_2\)O\(_3\)/AlGaN interface. Interface fixed charges which lead to threshold voltage shift is not the only interface states can affect the electron mobility. Deep traps in the bandgap [107][108][109][110] are also able to act as scattering centers which we were not able to detect in this study (fig. 42). Further analysis needs to be done for the deep trap characteristics. In the case of recessed MISHEMT, the window of PDA temperature below 500°C PDA, 400°C PMA and oxygen plasma also gives us the optimal fixed charge density, C-V hysteresis and electron mobility for E-mode MISHEMT design.
Figure 40 Impact of PMA treatment in (a) interface fixed charge density and (b) electron mobility.
Figure 41 Impact of PDA treatment in (a) interface fixed charge density and (b) electron mobility.

Figure 42 Energy band diagram indicating deep trap states and electrostatic chart of MISHEMT.
In this study, we discussed the MISHEMT characteristic optimization of interface fixed charge density, C-V hysteresis and electron mobility by oxygen plasma, PDA and PMA treatments. Photoresist was firstly found to increase the interface fixed charge density; therefore an ALD Al₂O₃ sacrificial layer is needed to protect the PR contamination. The treatment with oxygen plasma, PDA temperature below 500°C PDA and 400°C PMA was found to be the best window to obtain the optimal ΔV, fixed charge density and mobility in both non-recessed and recessed MISHEMTs. The study of mobility profiles in different temperatures of PDA shows that the remote impurity scattering centers were not only contributed from the interface fixed charge but deep traps at interface. Further detail regarding deep traps needs to be investigated carefully. Nevertheless, we provided useful information for both D-mode and E-mode MISHEMT design and fabrication.

3.6 Lateral energy band engineering

In the previous sections, we observed high density of Al₂O₃/III-Nitride interface fixed charge. Oxygen plasma, PDA and PMA treatments enable to engineer the interface charges. Successfully mitigating Al₂O₃/III-Nitride interface charges enables energy band engineering in lateral direction by patterning ALD Al₂O₃. In this work, lateral energy band engineering by patterning ALD Al₂O₃ is demonstrated. This technology provides a new approach to etch-free and doping-free normally-off MOSFETs/MISHEMTs.
3.6.1 Lateral charge engineering enhanced E-Mode MOSFET

Fig. 43 shows schematic of lateral charge engineering assisted E-Mode MOSFET. In access region of the MOSFET, 2DEG is induced by positive interface fixed charges; while there is no charge under the gate since interface fixed charges are efficiently mitigated by oxygen plasma and PMA. The electrical characteristics of the device were checked step by step to confirm the idea of lateral band engineering.

![Schematic of lateral charge engineering enhanced E-Mode MOSFET](image)

Figure 43 Schmatice and energy band diagrams of E-mode MOSFET by lateral charge engineering

For the MOSFET fabrication, a commercially obtained HEMT (29 nm Al$_{0.3}$Ga$_{0.7}$N/1 nm AlN/GaN) grown on Si substrate (NTT Inc) was used in this study. After the fabrication of the annealing Ti/Al/Ni/Au ohmic contact and mesa isolation, the
Al$_{0.3}$Ga$_{0.7}$N/AlN layer was recessed to different thicknesses using chlorine-based ICP-RIE etch. 10 nm of ALD Al$_2$O$_3$ was then deposited with water and TMA as precursors at 300 °C. The Al$_2$O$_3$/GaN interface fixed charges were able to induce the 2DEG in GaN. To achieve E-mode, the Al$_2$O$_3$ under the gate was removed by BOE 10:1 and annealed at 800 °C followed by 20 W oxygen plasma for 2 minutes. The second layer of ALD Al$_2$O$_3$ was then deposited as gate dielectric. A Ni/Au/Ni gate was evaporated and PMA was done under 5% H$_2$ ambient at 400°C. The Process flow of lateral charge engineering assisted E-mode MISHEMT is shown in fig. 44. In this device, the access region still remains 2DEG close to the interface; in the contrary, no current under the gate because of the oxygen plasma treatment.
The two-terminal I-V measurement was done in the TLM pattern with 6 μm of source-to-drain spacing before and after the first Al₂O₃ deposition (fig. 45). There was no current after the AlGaN removal dry ICP-RIE etching. However, 180 mA/mm of drain current density at V_d = 10 V was observed after the ALD Al₂O₃ deposition. It reveals that
2DEG was induced by the Al$_2$O$_3$/GaN positive interface fixed charges. The structure and $I_d$-$V_d$ family curves of E-mode MOSFET are shown in the fig. 46. Before the 400ºC PMA, the transistor with 2.8 $\mu$m of gate length and 6 $\mu$m of source-to-drain spacing shows low current density (40 mA/mm at $V_g = 12$ V). In the previous section, we found PMA treatment can efficiently increase the electron mobility thus increase the current density. In this case, the drain current density was increased substantially close to 200 mA/mm at $V_g = 12$ V. Fig. 47 shows the transfer characteristics of the lateral charge engineering assisted MOSFET before and after the PMA treatment. A positive threshold voltage was found; however, a large hysteresis (~6 V) and 0.2 mA/mm of the off-state leakage were observed before the PMA. A much lower hysteresis (~1 V) and off-state current density (10 $\mu$A/mm) were measured after the 400ºC PMA indicating that PMA can efficiently reduce the hysteresis and reverse current leakage as we discussed in the previous section. The threshold voltage in our lateral charge engineering assisted MOSFET after PMA is +0.5 V defined by the voltage at 1 $\mu$A/mm which is five-orders lower than the maximum drain current density.

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Figure 45 The two terminal I-V measurement before and after the first Al₂O₃ deposition.
Figure 46 The device dimensions and Id-Vd family curves before and after PMA treatment.

Figure 47 The transfer characteristics before and after the PMA treatment.
In this study, we successfully demonstrated an E-mode MOSFET by lateral energy band engineering. 2DEG was found to be induced by the positive interface fixed charge. An E-mode GaN MOSFET with +0.5 V threshold voltage is achieved by patterning ALD Al₂O₃. Treatments of PMA and oxygen plasma in the Al₂O₃/GaN interface are capable to improve the electron mobility, hysteresis and off-state current leakage. Better performance of normally-off device can be improved by using MISHEMT structure. Other applications for both electronics and optoelectronics are also possibly achieved by this dielectric-assisted lateral band engineering technology.

