Nitride Based Metal Insulator Semiconductor Heterostructure

Material and Device Design and Characterization

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Materials Science and Engineering

by

Jiechen Wu

2014
ABSTRACT OF THE DISSERTATION

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Doctor of Philosophy in Materials Science and Engineering

University of California, Los Angeles, 2014

Professor Dwight C. Streit, Chair

Al₂O₃/AlGaN/GaN metal-insulator-semiconductor-heterostructures (MISH) were designed, fabricated, and characterized. The effects of different dielectric deposition techniques, surface treatments, and post deposition treatments were investigated by comprehensive material and electrical characterization to understand the Al₂O₃ dielectric and Al₂O₃/AlGaN interfacial properties.

Thermal ALD and PEALD Al₂O₃ thin films were successfully deposited on MBE grown AlGaN/GaN layers. An XPS study reveals the band offset of Al₂O₃/AlGaN interface. In addition, pre-deposition treatments show a reduction of Ga-O bonds at the interface after ALD growth.

The fabrication of Al₂O₃/AlGaN/GaN MISH diodes were achieved with deposition of Ti/Al/Ni/Au ohmic contacts and Ni/Au gate contacts. C-V characterization of MISH diodes was applied to
evaluate Al$_2$O$_3$/AlGaN interface states. Traps with different energy levels were differentiated by C-V hysteresis curves and multi-frequency C-V. C-V analysis suggests that PEALD provides better film quality with lower defect densities than thermal ALD. The implementation of NH$_3$ and N$_2$ pre-deposition surface plasma treatment and N$_2$ post-deposition annealing can also improve interfacial properties.

Al$_2$O$_3$ dielectric thin film leakage current and conduction mechanisms were also studied by I-V characterization. PEALD Al$_2$O$_3$ thin films exhibit better leakage current suppression compared to thermal ALD films. Temperature dependent I-V characterization shows that Poole-Frenkel emission dominates in dielectric current transport at medium electric fields, while at high electric fields, Fowler-Nordheim tunneling and trap-assisted tunneling dominate at low and high temperatures, respectively. Various dielectric reliability tests were employed on Al$_2$O$_3$ thin films. The results of time dependent dielectric breakdown (TDDB) test can be fit into 1/E field dependent model and a Weibull slope of 2.87 is extracted for PEALD Al$_2$O$_3$ thin films. The dielectric breakdown field distribution statistics show that PEALD Al$_2$O$_3$ films have a larger average dielectric breakdown field than thermal ALD films, and the plasma N$_2$O post deposition annealing improves the average breakdown field. The improvements from integration of pre-deposition and post deposition treatments may offer a better device performance and reliability in MIS-HEMTs, and enable further progress and development of nitride based power electronics.
The dissertation of Jiechen Wu is approved.

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2014
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Acknowledgements

I would like to express my gratitude to all the people who have helped and supported me during my Ph.D. research. It is my luck to have these nice people around for four years. They encourage me to pursue my career, inspire me with their knowledge and experience, and help me out when difficulties came. The Ph.D. life also taught me to be a good collaborator and team-worker. Without these efforts spent together, it would be much harder to accomplish my journey in the academic research.

I would like to give my special thanks to my advisor, Professor Dwight Streit. He has been always supportive to my research. As a successful professional in semiconductor industry, he not only guides me on my research, but also broadens my vision to the entire industry. I have learned more than enough from him in terms of interpersonal skills, communication skills and problem-solving skills. His great personality will always be an excellent example to me. I would also like to thank Professor Mark Goorsky, Professor Jane Chang and Professor Oscar Stafsudd for being on my thesis committee and providing precious opinions and comments to my research.

As the first member in my research group, I cannot build my lab and start my research without other students’ help. I want to thank Charles Reyner and Pradeep Senanayake for helping me with the measurement setups. I also want to thank Jeff Mckay and Xiaolu Kou for the X-ray measurements and discussions. I am thankful to my labmates, Shenglin Ye, Xiaoxing Lu and Jinhee Park for all the help and support on my work. It was a pleasure working with all these guys together at UCLA.

Last but not least, I am deeply grateful to my parents, my family, and my girlfriend, Wei Hu. They have always stood behind me and firmly supported me. I truly appreciate their love and dedication.
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Chapter 1 Introduction

1.1 Motivation

With the continuous development of power conversion technology and rapid growth of wireless communication market, high power and high frequency transistors are arousing significant interests for emerging applications.

The expectation for modern power transistors becomes higher and higher as new technologies are boosted up rapidly. The next generation mobile phone needs a wider bandwidth. The receiver requires a lower noise while maintaining a high gain. The broadband wireless internet connection and TV broadcasting require a higher frequency for faster data transmission. The traditional power switch and diode also need to improve power handling and minimize energy loss, and therefore achieve a higher efficiency [1], [2].

To summarize, modern power semiconductor devices require higher efficiency, better power handling, lower noise and wider bandwidth. Due to these demands, significant research efforts and investments have been made to develop high power and high frequency transistors. And it has been found that GaN based power devices are the solution to this problem.