3.7 Summary

In this chapter, we comprehensively discussed the methods of interface charge engineering which were post metallization anneal and oxygen plasma treatments. Interface fixed charges could be efficiently mitigated in Al₂O₃/GaN and Al₂O₃/AlGaN interfaces by these techniques. E-mode MISHEMT with 1.5V of threshold voltage was demonstrated. The best PMA, PDA and oxygen plasma window was found as 400°C of PMA, PDA below 500°C and with oxygen plasma treatment to give the optimal characteristics of MISHEMT. Passivation of Ga dangling bonds by oxygen leading to reduction of interface fixed charges was investigated by XPS measurement. New idea of lateral energy band engineering was shown by patterning ALD Al₂O₃ with oxygen plasma and PMA treatments. Our study provides important information for the development of ALD Al₂O₃ on III-Nitride devices.
Chapter 4
Interface Properties of ALD Al₂O₃ on InGaN and Other Wide Bandgap Materials

Al₂O₃ on AlGaN/GaN MISHEMT has been discussed in the previous chapter. By optimizing the Al₂O₃/AlGaN and Al₂O₃/GaN interfaces with various treatments, this high-k gate dielectric is capable to efficiently suppress leakage current but also achieve E-mode operation. ALD Al₂O₃ can be also useful as a gate dielectric in MOSFETs or MISHEMTs with new channel materials. In this chapter, we introduce energy band line-up of ALD Al₂O₃ on high composition InGaN, high composition AlGaN and β-Ga₂O₃. By understanding the dielectric/semiconductor interface properties, it is helpful for device design in high frequency or power switching application.

4.1 Energy band line-up of ALD Al₂O₃ on high composition InGaN

InGaN (InN) channel has been theoretically demonstrated to have higher steady-state peak drift velocity than GaN channel because of its low electron effective mass [111][112][113]. Both In-polar and N-polar InGaN channel are proposed to replace the conventional GaN channel to improve the high frequency performance [114][115]. Growth of InGaN channel structures with high mobility has been challenging due to
InGaN instability at high substrate temperatures [116][117][118]. For InGaN channel transistors, introducing a high-k dielectric as gate can efficiently suppress the gate leakage current and maintain the device performance as well. However, the energy band line-up needs to be investigated before designing and fabricating devices. In this section, we demonstrate the growth of high composition In-polar InGaN (up to 20%) with smooth surface. Metal-insulator-semiconductor (MIS) Al$_2$O$_3$/InGaN diode was fabricated for the study of energy band alignment.

4.1.1 In-polar InGaN growth and material properties

Samples used in this study were grown by plasma assisted molecular beam epitaxy (PAMBE) in a Veeco Gen 930 system equipped with standard effusion cells for Ga and In. Active nitrogen was supplied using a Veeco rf plasma source. Commercially available Ga-polar free-standing n-doped GaN substrates (threading dislocation density (TDD) 5x10$^7$ cm$^2$ ) from St. Gobain were used for the growths. The growth temperature was monitored by an optical pyrometer with readings calibrated against the melting point of Al. The In flux was kept constant at 2.25x10$^{-7}$ torr and Ga flux 5x10$^{-8}$ torr (sample 1) and 3.38x10$^{-8}$ (sample 2) torr for two different samples. The growth temperature was 550°C for both of the cases. High-resolution X-ray diffractometer (XRD) scans were done to verify the thicknesses and compositions of epitaxial layers. The In-composition as well as the optical quality of the InGaN films is also assessed by room temperature photoluminescence PL measurements. All measurements were done at room temperature.
Surface morphologies of InGaN samples were observed by atomic force microscopy (AFM).

![Graph showing XRD measurement of sample 1](image)

**Figure 48 XRD measurement of the sample 1**

Fig. 48 shows the XRD of the sample 1. By fitting the measurement data to the theoretical curve, the 45 minutes of InGaN growth gave 72 nm of fully strained InGaN, and the In composition was 18%. PL measurement was done for confirming the InGaN material properties (fig. 49). The InGaN peak wavelength was at 469 nm (2.64 eV) and full width half maximum of the peak (FWHM) was 21 nm which shows good quality of the InGaN layer. The peak at 725 nm was the second harmonic peak of GaN. By applying
bowing parameter of 1.65 [119][120], the In composition of sample 1 was 18.8 which matched the result from the XRD measurement.

![Graph](image)

Figure 49 The PL measurement of the sample 1

The other sample (sample 2) was also measured by both XRD (fig. 50) and PL (fig. 51) measurements to characterize the In composition. By fitting the measurement data to the theoretical curve, the 45 minutes of InGaN growth gave 50 nm of fully strained InGaN, and the In composition was 20%. The PL wavelength peak of InGaN was at 477 nm (2.6 eV) giving the 20% In composition which was also consistent to the XRD result.
Figure 50 The XRD measurement of sample 2
The surface morphology for both sample 1 and 2 were investigated by the AFM measurements. The upper image of fig. 52 shows the smooth surface in sample 1 with RMS roughness of 0.32 nm. Similarly, smooth surface with RMS roughness of 0.21 nm was also observed in the sample 2. From the XRD, PL and AFM measurements, high qualities of high composition InGaN were successfully grown.
Figure 52 The AFM images of (upper) sample 1 and (lower) sample 2
4.1.2 Energy band line-up of Al2O3/InGaN

To understand the energy band line-up of Al2O3/InGaN, MIS diodes with different Al2O3 thickness in sample 1 (18% InGaN) were made. Before Al2O3 deposition, solvent clean (acetone/isopropanol/DI water) was carried out followed by HCl dip for 10 minutes. 15 nm, 20 nm and 25 nm ALD Al2O3 layers were deposited respectively at 300 ºC with trimethylaluminum (TMA) and water as precursors. The Al2O3 growth was started with five times of water pulses (0.1 second for each pulse) and followed by TMA and water pulse cycles. After the Al2O3 deposition, we used ellipsometry (Woollam alpha-SE Spectroscopic Ellipsometer) to confirm the Al2O3 thickness. Large area Ti/Au/Ni ohmic contacts and Ni/Au/Ni gate contacts were defined by photolithography and deposited by e-beam evaporator. The C-V (1 MHz) and current-voltage (I-V) characteristics of Ni/Al2O3/In0.18Ga0.82N diodes were measured using Agilent B1500 semiconductor device analyzer equipped with medium power source/monitor units (MPSMUs) and multi frequency capacitance measurement unit (MFCMU).
Fig. 53 Two terminal Ig-Vg characteristics of Al₂O₃/In₀.₁₈Ga₀.₈₂N diodes