1.2 GaN

Gallium Nitride (GaN) is considered one of the most important semiconductor materials after silicon. It has three possible structures: wurtzite, zinc blende and rock salt. Among them, wurtzite structure is thermodynamically favorable under ambient atmosphere. The wurtzite GaN is constructed from two interpenetrating hexagonal close packed structures of gallium and nitrogen
atoms displaced from each other by 3/8 c. The typical 2H type structure material has very strong polar bonds because of strong electronegativity of nitrogen atoms.

GaN is a perfect candidate in high power transistor domain. It possesses supreme electronic properties such as wide bandgap (3.42eV), excellent electron saturation velocity ($2.7 \times 10^7$ cm/s), good electron mobility (2000 cm$^2$/Vs), high 2 dimensional electron gas (2DEG) density ($10^{13}$ cm$^{-2}$), high breakdown field ($3.3 \times 10^6$ V/cm) and good thermal conductivity (170 W/mK). Table 1-1 shows a comparison of electronic properties of four widely used power transistor materials from high power device perspective. There is no doubt that GaN owns excellent properties compared to other semiconductor materials. Table 1-2 lists Baliga’s figure of merit and Johnson’s figure of merit, two calculated parameters based on material properties such as electron saturation velocity and breakdown field, which are normally used for high power and high frequency transistors comparison [2]. An intuitive comparison of device properties can be reflected on the following graph (figure 1-1). At the regime that requires both high power and high frequency operating, the GaN transistor owns unique advantages and few techniques can compete with it.
Table 1-1 Semiconductor material properties at high frequency and high power operation.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Si (----)</th>
<th>GaAs (AlGaAs / InGaAs)</th>
<th>4H-SiC (----)</th>
<th>GaN (AlGaN / GaN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandgap (eV)</td>
<td>1.11</td>
<td>1.42</td>
<td>3.26</td>
<td>3.42</td>
</tr>
<tr>
<td>( \mu_e ) (cm(^2)/Vs)</td>
<td>1500</td>
<td>8500 (10000)</td>
<td>700</td>
<td>900 (2000)</td>
</tr>
<tr>
<td>( V_{sat} ) (( \times 10^7 ) cm/s)</td>
<td>1</td>
<td>1 (2.1)</td>
<td>2</td>
<td>1.5 (2.7)</td>
</tr>
<tr>
<td>2DEG density (cm(^2))</td>
<td>NA</td>
<td>&lt; 4( \times 10^{12} )</td>
<td>NA</td>
<td>1-2( \times 10^{13} )</td>
</tr>
<tr>
<td>( E_B ) (10(^6) V/cm)</td>
<td>0.3</td>
<td>0.4</td>
<td>2</td>
<td>3.3</td>
</tr>
<tr>
<td>Dielectric constant</td>
<td>11.8</td>
<td>12.8</td>
<td>10</td>
<td>9</td>
</tr>
<tr>
<td>Thermal conductivity (W/mK)</td>
<td>150</td>
<td>50</td>
<td>490</td>
<td>170</td>
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Table 1-2 Power semiconductor devices Figure of Merit

<table>
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<th>Si</th>
<th>GaAs</th>
<th>SiC</th>
<th>GaN</th>
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<td>Tmax</td>
<td>300</td>
<td>300</td>
<td>600</td>
<td>700</td>
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<tr>
<td>BFOM</td>
<td>1</td>
<td>9.6</td>
<td>3.1</td>
<td>24.6</td>
</tr>
<tr>
<td>JFM</td>
<td>1</td>
<td>3.5</td>
<td>60</td>
<td>80</td>
</tr>
</tbody>
</table>

**BFOM = k\mu_eE_B^3**
Baliga’s figure-of-merit
Evaluate resistive loss [3]

**JFM = E_CRV_{sat}/2\pi**
Johnson’s figure-of-merit
Evaluate switching delay [4]
1.3 GaN HEMT

The AlGaN/GaN heterojunction enables the development of GaN high electron mobility transistors (HEMT). Owing to spontaneous polarization and piezoelectric effect, a high density 2DEG is formed at AlGaN/GaN heterointerface, and it makes the GaN HEMT possible. The high electron density, combining with a high electron mobility due to reduced ionized impurity scattering, provides large current and high speed in device operations. GaN based HEMT offers many advantages comparing to existing technologies. Besides the advantages of high power handling, high frequency and high efficiency, the wide bandgap nature and its growth on SiC substrate allow good thermal management and high temperature operation of devices. In addition, the high power density feature makes transistor size and number much smaller. Low channel resistance and high electron saturation velocity offer the potential of low noise application. From the fabrication aspect, the chemical inertness of GaN and good ohmic contacts facilitate a reliable device fabrication. In the end, the potential of forming a good dielectric/GaN interface holds a promising future for insulated gate transistors.