Fig. 53 demonstrates two terminal I-V characteristics of the MIS diodes. Low reverse gate current was observed in all three samples showing that excellent insulating quality of ALD Al₂O₃ layers. Fig. 54 (a) shows the C-V characteristics of 15 nm, 20 nm and 25 nm Al₂O₃/In₀.₁₈Ga₀.₈₂N diodes. The carrier density profiles (fig. 54 b) derived from C-V by the equation 1 shows 2x10¹⁹ cm⁻³ of back ground doping density (n_D) in the In₀.₁₈Ga₀.₈₂N substrate and the thickness of Al₂O₃ layers.

\[ n_D = \frac{-2}{q \varepsilon_{Al_2O_3} \left[ d \left( \frac{1}{C^2} \right) / dV \right]} \]  

(1)

\[ x_D = \frac{\varepsilon_{Al_2O_3}}{C} \]

where \( \varepsilon_{Al_2O_3} \) is the Al₂O₃ permittivity and \( x_D \) is the depletion region width.
Figure 54 (a) C-V profiles of the Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N diodes. (b) The carrier density profiles derived from C-V

The conduction band diagram of Ni/Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N MIS structure is shown in the fig. 55 (a). The flat band voltage ($V_{FB}$) in the In$_{0.18}$Ga$_{0.82}$N for each of the Al$_2$O$_3$ thickness was determined from the first derivative of capacitance verses gate bias (fig. 55 b). The shift of the flat-band voltage as a function of Al$_2$O$_3$ thickness is a clear indication of charges either at the interface or in the gate dielectric. A simple analytical expression relating the applied flat band gate voltage to the interfacial parameters can be derived as

$$qV_{gi} = -qF_{ox}t_{ox} + (\varphi_b - \Delta E_c - \varphi_s) \quad (2)$$

where $\varphi_b$ is the Ni/Al$_2$O$_3$ conduction band barrier height, $F_{ox}$ the electric field in the oxide, $\varphi_s$ is the energy difference between conduction band and Fermi level in In$_{0.18}$Ga$_{0.82}$N, $\Delta E_c$ is the conduction band offset between Al$_2$O$_3$ and In$_{0.18}$Ga$_{0.82}$N, and $V_{gi}$ is the flat band gate bias for Al$_2$O$_3$ thickness $t_{ox}$. From C-V measurements, the $V_{FB}$ extracted was

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found to vary linearly with oxide thickness, confirming the validity of equation 2 (fig. 55 c) and indicating that the charge was distributed as a sheet, rather than throughout the oxide. Since the flat band voltage dependence on Al$_2$O$_3$ thickness is linear, the electric field in the oxide can be assumed to be independent of the oxide thickness, indicating the absence of a significant density of bulk oxide charges. From equation 2, the slope of this curve gives the field in the oxide under flat band conditions in the semiconductor, while the intercept can be used to determine the conduction band offset $\Delta E_c$. According to the analytical expression of the linear fit reported in the fig. 55 (b), the electric field dropping across the oxide ($F_{ox}$) at flat-band is 4.7 MV/cm and the band offset (given by $\varphi_b - \Delta E_c - \varphi_s$) is 0.33 eV. $\varphi_s$ is estimated close to zero using the doping density in In$_{0.18}$Ga$_{0.82}$N, determined from C-V profiling, and the Ni/Al$_2$O$_3$ conduction band barrier height $\varphi_b$ was estimated to be 3 eV from internal photoemission measurements$^{21}$. Therefore, the Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N conduction band offset $\Delta E_c$ is found to be 2.67 eV. Using $F_{ox}$ at the Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N interface, we estimate a net sheet charge density of $+2.3 \times 10^{13}$ cm$^{-2}$ which is larger than in the Al$_2$O$_3$/GaN interface (section 3.2.2). These positive interface charges leading to threshold voltage shift and remote impurity scattering bring significant impact in MOS devices$^{24}$. Post metallization anneal (PMA) and oxygen plasma treatments were used to mitigate interface charges efficiently which was discussed in the chapter 3. This experiment provides important information of both energy band alignment and interface property at Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N for future device design.
Figure 55 (a) The conduction band diagram of Ni/Al₂O₃/In₀.₁₈Ga₀.₈₂N MIS structure. (b) The first derivative of capacitance versus gate bias. (c) The flat band voltage in InGaN versus oxide thickness.
Excellent quality of high composition In-polar InGaN grown by MBE was demonstrated. A quantitative analysis of the ALD Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N interface was also shown in this study. Up to 20% of bulk InGaN with smooth surface was analyzes by XRD, PL and AFM measurements. Our experimental investigation shows that the ALD Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N heterointerface has a conduction band offset $\Delta E_c$ of 2.67 eV. A net sheet charge density of $2.3 \times 10^{13}$ cm$^{-2}$ was observed at the Al$_2$O$_3$/ In$_{0.18}$Ga$_{0.82}$N interface. Both of the analysis of InGaN growth and investigation of the Al$_2$O$_3$/In$_{0.18}$Ga$_{0.82}$N interface are important in future device development.

4.2 Energy band line-up of ALD Al$_2$O$_3$ on high composition AlGaN

E-mode Al$_2$O$_3$/AlGaN/GaN MISHEMT has been paid wide attention due to the high electron mobility, high breakdown performance and for compatibility with existing gate drive circuits. However, unlike SiO$_2$/Si interface which has excellent interface property [121][122][123][124], large number of trap density at Al$_2$O$_3$/AlGaN interface [125][126][127][128][129][130][65] leads to large hysteresis in E-mode operation. Several solutions have been proposed to solve the problems including optimization of the gate etch, change to other dielectrics or anneal treatment [94][86][131]. Nevertheless, since Al$_2$O$_3$/AlGaN/GaN MISHEMT possesses two interfaces, it is inevitable for electrons in the channel tunnel through the AlGaN barrier and see the Al$_2$O$_3$/AlGaN interface while the positive gate bias is applied. Fig. 56 (a) shows the energy band diagram of standard Al$_2$O$_3$/AlGaN/GaN MISHEMT in the positive gate bias operation. The energy barrier of Al$_2$O$_3$/AlGaN interface is able to block the electrons which could
be captured in the trap states. To solve this intrinsic problem, reduction or even eliminate the energy barrier of dielectric/III-Nitride interface is needed (Fig 56 b). ALD Al$_2$O$_3$ on high composition AlGaN or AlN theoretically has smaller ΔEc.