Figure 1-1 Operation range of high power and high frequency transistors.
Figure 1-2 shows a conventional GaN based HEMT structure. It uses a schottky gate to control 2DEG at AlGaN/GaN channel. However, some problems that degrade transistor performance have to be overcome [5]. First of all, dangling bonds at AlGaN surface form surface states. Charges are trapped in these states during device operation, which causes the reduction of the output current [6]. This phenomenon is called current collapse, one of the major obstacles in developing GaN HEMT. Another critical issue of GaN HEMT is the gate leakage current at high voltage operation. Electrons may jump over the potential barrier or directly tunnel through AlGaN barrier into gate electrode when they have high energy or local electric field is large enough [7]. Escaped electrons not only increase power consumption, but also accumulate at AlGaN surface to form a virtue gate, thereby resulting in loss of gate control at the channel [6]. Both surface states and gate leakage significantly limit the operation of GaN HEMT. To solve this problem, a new structure that combines advantages in insulated gate and heterostructure transistors, has been proposed for GaN power devices [8], [9], [10].

Figure 1-2 Conventional HEMT structure and problems. Figure 1-3 MIS-HEMT structure.
1.4 MIS-HEMT

1.4.1 MISH devices and interfaces

Figure 1-3 shows a general MIS-HEMT structure. A dielectric layer is added on top of AlGaN/GaN heterostructure. This layer acts as a gate dielectric separating gate metal and semiconductor and preventing the gate leakage, and it also passivates the semiconductor surface, eliminating surface dangling bonds and minimizing traps. One of the earliest papers of GaN MIS-HEMT published in 2003 shows a tremendous improvement of gate leakage without decreasing device performance by adding a dielectric layer (figure 1-4) [11]. The drain voltage ($V_{ds} = 20V$) here is a typical operating voltage for a power transistor. It was also reported that the SiN passivation layer in HEMT can eliminate current collapse and dispersion between the large signal direct current and alternating current characteristics [12].

Figure 1-4 Gate leakage current (a) and transfer characteristic (b) of HFET and MISHFET [11].

The dielectric layer may influence device performance by changing 2DEG density at AlGaN/GaN interface. The mechanism behind this effect is not fully understood. Some groups suggested stress induced piezoelectric effect due to the additional dielectric layer causes a 2DEG density change.
[13], [14], [15] while other groups considered that the surface states reduction [16], [17], [18] in passivation leads to surface trapped electrons transferring to AlGaN/GaN interface.

Another important point that we are interested in is the characterization of the dielectric/semiconductor interface [19], [20], [21], [22]. Although the dielectric layer decreases semiconductor surface states by reducing dangling bonds, it still leaves a small amount of unsatisfied bonds at the interface due to the material heterogeneity (figure 1-5). This type of bonds also behaves as interface states and traps electrons during device operation. Therefore, it is very important to characterize the dielectric/semiconductor interface to achieve a good device control.

However, since there are two interfaces in this structure (dielectric/AlGaN interface and AlGaN/GaN interface), it is especially hard to study the former one in MIS-HEMT structure because the potential modulation is essentially fairly complicated between the two interfaces. In this work, we focus on the dielectric/AlGaN interface characterization and study the physics inside and effects on device performance.

Figure 1-5 Schematic models of (a) atomic arrangements at SiN/AlGaN interface [17] and (b) band alignment.
Several techniques have been developed to characterize interface states. The conductance method was proposed by Nicollian and Goetzberger to relate a measured admittance with interface trap states in a silicon MOS capacitor [31]. The trap information can be extracted from the measured admittance by an equivalent circuit. This technique can also be applied in GaN MISH structure for interface study. Shih et al. reported an analysis of AlN/AlGaN interface properties using the conductance method and found an interface state density larger than $10^{13}$ cm$^{-2}$eV$^{-1}$ [29]. Gregusova et al. applied frequency dependent conductance measurement to characterize Al$_2$O$_3$/AlGaN interface in MISH structure, and the trap state density decreased from $10^{12}$ cm$^{-2}$eV$^{-1}$ at 0.27 eV to $3 \times 10^{10}$ cm$^{-2}$eV$^{-1}$ at 0.45 eV [32]. Generally speaking, conductance method is more sensitive and accurate than capacitance method, but with more complexity.

C-V technique is the most frequently used technique that evaluates insulator/semiconductor interface [33]. However, conventional methods, such as Gray-Brown technique and Terman method have met some difficulties in extracting interface state density due to the pyroelectric and wide bandgap nature of nitride based materials. Therefore, several modified C-V characterization techniques such as photo-assisted C-V and frequency dependent C-V measurements have been developed in both nitride based MIS and MISH structures.

Shih et al. also studied AlN/AlGaN interface using multi-frequency C-V measurement with frequency from 100Hz to 1MHz [22]. It was found that C-V curves disperse significantly at high forward bias, probably due to a large amount of electrons trapping at AlN/AlGaN interface states. The interface state density was not extracted in this characterization method. With this technique, an elaborated investigation of the dielectric/semiconductor interface is necessary. In this work, we perform frequency dependent C-V technique extensively to study interface states at Al$_2$O$_3$/AlGaN interface.
1.4.2 Dielectrics

The study of GaN dielectric materials benefits from the continuous progress in silicon transistor scaling, which pushes forward the development of various dielectric materials. Hafnium based dielectrics have emerged as next generation dielectrics for silicon with a careful balance of various requirements, while the best dielectric for GaN remains to be investigated.

The ideal candidate material for GaN based device should have a high bandgap ($E_g > 5$ eV), high dielectric constant comparable to AlGaN ($k \sim 9.5$), high breakdown field ($E > 10$ MV/cm) and high thermal conductivity. The most important criteria, as we discussed above for the dielectric material, is to form a good interface with AlGaN since a good gate control of the transistor depends on dielectric/AlGaN interfacial properties.