![Figure 56 Energy band diagrams of (a) Standard Al$_2$O$_3$/AlGaN/GaN MISHEMT and (b) On the other hand, to achieve higher threshold voltage (> 3V) in III-Nitride power switching application with higher breakdown voltage, AlGaN channel MISHEMT was proposed to replace GaN channel due to lower electron affinity or higher Schottky-barrier height at the gate, and its wider bandgap [132]. A high composition AlGaN or AlN is needed for the cap layer in AlGaN channel MISHEMT. Therefore, it is important to find out energy band line-up of Al$_2$O$_3$ on high composition AlGaN. In this section, we demonstrate the energy band line-up of ALD Al$_2$O$_3$ on Al$_{0.7}$/Ga$_{0.3}$N. Interface charges are also quantitatively investigated.

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4.2.1 Experimental details

MIS diodes with different Al$_2$O$_3$ thickness in n-doped 70% AlGaN substrate provided by Sandia National Labs were made. Before Al$_2$O$_3$ deposition, solvent clean (acetone/isopropanol/DI water) was carried out followed by HF dip for 10 minutes. A 50 nm ALD Al$_2$O$_3$ layer was deposited at 300 °C with trimethylaluminum (TMA) and water as precursors. The Al$_2$O$_3$ growth was started with five times of water pulses (0.1 second for each pulse) and followed by TMA and water pulse cycles. After the Al$_2$O$_3$ deposition, we used ellipsometry (Woollam alpha-SE Spectroscopic Ellipsometer) to confirm the Al$_2$O$_3$ thickness. To obtain different Al$_2$O$_3$ thickness in the same Al$_{0.7}$/Ga$_{0.3}$N substrate, inductively coupled plasma reactive ion etching (ICP-RIE) with 30 W RIE power and 50 sccm BCl$_3$ was applied. The etched Al$_2$O$_3$ thickness was confirmed by both AFM profile and capacitance-voltage (C-V) measurements which showed 40 nm, 30 nm, 20 nm and 10 nm of Al$_2$O$_3$ with smooth surface. Large area Al/Ni/Au ohmic contacts and Ni/Au/Ni gate contacts were defined by photolithography and deposited by e-beam evaporator. The C-V (1 MHz) and current-voltage (I-V) characteristics of Ni/Al$_2$O$_3$/Al$_{0.7}$/Ga$_{0.3}$N diodes were measured using Agilent B1500 semiconductor device analyzer equipped with medium power source/monitor units (MPSMUs) and multi frequency capacitance measurement unit (MFCMU).
4.2.2 Energy band line-up of $\text{Al}_2\text{O}_3/\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$

Figure 57 (a) C-V characteristics of 10 nm, 20 nm, 30 nm, 40 nm and 50 nm $\text{Al}_2\text{O}_3/\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$ diodes. (b) Band diagram of Ni/$\text{Al}_2\text{O}_3/\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$ MIS structure.
Fig. 57 (a) shows the C-V characteristics of 10 nm, 20 nm, 30 nm, 40 nm and 50 nm Al$_2$O$_3$/Al$_{0.7}$Ga$_{0.3}$N diodes. The carrier density profiles derived from C-V by the equation 1 shows $4 \times 10^{18}$ cm$^{-3}$ of n-doping density ($n_D$) in the Al$_{0.7}$/Ga$_{0.3}$N substrate and the thickness of Al$_2$O$_3$ layers.

$$n_D = \frac{-2}{q \varepsilon_{Al_2O_3} \left[ d \left( \frac{1}{C^2} \right) / dV \right]}$$  \hspace{1cm} (1)

$$x_D = \frac{\varepsilon_{Al_2O_3}}{C}$$

where $\varepsilon_{Al_2O_3}$ is the Al$_2$O$_3$ permittivity and $x_D$ is the depletion region width. The conduction band diagram of Ni/Al$_2$O$_3$/Al$_{0.7}$Ga$_{0.3}$N metal-oxide-semiconductor (MOS) structure is shown in the fig. 57 (b). The flat band voltage ($V_{FB}$) in the Al$_{0.7}$/Ga$_{0.3}$N for each of the Al$_2$O$_3$ thickness was determined from the first derivative of capacitance verses gate bias (fig. 58 a). The shift of the flat-band voltage as a function of Al$_2$O$_3$ thickness is a clear indication of charges either at the interface or in the gate dielectric. A simple analytical expression relating the applied flat band gate voltage to the interfacial parameters can be derived as

$$qV_{gi} = -qF_{Ox}t_{ox} + (\varphi_b - \Delta E_C - \varphi_s)$$  \hspace{1cm} (2)

where $\varphi_b$ is the Ni/Al$_2$O$_3$ conduction band barrier height, $F_{Ox}$ the electric field in the oxide, $\varphi_s$ is the energy difference between conduction band and Fermi level in Al$_{0.7}$/Ga$_{0.3}$N, $\Delta E_C$ is the conduction band offset between Al$_2$O$_3$ and Al$_{0.7}$/Ga$_{0.3}$N, and $V_{gi}$ is the flat band gate bias for Al$_2$O$_3$ thickness $t_{ox}$. From C-V measurements, the $V_{FB}$ extracted was found to vary linearly with oxide thickness, confirming the validity of equation 2 (fig. 58 b) and
indicating that the charge was distributed as a sheet, rather than throughout the oxide. Since the flat band voltage dependence on $\text{Al}_2\text{O}_3$ thickness is linear, the electric field in the oxide can be assumed to be independent of the oxide thickness, indicating the absence of a significant density of bulk oxide charges. From equation 2, the slope of this curve gives the field in the oxide under flat band conditions in the semiconductor, while the intercept can be used to determine the conduction band offset $\Delta E_c$. According to the analytical expression of the linear fit reported in the fig. 58 (b), the electric field dropping across the oxide ($F_{\text{ox}}$) at flat-band is 0.5 MV/cm and the band offset (given by $\varphi_b - \Delta E_c - \varphi_s$) is 2.0 eV. $\varphi_s$ is estimated as 5 meV using the doping density in $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$, determined from C-V profiling, and the Ni/$\text{Al}_2\text{O}_3$ conduction band barrier height $\varphi_b$ was estimated to be 3 eV from internal photoemission measurements [133]. Therefore, the $\text{Al}_2\text{O}_3$/ $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$ conduction band offset $\Delta E_c$ is found to be 1 eV. Using $F_{\text{ox}}$ at the $\text{Al}_2\text{O}_3$/ $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$ interface, we estimate a net sheet charge density of $+2.5 \times 10^{12}$ cm$^{-2}$. Similar to the previous study of $\text{Al}_2\text{O}_3$/GaN interface, these positive interface charges leading to threshold voltage shift and remote impurity scattering bring significant impact in MOS devices [86]. Post metallization anneal (PMA) and oxygen plasma treatments can be used to mitigate interface charges efficiently [94][131] in this case.
Figure 58 (a) First derivative of capacitance verses gate bias. (b) $V_{FB}$ in AlGaN versus oxide thickness
A quantitative analysis of the ALD Al$_2$O$_3$/Al$_{0.7}$Ga$_{0.3}$N interface was shown in this study. A conduction band offset $\Delta E_c$ of 1 eV of the ALD Al$_2$O$_3$/Al$_{0.7}$Ga$_{0.3}$N heterointerface was investigated. A sheet charge density of $2.5 \times 10^{12}$ cm$^{-2}$ was observed at the Al$_2$O$_3$/ Al$_{0.7}$Ga$_{0.3}$N interface. The understanding of Al$_2$O$_3$/Al$_{0.7}$Ga$_{0.3}$N energy band alignment is useful for the design of low hysteresis GaN-based MIHEMT and AlGaN channel MISHEMT for power switching applications.

4.3 Energy band line-up of ALD Al$_2$O$_3$ on Ga$_2$O$_3$

$\beta$-Gallium oxide ($\beta$-Ga$_2$O$_3$) is one of the promising material systems for applications of power switching [134][135] and UV detectors [136][137] due to a high breakdown electric field of 8 MV/cm and a wide bandgap of 4.7-4.9 eV in $\beta$-Ga$_2$O$_3$ [138][139][140]. Controllable doping in $\beta$-Ga$_2$O$_3$ from semi-insulating to n-type concentration of $10^{19}$ cm$^{-3}$ has been demonstrated which provides flexibility for device design [141][142][143][144]. The bulk electron mobility of $\beta$-Ga$_2$O$_3$ is estimated to be 300 cm$^2$V$^{-1}$s$^{-1}$ for carrier densities in the range of $10^{15}$-$10^{16}$ cm$^{-3}$ [145], and the Baliga figure of merit for $\beta$-Ga$_2$O$_3$ is more than four times larger than that for other technologies such as GaN and SiC [145]. An important advantage of $\beta$-Ga$_2$O$_3$ is that it can be grown in bulk crystal form by relatively inexpensive float-zone (FZ) edge-defined film-fed growth (EFG) and Czochralski (CZ) methods, and in epitaxial thin films by molecular beam epitaxy [146][147][148][149]. The availability of bulk semiconductor crystals is important for future commercial utilization that would benefit from low defect density and large area bulk crystals.
The demonstration of β-Ga$_2$O$_3$ depletion-mode metal-oxide-semiconductor field effect transistors (MOSFETs) on single crystal β-Ga$_2$O$_3$ on-off ratio over ten orders of magnitude at room temperature has been reported$^2$. Atomic layer deposited (ALD) Al$_2$O$_3$, which has larger bandgap (~8.8 eV) [73] and conformal coverage, was used as gate dielectric to efficiently suppress gate leakage [135][73][94]. However, the band offset and other electrical properties of ALD Al$_2$O$_3$/ β-Ga$_2$O$_3$ interfaces have not been investigated in detail. In this work, we quantitatively investigated conduction band offset (ΔEc) and interface fixed charges in Al$_2$O$_3$/β-Ga$_2$O$_3$, following methods used previously for ALD Al$_2$O$_3$/III-Nitride interfaces which led to experimental determination of the conduction band offset (ΔEc) and existence of interface fixed charges [73][94][150].

### 4.3.1 Experimental details

Edge-defined film-fed growth (EFG) method [147], which uses a die to define thickness of β-Ga$_2$O$_3$ to avoid the cutting process, was used for the bulk Sn-doped β-Ga$_2$O$_3$ growth. The X-ray diffraction (XRD) pattern of bulk β-Ga$_2$O$_3$ (fig. 59 a) demonstrates the sharp (-201) and (-402) β-Ga$_2$O$_3$ peaks while atomic force microscope (AFM) scans (fig. 59 b) show smooth surface morphology (roughness = 0.13 nm). In our experiment, we used n-type β-Ga$_2$O$_3$ wafers with a polished surface to investigate the band offsets. Before Al$_2$O$_3$ deposition, solvent clean (acetone/isopropanol/DI water) was carried out followed by HF dip for 10 minutes. A 50 nm ALD Al$_2$O$_3$ layer was deposited at 300 ºC with trimethylaluminum (TMA) and water as precursors. The Al$_2$O$_3$ growth was started with five times of water pulses (0.1 second for each pulse) and followed by TMA
and water pulse cycles. After the Al₂O₃ deposition, we used ellipsometry (Woollam alpha-SE Spectroscopic Ellipsometer) to confirm the Al₂O₃ thickness.

Figure 59 (a) XRD pattern of bulk β–Ga₂O₃. (b) AFM image of β–Ga₂O₃ surface. (c) AFM profile of 38 nm dry-etched ALD Al₂O₃.

To obtain different Al₂O₃ thickness in the same β-Ga₂O₃ substrate, inductively coupled plasma reactive ion etching (ICP-RIE) with 30 W RIE power and 50 sccm BCl₃ was applied. The etched Al₂O₃ thickness was confirmed by both AFM profile (fig. 59 c) and capacitance-voltage (C-V) measurements which showed 32 nm and 12 nm of Al₂O₃ with smooth surface. Large area Ti/Au/Ni ohmic contacts Ni/Au/Ni gate contacts were defined by photolithography and deposited by e-beam evaporator. The C-V (1 MHz) and current-voltage (I-V) characteristics of Ni/Al₂O₃/β-Ga₂O₃ diodes were measured using Agilent B1500 semiconductor device analyzer equipped with medium power
source/monitor units (MPSMUs) and multi frequency capacitance measurement unit (MFCMU).

4.3.2 Energy band line-up of Al₂O₃/Ga₂O₃

Figure 60 (a) C-V profile for Al₂O₃/β–Ga₂O₃ and carrier density profile (inset) derived from C-V. (b) Energy band structure of Ni/Al₂O₃/β–Ga₂O₃ diodes.