Insulating materials such as SiO$_2$, SiN, Al$_2$O$_3$, HfO$_2$, AlN, Ga$_2$O$_3$ and Sc$_2$O$_3$ have been reported as gate dielectrics and passivation layers [8], [9], [10], [22], [23], [24]. Table 1-3 summarizes related properties and research progresses of several frequently investigated materials. Until now none of these materials performs significantly better than the others. Our study mainly focus on ALD Al$_2$O$_3$ dielectric thin films.
The ALD Al₂O₃ thin film is one of the pioneer materials studied in this field and it has made impressive progress recently. Many groups have demonstrated GaN based MISH, MIS-HEMT and similar structures using Al₂O₃ as the insulating material. As a gate dielectric material, the high band gap (7 eV – 9 eV), high dielectric constant (8 – 10) and high breakdown field (> 10 MV/cm) properties are especially attractive to high power and high voltage devices. However, although ALD Al₂O₃ techniques are rather mature, the discrepancies existing between thermal ALD films and plasma enhanced ALD (PEALD) films are still worth investigating. Furthermore, interfacial properties of the Al₂O₃/AlGaN are far from perfect and a large number of problems need to be resolved in terms of pre-deposition treatments and post-deposition annealing. This work on Al₂O₃/AlGaN/GaN structures compares Al₂O₃ thin films using thermal ALD and PEALD techniques, and discusses film qualities and interfacial properties using material and electrical characterization methods. Several solutions are provided to improve the dielectric material and dielectric/semiconductor interface as well.
1.5 Dissertation outline

In this thesis, the full picture of Al₂O₃/AlGaN/GaN MISH structure fabrication and characterization is provided. Chapter 2 emphasizes on materials and fabrication. Al₂O₃ thin films grown by thermal ALD and PEALD are studied and the films are investigated by different material characterization tools. The device fabrication and process flow are discussed in the same chapter. Chapter 3 focuses on electrical characterization using capacitance voltage measurements. The C-V curves are interpreted, and the information on carrier concentration, dielectric constant and interface state density are extracted. Special emphases are given to Al₂O₃/AlGaN interface states characterization using frequency dependent C-V tests. In chapter 4, Al₂O₃ dielectric conduction mechanisms are investigated with temperature dependent measurements in the first part. Dielectric reliability is studied and analyzed in the second part of chapter 4. Chapter 5 concludes the entire work and proposes several ideas for the future work.

1.6 References


Chapter 2 Materials and Fabrication

2.1 AlGaN/GaN epitaxial layer

In a GaN based material system, an AlGaN/GaN heterostructure is widely used in high speed devices due to the high density of 2D electron gas (2DEG) confined at AlGaN/GaN interface. The quality of the GaN epitaxial layer and the AlGaN pseudomorphic cap plays a significant role on device performance and reliability. Usually, metal organic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE) are the two methods of growing AlGaN/GaN epi-layers. MOCVD involves a dynamic process of semiconductor formation. Gaseous reactants flow into the chamber, and the chemical reaction occur onto a heated substrate. MBE employs an ultrahigh vacuum and non-equilibrium growth condition at which reactions happen between atomic, molecular or ionized beams of corresponding elements [1].

Our AlGaN/GaN epi sample was obtained from Northrop Grumman and grown by MBE technique. The epitaxial growth was performed on a three inches sapphire substrate. A 30 nm AlN nucleation layer was first formed on sapphire, followed by a 500 nm GaN buffer layer. The AlGaN/GaN heterostructure was then grown on the GaN buffer layer, with a film thickness of 23 nm of Al$_{0.23}$Ga$_{0.77}$N and 140 nm of GaN. The entire epi-film structure is illustrated below in figure 2-1.
Several material and surface characterization including atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM) and X-ray diffraction (XRD) techniques were performed on the epitaxial sample to analyze the film quality, surface properties and constituents.

Cross section TEM graphs of the epi-layer are shown in figure 2-2. We can clearly find the GaN, AlN nucleation layer and sapphire substrate in the left image. The right picture shows a small scale image of the AlGaN and GaN layer.
AFM scans were also carried out on the bare epi-film surface after necessary surface cleaning, but without any surface treatment. Figure 2-3 shows an image of a 10 micron by 10 micron square area scan of the AlGaN/GaN/AlN nucleation layer/Sapphire sample. A root mean squared (RMS) surface roughness of this area is 18.1Å.
Figure 2-3 AFM graph of the AlGaN surface of the AlGaN/GaN/AlN nucleation layer/Sapphire substrate epitaxial layer.

Figure 2-4 Triple axis crystal X-ray diffraction curve of AlGaN/GaN/AlN nucleation layer/Sapphire substrate epitaxial layer.
Omega-2theta X-ray diffraction scan was performed using triple axis crystal diffractometer. There are three peaks in this picture in a given scanning range. From the scan, we can observe the presence of epitaxially grown AlGaN and GaN films. The highest intensity peak corresponds to GaN epi-film. It also exhibits a small full width at half maximum since the GaN film has a large thickness of 640 nm. The more broaden peak next to the GaN is the AlGaN peak with the AlGaN thickness of only 23 nm. The peak at right of the picture indicates the signal from AlN nucleation layer. It has a low intensity and a broad width because the nucleation layer locates at the bottom of the epitaxial layer and only has 30 nm thickness.