Fig. 60 (a) shows the C-V characteristics of 12 nm, 32 nm and 50 nm Al₂O₃/β-Ga₂O₃ diodes. The carrier density profiles (fig. 60 a inset) derived from C-V by the equation 1 shows 6x10¹⁸ cm⁻³ of Sn doping density (n₀) in the β-Ga₂O₃ substrate and the thickness of Al₂O₃ layers.
where $\varepsilon_{\text{Al}_2\text{O}_3}$ is the Al$_2$O$_3$ permittivity and $x_D$ is the depletion region width. The conduction band diagram of Ni/Al$_2$O$_3$/β-Ga$_2$O$_3$ metal-oxide-semiconductor (MOS) structure is shown in the fig. 60 (b). The flat band voltage ($V_{\text{FB}}$) in the β-Ga$_2$O$_3$ for each of the Al$_2$O$_3$ thickness was determined from the first derivative of capacitance verses gate bias (fig. 61 a). The shift of the flat-band voltage as a function of Al$_2$O$_3$ thickness is a clear indication of charges either at the interface or in the gate dielectric. A simple analytical expression relating the applied flat band gate voltage to the interfacial parameters can be derived as

$$qV_{gi} = -qF_{\text{ox}}t_{\text{oxi}} + (\varphi_b - \Delta E_C - \varphi_S) \quad (2)$$

where $\varphi_b$ is the Ni/Al$_2$O$_3$ conduction band barrier height, $F_{\text{ox}}$ the electric field in the oxide, $\varphi_s$ is the energy difference between conduction band and Fermi level in β-Ga$_2$O$_3$, $\Delta E_C$ is the conduction band offset between Al$_2$O$_3$ and β-Ga$_2$O$_3$, and $V_{gi}$ is the flat band gate bias for Al$_2$O$_3$ thickness $t_{\text{oxi}}$. From C-V measurements, the $V_{\text{FB}}$ extracted was found to vary linearly with oxide thickness, confirming the validity of equation 2 (fig. 61 b) and indicating that the charge was distributed as a sheet, rather than throughout the oxide. Since the flat band voltage dependence on Al$_2$O$_3$ thickness is linear, the electric field in the oxide can be assumed to be independent of the oxide thickness, indicating the absence of a significant density of bulk oxide charges. From equation 2, the slope of this curve
gives the field in the oxide under flat band conditions in the semiconductor, while the intercept can be used to determine the conduction band offset $\Delta E_c$. According to the analytical expression of the linear fit reported in the fig. 61 (b), the electric field dropping across the oxide ($F_{ox}$) at flat-band is 0.7 MV/cm and the band offset (given by $\varphi_b - \Delta E_c - \varphi_s$) is 1.3 eV. $\varphi_s$ is estimated as 5 meV using the doping density in $\beta$-Ga$_2$O$_3$, determined from C-V profiling, and the Ni/Al$_2$O$_3$ conduction band barrier height $\varphi_b$ was estimated to be 3 eV from internal photoemission measurements[133]. Therefore, the Al$_2$O$_3$/β-Ga$_2$O$_3$ conduction band offset $\Delta E_c$ is found to be 1.7 eV. This offset is different from the offset predicted by the electron affinity difference between ALD Al$_2$O$_3$ (2.5 eV) [151] and β-Ga$_2$O$_3$ (4 eV) [152]. The deviation from the electron affinity rule[153]$^{29}$ may be due to interfacial charge and mid-gap state effect [153][154], but a detailed analysis of this is beyond the scope of the paper. Using $F_{ox}$ at the Al$_2$O$_3$/β-Ga$_2$O$_3$ interface, we estimate a sheet fixed charge density of $+3.6 \times 10^{12}$ cm$^{-2}$. In Al$_2$O$_3$/III-nitride interface, a large number of fixed charges ($> 2\times10^{13}$ cm$^{-2}$) were found [73][94][150]. These positive interface charges leading to threshold voltage shift and remote impurity scattering bring significant impact in MOS devices [86]. Post metallization anneal (PMA) and oxygen plasma treatments were used to mitigate interface charges efficiently [94][131] in the III-nitride system, and may lead to similar effects in the oxide system.
Figure 61 (a) First derivation of capacitance versus gate bias of 50 nm, 32 nm and 12 nm Al$_2$O$_3$/$\beta$–Ga$_2$O$_3$ diode. (b) Linear relationship of flat band voltage and Al$_2$O$_3$ thickness for Al$_2$O$_3$/$\beta$–Ga$_2$O$_3$ diodes.

4.3.3 I-V characteristics and tunneling mechanism

To analyze forward I-V characteristics, several mechanisms were used in ALD-Al$_2$O$_3$/AlGaN/GaN metal-insulator-semiconductor high electron mobility transistors (MISHEMTs) [55]. At T>0$^\circ$C, Trap-assisted tunneling (TAT) was found to be dominant for the forward gate current transport. In the Al$_2$O$_3$/$\beta$-Ga$_2$O$_3$ diodes, the TAT model was used to analyze the forward I-V characteristics. Fig. 62 (a) shows the I-V characteristics of Ni/Al$_2$O$_3$/$\beta$-Ga$_2$O$_3$ diodes. The forward turn-on voltages are 2 V, 3 V and 5 V with respect to the 12 nm, 32 nm and 50 nm Al$_2$O$_3$/$\beta$-Ga$_2$O$_3$ diodes. The current density of TAT ($J_{TNT}$) is given by:

\[ V_{FB} = 1.3 - 0.07x \]
where $m_{ox}^* = 0.16 \, m_0$ [150] is the effective electron mass in ALD Al$_2$O$_3$, $q$ is the electron charge, $h$ is the Planck’s constant, $E_{ox}$ is the electrical field in the Al$_2$O$_3$, and $\phi_t$ is the trap energy level. The TAT plot [ln$(J_{TAT})$ vs. $1/ E_{ox}$] is shown in fig. 62 (b) and energy band structure during forward turn-on is shown in the inset of fig. 62 (b). The extracted trap energy level ($\phi_t$) is 1.1 eV. These interface traps are able to assist forward tunneling, but may also possibly act as donor states which form positive interface fixed charges. Further interface analysis needs to be done to confirm the role of the interface traps.

$$J_{TAT} \propto \exp\left(-\frac{8\pi \sqrt{2qm^*_{ox}} \phi_t^{3/2}}{3hE_{ox}}\right)$$

Figure 62 (a) I-V characteristics of Ni/Al$_2$O$_3$/β–Ga$_2$O$_3$ diodes. (b) Trap-assisted-tunneling (TAT) plot of the experimental (symbols) and fitted (lines) forward I-V characteristics. (inset) Schematic of trap-assisted-tunneling at forward turn-on.
In conclusion, a quantitative analysis of the ALD Al₂O₃/β-Ga₂O₃ interface was demonstrated. High quality of β-Ga₂O₃ grown by EFG method with 6x10¹⁸ cm⁻³ of Sn doping density was used in this study. Our experimental investigation shows that the ALD Al₂O₃/β-Ga₂O₃ heterointerface has a conduction band offset ΔEₜ of 1.7 eV. A fixed sheet charge density of 3.6 x 10¹² cm⁻² was observed at the Al₂O₃/β-Ga₂O₃ interface. Trap-assisted tunneling model is used to analyze the forward I-V characteristics which show a dominant trap energy level at 1.1 eV. The investigation of the dielectric semiconductor interface for Al₂O₃/β-Ga₂O₃ junctions could be important in future device development based on the β-Ga₂O₃.

4.4 Summary

In this chapter, we studied interface properties of ALD Al₂O₃ on high composition InGaN, high composition AlGaN and Ga₂O₃. MOS devices with high composition InGaN is attractive for high frequency application due to high electron velocity while high composition AlGaN and Ga₂O₃ are promising for power switching application. The energy band offset ΔEₜ of Al₂O₃/In₀.₁₈Ga₀.₈₂N, Al₂O₃/Al₀.₇Ga₀.₃N and Al₂O₃/β-Ga₂O₃ was found to be 2.67 eV, 1 eV and 1.1 eV, respectively. Interface charges in these materials were also observed (2.3 x 10¹³ cm⁻², 2.5 x 10¹² cm⁻² and 3.6 x 10¹² cm⁻² for Al₂O₃ on In₀.₁₈Ga₀.₈₂N, Al₀.₇Ga₀.₃N and β-Ga₂O₃, respectively). Techniques of interface charge engineering developed in the previous chapter could be useful to improve the device characteristics. This information gave us a guide line for the device design and performance optimization in the future.
Chapter 5
Conclusions and future work

5.1 Conclusions

To achieve high performance and low gate leakage of both D-mode and E-mode GaN-based HEMT for power switching application, atomic layer deposited Al₂O₃ with high dielectric constant and wide bandgap was applied to the GaN HEMT. The energy band line-up and interface properties were firstly investigated. The energy band offset (Δₐ鸁) between ALD Al₂O₃ and different polarities of GaN (Ga-polar, N-polar and non-polar) were observed as 2.1 eV. A very high positive interface fixed charge density (larger than 2x10¹³ cm⁻²) was found at Al₂O₃/III-Nitride interface. These positive fixed charges could induce electrical field in the oxide thus increase the reverse gate current leakage, but also prevent the normally-off operation by shifting the threshold to negative making E-mode device fabrication more challenging. The effect of interface charges on electron mobility in MISHEMT was theoretically studied. The remote impurity scattering was used as the model in the calculation along with other scattering mechanisms such as phonon scattering, dislocation scattering, dislocation strain field and surface roughness scattering. Our calculation results showed that the electron mobility in the MISHEMT degraded substantially as the Al₂O₃/III-Nitride interface charge density was greater than
5x10^{12} \text{ cm}^{-2} \text{ and } 2\text{DEG density less than } 5x10^{12} \text{ cm}^{-2}. \text{ Furthermore, remote impurity scattering could affect electron mobility exponentially when we vertically scale down MISHEMT. Therefore, finding a method to efficiently reduce the positive fixed charges became very critical.}

Comprehensive study of interface charge engineering was then investigated. Post metallization anneal (PMA) was firstly proposed to suppress the interface charges. Higher temperature of PMA, up to 550°C, showed that the interface net charge density was reduced to less than 1x10^{12} \text{ cm}^{-2}. The two-terminal I-V characteristics showed lower reverse gate current after PMA indicating reduction of interface fixed charges as well. However, PMA had only limited effect on Al_{2}O_{3}/AlGaN interface. Therefore, oxygen plasma treatment was another approach for interface charge engineering. Investigated from the XPS measurement, the oxygen plasma efficiently oxidized the AlGaN surface enabling to neutralize the Ga dangling bonds which act as donor states. This Ga-O bond was stable observed by XPS analysis after long term and thermal stress. The C-V measurement in both of the non-recessed and recessed MISHEMT showed positive shift of the flat band voltages after oxygen plasma treatment. Interface net charge density which was extracted by fitting the theoretical C-V curve to the experiment was suppressed to -1x10^{13} \text{ cm}^{-2} after the combination of PMA and oxygen plasma treatments.

The drift mobility versus 2DEG density in the MISHEMT was experimentally investigated showing that the electron mobility recovered after the treatments of PMA and oxygen plasma. An E-mode MISHEMT with 1.5 V of threshold voltage and 140 mA/mm of drain current density at 10V of gate bias was demonstrated by interface
charge engineering. The transfer characteristics of the oxygen plasma/PMA treated MISHEMT also showed stable threshold voltage after time dependent measurement.

The study of device optimization by interface charge engineering was done. We found the III-Nitride surface with photoresist exposure created more interface fixed charges; therefore a sacrificial layer was needed to protect the surface. By investigating the optimal characteristics of C-V hysteresis, interface fixed charge density and electron mobility, we found the best treatment window was 400°C PMA, PDA temperature below 500°C and with oxygen plasma. After comprehensively understanding the technology of interface charge engineering, lateral energy band engineering by patterning ALD was demonstrated. An E-mode MOSFET with 0.5 V of threshold voltage and 200 mA/mm of drain current density at 12 V of gate bias was fabricated by lateral energy band engineering. Other applications for both electronics and optoelectronics are also possibly achieved by this dielectric-assisted lateral band engineering technology.

By applying the knowledge from the Al₂O₃/III-Nitride interface study, Al₂O₃ on high composition InGaN, high composition AlGaN and Ga₂O₃ were characterized. High composition InGaN has low electron effective mass which is promising for high frequency device. Understanding the energy band line-up of Al₂O₃/InGaN is beneficial for the design of InGaN channel MOSFET/MISHEMT. Smooth 18% and 20% of InGaN were grown by the MBE. In compositions were confirmed by XRD and PL analysis. The Al₂O₃/InGaN ΔEₓ was found as 2.67 eV. High composition AlGaN could be useful as a cap layer to reduce the hysteresis in GaN MISHEMT, and also potential in AlGaN channel MISHEMT for even higher threshold voltage. The Al₂O₃/AlGaN ΔEₓ was found
as 2.67 eV. Ga$_2$O$_3$, which has high breakdown electric field of 8 MV/cm and a wide bandgap of 4.7-4.9 eV, is a very promising material for next generation power switching. Charactering the Al$_2$O$_3$/Ga$_2$O$_3$ interface property could be helpful for the design of MOS devices. We found the Al$_2$O$_3$/Ga$_2$O$_3$ $\Delta E_c$ was 1.7 eV. Mechanism of trap assisted tunneling was investigated by analyzing the forward gate current.

Comprehensive study of high-k dielectric enhanced III-Nitride devices and interface characterization were proposed in this dissertation. The information could be useful for the development of GaN based MISHEMT/MOSFET in power switching and high speed applications.