![XPS survey of the AlGaN surface.](image)

Figure 2-5 XPS survey of the AlGaN surface.

X-ray photoelectron spectroscopy (XPS) measurements were carried out using a monochromatic Al Kα X-ray source of energy 1486.7 eV (Axis Ultra DLD, Kratos Analytical). The XPS spectra
reported here are referenced to the surface C 1s peak at the binding energy (BE) of 285.0 eV and the spectra are curve-fitted with a combination of Gaussian and Lorentzian line shapes(GL30), using a Shirley-type background subtraction. Figure 2-5 shows an XPS survey of the AlGaN surface. A stoichiometry analysis suggests an Al to Ga composition ratio of ~1:3, very close to the given ratio of the Al$_{0.23}$Ga$_{0.77}$N compound.

2.2 ALD Al$_2$O$_3$ thin film

2.2.1 Thin film growth

The atomic layer deposition (ALD) technique has been developed and accepted by semiconductor industry for high K dielectric application. It has a deposition process that consists a sequent of self-terminating chemical reaction steps and each limiting step dominates in the formation and saturation of a monolayer. In each of the partial reaction, a surface functional group reacts with a gas phase precursor. This reaction keeps forming a new functional group on the surface until it fully replaces the previous group. Therefore, only one monolayer is generated.

In our work, the ALD technique was implemented to Al$_2$O$_3$ dielectric thin film growth. Al$_2$O$_3$ films grown by thermal ALD and plasma enhanced ALD (PEALD) were evaluated using several material characterization methods. We also fabricated similar device structures for these two films and compared electrical performance of the devices. The chemical reaction and precursors for thermal ALD and PEALD Al$_2$O$_3$ techniques are actually different from each other.

The thermal ALD Al$_2$O$_3$ process is conducted in a heated chamber using trimethylaluminum (TMA) as precursor and H$_2$O as oxidizing agent [2]. The surface reaction formula is described as following:
\[(A) \text{AlOH}^* + \text{Al(CH}_3\text{)}_3 \rightarrow \text{AlOAl(CH}_3\text{)}_2^* + \text{CH}_4\]

\[(B) \text{AlCH}_3^* + \text{H}_2\text{O} \rightarrow \text{AlOH}^* + \text{CH}_4\]

where surface groups are expressed with asterisks. The self-limiting Al\textsubscript{2}O\textsubscript{3} growth occurs during TMA and H\textsubscript{2}O alternating exposures. The overall reaction chemistry is:

\[\text{Al(CH}_3\text{)}_3 + 3\text{H}_2\text{O} \rightarrow \text{Al}_2\text{O}_3 + 3\text{CH}_4\]

PEALD has a unique process that a self-limiting deposition is followed by a surface activation or ligand extraction step with radicals generated from a plasma. The radical in the plasma induces the reaction with surface ligands with a low activation energy and therefore it increases the deposition rate and allows a lower deposition temperature. The PEALD Al\textsubscript{2}O\textsubscript{3} process is conducted using TMA as precursor and plasma oxygen as oxidizing agent.

In this work, all the dielectric deposition processes were performed at UCLA Nanolab. We utilized two ALD systems: Savannah and Fiji both from Cambridge Nanotech Inc. Savannah was only used for thermal ALD while Fiji for both thermal and plasma ALD. The recipes are shown in the following tables.

Table 2-1 Thermal ALD Al\textsubscript{2}O\textsubscript{3} process in Savannah system.

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<th>Valve</th>
<th>Time (s)</th>
<th>Pump (s)</th>
<th>Sccm</th>
<th>Delay (min)</th>
</tr>
</thead>
<tbody>
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<td>20</td>
<td>10</td>
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<td>2 (Al)</td>
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Table 2-2 Thermal ALD Al₂O₃ process in Fiji system.

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</thead>
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</tr>
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Table 2-3 PEALD $\text{Al}_2\text{O}_3$ process in Fiji system.

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<td>doorpurge</td>
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2.2.2 Al₂O₃ thin film characterization

2.2.2.1 Surface morphology

AFM was applied to study surface morphology for Al₂O₃ films grown by different techniques. Figure 2-6 presents four surface images that compare Al₂O₃ films on the AlGaN/GaN layer. The surface of thermal ALD Al₂O₃ films is shown in figure (a) and (b) and the surface of PEALD Al₂O₃ films is shown in figure (c) and (d). Samples in figure (a) and (c) were as-deposited condition while samples in figure (b) and (d) were annealed for 5 minutes in 1000°C nitrogen atmosphere after deposition. Compared with bare AlGaN/GaN surface in figure 2-3, all the deposited Al₂O₃ films exhibit much lower surface roughness, which indicates a conformal and smooth coating of thin film by ALD. Among them, PEALD films show a slightly lower roughness than thermal ALD films. But the difference between the as-deposited samples and annealed samples is within 0.5Å, which is almost negligible.
2.2.2.2 XPS

XPS measurements were carried out to study bonding information and band alignment for both \( \text{Al}_2\text{O}_3 \) thin films and \( \text{Al}_2\text{O}_3/\text{AlGaN} \) interfaces. To observe the signal from \( \text{Al}_2\text{O}_3/\text{AlGaN} \) interfaces, very thin \( \text{Al}_2\text{O}_3 \) layers were deposited by both thermal ALD and PEALD techniques [3], and the results were compared with those on AlGaN layer surface and thick \( \text{Al}_2\text{O}_3 \) films.
Figure 2-7 shows Ga 3d and Al 2p core-level spectra for AlGaN, thermal ALD Al₂O₃ thin film on AlGaN and PEALD Al₂O₃ thin film on AlGaN.

Figure 2-7 shows Ga 3d and Al 2p core-level spectra for AlGaN, PEALD Al₂O₃ thin film on AlGaN and thermal ALD Al₂O₃ thin film on AlGaN. The detail thickness of films and the binding energy are given in table 2-4 below. It can be seen that Ga 3d peak positions shift towards smaller binding energy for thermal ALD and PEALD Al₂O₃ thin films. These shifts might be attributed to dipole formation at Al₂O₃/AlGaN interface that change the AlGaN surface potential.

It should also be noted that Ga-O to Ga-N bond ratio increases from 0.057 for AlGaN to 0.196 for PEALD film and 0.25 for thermal ALD film. The rising ratio implies that GaOₓ forms at interface during both ALD Al₂O₃ growth. The lower GaOₓ composition in PEALD grown sample suggests that plasma process has a better control to the surface oxide formation.
Table 2-4 Thickness, binding energy and Ga-O/Ga-N ratio of AlGaN, thermal ALD Al₂O₃ thin film on AlGaN and PEALD Al₂O₃ thin film on AlGaN.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Al₂O₃ thickness(nm)</th>
<th>Ga-N</th>
<th>Ga-O</th>
<th>Al-O</th>
<th>Al-N</th>
<th>GaOx/GaN</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlGaN</td>
<td>0</td>
<td>20.02</td>
<td>20.84</td>
<td>74.33</td>
<td>73.67</td>
<td>0.057</td>
</tr>
<tr>
<td>PEALD</td>
<td>3.90</td>
<td>19.69</td>
<td>20.37</td>
<td>74.41</td>
<td>73.68</td>
<td>0.196</td>
</tr>
<tr>
<td>Thermal</td>
<td>3.75</td>
<td>19.87</td>
<td>20.55</td>
<td>74.61</td>
<td>73.81</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Figure 2-8 XPS O1s energy loss spectrum of 50 nm PEALD Al₂O₃ thin film on AlGaN.

The bandgap of the Al₂O₃ film can be estimated using O 1s energy loss spectrum. Figure 2-8 shows a spectrum for the 50 nm PEALD Al₂O₃ film. The separation of energy between O 1s peak and
plasmon loss onset represents the minimum energy for an electron to reach conduction band and result in plasmonic oscillation, and is approximately the energy bandgap. Here, the bandgap for the PEALD Al$_2$O$_3$ film is measured as 7.0 eV. Table 2-5 shows a comparison of the bandgap for both thermal ALD and PEALD Al$_2$O$_3$ films as-deposited and after 1000°C annealing. The increase of Al$_2$O$_3$ bandgap after annealing is due to that Al$_2$O$_3$ thin films change from amorphous to polycrystalline at high annealing temperatures.

Table 2-5 Band gap of 50 nm thermal ALD Al$_2$O$_3$ thin films and PEALD Al$_2$O$_3$ thin films with and without annealing.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Bandgap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal ALD</td>
<td>6.7</td>
</tr>
<tr>
<td>Thermal ALD + Annealing</td>
<td>7.0</td>
</tr>
<tr>
<td>PEALD</td>
<td>7.0</td>
</tr>
<tr>
<td>PEALD + Annealing</td>
<td>7.3</td>
</tr>
</tbody>
</table>

The refractive index measurement also gave us an Al$_2$O$_3$ film density of ~1.5 in thermal ALD, much lower than the normal ALD Al$_2$O$_3$ density (1.6 - 1.65). This might be due to the existence of excessive CH$_3$ ligands from Al(CH$_3$)$_3$ precursor, and they are not fully dissociated during the thermal based deposition. The light atoms from the ligands such as carbon and hydrogen lead to a low Al$_2$O$_3$ film density. Since the density of TMA precursor is about 1/5 of the Al$_2$O$_3$ density, the impurity concentration can be estimated around 10% - 12% assuming refractive index is linearly proportional to film density, since we have observed an 8% - 10% reduction of refractive index.
Valence band spectra of both thermal ALD and PEALD Al$_2$O$_3$ films with and without post annealing are depicted in figure 2-9. The valence band maximum (VBM) of each sample is extrapolated by crossing the leading edge of the spectrum over the baseline.