5.2 Future work

Improvement of high-k dielectric/III-Nitride interface properties makes various applications promising. Besides power switching, III-Nitride based high frequency device by integrating high-k dielectric can be a promising topic. Passivation study in GaN based MISHEMT is also very important for the improvement of the device performance. Lateral energy engineering could be further investigated in MISHEMT or other applications.

5.2.1 Ultra-thin HfO$_2$/Al$_2$O$_3$ stacks on III-Nitride

N-polar HEMT is promising for high frequency device because the top GaN cap layer can be highly scaled down for high transconductance without reducing 2DEG density. However, gate leakage becomes an issue with schottcky metal gate. Thin high-k
dielectric is able to directly solve the leakage problem without substantially sacrificing the device performance. Since post-metallization anneal and oxygen plasma treatments were found to optimize the Al₂O₃/III-Nitride surface, HfO₂, which has ultra high dielectric constant (~22 [155][155][156]), on Al₂O₃ dielectric stacks can be used as gate dielectric in N-polar MISHEMT. Different effective oxide thickness (EOT), which is the effective SiO₂ thickness giving the same capacitance, of HfO₂/Al₂O₃ stacks on Ga-polar GaN diodes have preliminarily studied. Fig. 63 shows the two terminal I-V characteristics of the diodes before and after 400°C PMA. Low reverse leakage which (below 10 μA/cm²) was observed with and without PMA. However, forward current turned on near the zero bias while the EOT was below 2.6 nm. C-V characteristics show 1.5 μF/cm² of accumulation capacitance was achieved with 1.3 nm of EOT (fig. 64). Further optimization of the ultra thin dielectric stacks is needed for high performance highly scaled N-polar MISHEMT.
Figure 63 The I-V characteristics of HfO$_2$/Al$_2$O$_3$ stacks on Ga-polar GaN diodes with different EOT before and after PMA.
Figure 64 The C-V characteristics of HfO$_2$/Al$_2$O$_3$ stacks on Ga-polar GaN diodes with different EOT.

5.2.2 Passivation study in GaN-based MISHEMT

In the previous study, we only discussed about ALD Al$_2$O$_3$ as gate dielectric. Dielectric/III-Nitrde interface property in the access region is also very important since
the trap dispersion is capable to impact device performance and reliability. Study of SiN passivation in GaN HEMT has been reported. Investigating different high-k dielectrics as passivation layers could be useful. Three terminal breakdown and pulse measurements can be done for the interface analysis. Effect of interface charge engineering such as PMA and oxygen plasma treatments can be also investigated. The study of high-k dielectric enhanced GaN-based MISHEMT could be more comprehensive by adding passivation analysis.

5.2.3 Recess-free E-mode MISHEMT by lateral energy band engineering

We discussed the lateral energy band engineering in the section 3.6. In the experiment, the alloy ohmic contacts were firstly made followed by ICP-RIE dry etch for the removal of the AlGaN layer; ALD Al₂O₃ then induced the 2DEG. However, ICP-RIE can always create some damage which affects the device performance. To achieve a recess-free MISHEMT by lateral charge engineering, ohmic contacts though the Al₂O₃ layer is needed. There are two possible directions to achieve that. The first method is to optimize the ohmic alloy which may be done by changing the metal stacks or anneal temperature. The other one would be the ohmic contact regrowth technology. The Al₂O₃ and GaN in the ohmic region could be removed first followed by the MBE growth of n+ GaN to make side contact. Once the ohmic contact technology is developed, not only E-mode MISHEMT but lateral n-p-n BJT could be possibly achieved by patterning the ALD.
5.2.4 High composition InGaN channel HEMT

High quality of high composition In-polar InGaN growth was introduced in the section 4.1. The study of Al₂O₃/InGaN diodes showed that the interface was pinned-free thus modulation was observed. High composition InGaN channel HEMT becomes very promising. In-polar AlGaN/InGaN HEMT could be firstly investigated. Hall measurement is able to give us sheet charge density and carrier mobility. Therefore we can optimize our material based on it along with XRD and PL characterizations. Saturation velocity of the InGaN channel HEMT could be obtained from the pulsed I-V measurement in the constrained channel width under high electrical field. Device characterization including I-V and C-V measurement can be analyzed after putting the gate. Study of N-polar InGaN channel could be done by similar material and electrical characterizations. ALD Al₂O₃ could be useful in the N-polar case to efficiently suppress the gate leakage. Interface optimization could be done later to achieve N-polar MISHEMT with better performance.

5.2.5 Theoretical model development for electron transport

As discussed in the section 3.5.3, our theoretical model including remote impurity scattering was not able to completely explain and predict the electron mobility in MISHEMT. To improve our model, firstly the Al₂O₃/AlGaN interface trap profile across the bandgap needs to be investigated to give precise interface charge density for the calculation. Furthermore, since we treated the interface fixed charges as sheet charges in the remote scattering model, effect of fixed charge’s Bohr radius could be an issue in the
highly scaled case. Fig. 65 shows the Bohr radius is the mean radius of the orbit of an electron around the nucleus of a hydrogen atom at its ground state. It can be expressed as

\[ a_0 = \frac{4\pi \varepsilon_0 \hbar^2}{m_e e^2} \]

where \( \varepsilon_0 \) and \( m_e \) are permittivity of free space and electron rest mass. It can be also applied to other materials by changing \( \varepsilon \) and \( m \). In the case of Al\(_2\)O\(_3\), \( m_{\text{Al}_2\text{O}_3} = 0.23 \, m_e \) and \( \varepsilon_{\text{Al}_2\text{O}_3} = 9 \, \varepsilon_0 \), so the Bohr radius of Al\(_2\)O\(_3\) is \( \sim 2 \) nm. To explain clearer, there is potential distribution surrounding the center of positive interface fixed charge (fig. 65). The mean radius of the potential well can be regarded as Bohr radius in Al\(_2\)O\(_3\).

![Figure 65 The schematic of potential distribution interface fixed charges.](image)

In the highly scaled GaN MISHEMT, the AlGaN/AlN cap is usually smaller than 4 nm. As a result, the remote scattering model may need to consider of the Bohr radius of fixed charges. On the other hand, the Fang-Howard 2DEG wavefunction used in our scattering model did not include the electron penetration into the AlGaN/AlN layer which is around 1.5 nm deep. Although it is a small portion compared to whole 2DEG distribution, it may be affected by interface charges in highly scaled case to reduce the mobility.
The improvement of our theoretical scattering model may be started from the Bohr radius of fixed charges and 2DEG distribution to make our calculated mobility more precisely.
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