Figure 2-9 Valence band spectra of 50 nm (a) PEALD Al$_2$O$_3$ thin film after annealing, (b) PEALD Al$_2$O$_3$ thin film as-deposited, (c) thermal ALD Al$_2$O$_3$ thin film after annealing and (d) thermal ALD Al$_2$O$_3$ thin film as-deposited.
To calculate the valence band offset (VBO), we have

\[
VBO = \left[ E_{CL}^{Al_{2}O_{3}}(b) - E_{V}^{Al_{2}O_{3}}(b) \right] - \left[ E_{CL}^{AlGaN}(b) - E_{V}^{AlGaN}(b) \right] - \left[ E_{CL}^{Al_{2}O_{3}}(i) - E_{CL}^{AlGaN}(i) \right]
\]

The letter E indicates the binding energy. The subscript CL and V stand for core-level and VBM, respectively. The letter b stands for the bulk Al\(_2\)O\(_3\) and AlGaN signal while i for the interface signal. The binding energy difference between bulk AlGaN core-level and VBM is presented in figure 2-10. By substituting all the numbers into the equation above, we can obtain the valence band offset (\(\Delta E_v\)) for Al\(_2\)O\(_3\) films. Since we have measured the dielectric bandgap, the conduction band offset can also be calculated below:

\[
\Delta E_c = E_g(Al_2O_3) - E_g(AlGaN) - \Delta E_v
\]

where the bandgap of Al\(_{0.25}\)Ga\(_{0.77}\)N is [4]:

Figure 2-10 Ga 3d core-level and valence band spectra of AlGaN.
\[ E_g(Al_xGa_{1-x}N) = 3.42 \, eV + x \cdot 2.86 \, eV - x(1-x) \cdot 1.0 \, eV \]

Figure 2-11 Schematic band alignment of Al\(_2\)O\(_3\)/AlGaN.

Figure 2-11 shows a schematic band alignment of Al\(_2\)O\(_3\)/AlGaN interface and band offset. The number of \(\Delta E_v\) and \(\Delta E_c\) are summarized in table 2-6 for the as-deposited and annealing samples. The valence band offsets of the Al\(_2\)O\(_3\) films after annealing are in agreement with reported studies.

<table>
<thead>
<tr>
<th>Sample</th>
<th>(\Delta E_v) (eV)</th>
<th>(\Delta E_c) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal ALD</td>
<td>1.2</td>
<td>1.6</td>
</tr>
<tr>
<td>Thermal ALD + Annealing</td>
<td>0.8</td>
<td>2.3</td>
</tr>
<tr>
<td>PEALD</td>
<td>1.0</td>
<td>2.1</td>
</tr>
<tr>
<td>PEALD + Annealing</td>
<td>0.7</td>
<td>2.7</td>
</tr>
</tbody>
</table>

Table 2-6 Summary for valence band offset and conduction band offset of thermal ALD and PEALD Al\(_2\)O\(_3\) thin film samples with and without annealing.
### 2.2.2.3 Crystal structure

To understand the crystal structure of $\text{Al}_2\text{O}_3$ thin films, we deposited 50 nm $\text{Al}_2\text{O}_3$ films using PEALD on p-type silicon substrate. The deposition was followed by 5 minutes rapid thermal annealing in nitrogen atmosphere with various temperature conditions from 600°C to 1000°C. The crystal structure and crystallization behavior of as-deposited and annealed $\text{Al}_2\text{O}_3$ thin films were investigated using grazing incidence X-ray diffraction.

The scans were conducted from low angle to high angle (10° to 80°). The intensity curves do not show any peaks along the scanning range for samples without annealing or annealed at 600°C and 800°C, which might suggest that $\text{Al}_2\text{O}_3$ thin films under these conditions are amorphous. However,
the sample annealed at 1000°C shows a peak at two theta of 67° in figure 2-12. The appearance of this peak may indicate the crystallinity has changed for Al₂O₃ thin films at high temperatures. The Al₂O₃ thin film probably transforms from amorphous to polycrystalline at a temperature between 800°C and 1000°C. Our result is also in agreement with other reported ALD Al₂O₃ studies [5], [6]. It is suggested that the Al₂O₃ thin film has a crystallization temperature around 900°C and the film structure changes from amorphous to γ-Al₂O₃.

2.3 Fabrication

2.3.1 GaN process

Many efforts have been spent on solving GaN process issues since nitride based III-V material and process technology is significantly different from traditional silicon and gallium arsenide technology. In general, a successful process requires a good uniformity, reproducibility and reliability. Before realizing a stable process flow, some of special requirements have to be satisfied for high performance GaN FETs. The following points are particularly important in GaN process [7]:

- Surface cleaning, pre-treatment and post annealing to remove native oxide and reduce interface defect states
- Good device isolation to avoid device crosstalk
- Low resistance contacts for high performance transistors
- Good dielectric materials to achieve low leakage current
2.3.2 Process flow for MISH devices

Some of the issues mentioned above were investigated when we start to build our own GaN process flow in UCLA nanolab. Problems including pre-treatment and post annealing will be addressed in following paragraphs. Before we discuss these processes, the entire process flow of our GaN MISH device is presented.

![Diagram of MISH test device structure](image)

Figure 2-13 Schematic cross section of metal/Al₂O₃/AlGaN/GaN MISH structure.

Figure 2-13 shows an MISH test device structure. The detail steps are listed below.

- Surface cleaning
- Ohmic contacts formation
- Rapid thermal annealing
- Pre-deposition treatment
- Dielectric deposition
- Post-deposition annealing
- Gate contacts formation
A short description of each steps is summarized here.

An AlGaN/GaN bare substrate was first rinsed by acetone and IPA to remove organic species. The sample was then dipped into HF solution for 5 minutes and HCl solution for 2 minutes to remove native oxide and metal contaminants, and followed by DI water rinse.

After surface cleaning, the sample was patterned and ohmic contacts were deposited using e-beam evaporator in nanolab. Ring pattern Ti/Al/Ni/Au metal stacks were evaporated on sample surface. The thickness of this four layers was 20nm/120nm/40nm/50nm. Ti/Al metal stack was also fabricated and compared to the Ti/Al/Ni/Au contact.

To obtain ohmic contacts, rapid thermal annealing was performed at 830 °C for 1 minute in nitrogen atmosphere.

A plasma surface treatment was carried out prior to the ALD process. We applied plasma N₂ and NH₃ on AlGaN surface to improve Al₂O₃/AlGaN interfacial properties. ALD Al₂O₃ film was then grown on the sample using standard procedure shown previously, and it was followed by a post annealing in different ambient with varied temperature. The annealing impact on devices will be shown in detail in next chapter.

The final step was the Ni/Au gate contact formation. A 40nm/50nm metal contact was deposited using e-beam evaporator as well.

All the steps above were finished in UCLA nanolab.
2.3.3 Pre-deposition treatment

Since the dielectric/semiconductor interface quality is crucial to transistor performance, special processes and treatments have been applied before or after dielectric deposition to reduce defect states and improve device behavior. From the experience in traditional silicon industry, we learn that surface plasma treatments prior to dielectric deposition may significantly affect number of interface states and fixed charges at the interface. Depending on the type of plasma treatment, the process may remove native oxide, form an interlayer that assists following deposition or modify surface states to achieve a desirable band alignment [8], [9].

In our work, we incorporated two types of surface pre-treatments that may be favorable to Al$_2$O$_3$/AlGaN interfacial behavior. The plasma species we chose here were ammonia and nitrogen. A brief introduction of these plasmas and their background in semiconductor applications are given below.

NH$_3$ plasma treatment has been employed in silicon industry because of its ability to form nitridation layer. This nitridation layer allows the following growth of silicon nitride or silicon oxynitride. This method was also introduced in GaN based HEMT devices as a pre-treatment step prior to SiN passivation. It was reported that the treatment effectively reduced gate lag and current collapse, and improved AlGaN/GaN HEMT reliability [10].

Nitrogen plasma is an alternative source to the nitridation layer formation. In addition, different usage of N$_2$ plasma has been widely reported on GaN based electronic devices. It was not only performed to remove surface residue contaminants such as carbon and oxides, but also to reduce gate leakage and mitigate device I-V dispersion [11], [12], [13], [14].
In addition, oxygen plasma surface pre-treatment was another method that intensively applied on sample cleaning and oxidation layer growth. Studies on AlGaN or GaN O\textsubscript{2} plasma surface treatments show a lower surface impurity concentration but an increased oxygen content. The high power O\textsubscript{2} plasma may assist to form a surface oxidation layer, and this layer aims to reduce gate leakage current and RF collapse. It was also suggested that oxygen treatment is beneficial to ohmic contact formation on the n-type GaN surface. In our case, however, the plasma oxygen treatment favors the growth of GaO\textsubscript{x} surface oxide layer. This layer creates more dangling bonds and increases the density of interface states at Al\textsubscript{2}O\textsubscript{3}/AlGaN interface [15], [16], [17].

The plasma NH\textsubscript{3} and N\textsubscript{2} pre-deposition surface treatment were performed before ALD Al\textsubscript{2}O\textsubscript{3} film growth. Various power and time were applied to the treatments. The process temperature was set at 300°C and chamber pressure was 300 mTorr.

![Figure 2-14 XPS Ga 3d core-level spectra of PEALD Al\textsubscript{2}O\textsubscript{3} thin films on AlGaN with plasma NH\textsubscript{3}, N\textsubscript{2} and without surface plasma treatment.](image-url)
Figure 2-14 shows the XPS results of the plasma treated samples. These samples were subject to 5 minutes and 50W N\textsubscript{2} and NH\textsubscript{3} treatments, and followed by a thin PEALD Al\textsubscript{2}O\textsubscript{3} film deposition. One sample with only PEALD growth was also measured as comparison. It can be seen that the Ga-O peak intensity in both N\textsubscript{2} and NH\textsubscript{3} treated samples is lower than the non-treated sample. Table 2-7 summarizes the binding energy and Ga-O/Ga-N ratio of each sample. We can clearly observe that GaO\textsubscript{x}/GaN ratio reduces when the plasma treatment is performed before deposition. The N\textsubscript{2} treatment is more effective since the ratio is nearly identical to the one measured with bare AlGaN surface. The XPS data suggests that nitrogen based plasma treatments lead to a good suppression of GaO\textsubscript{x} layer which is detrimental to Al\textsubscript{2}O\textsubscript{3}/AlGaN interfacial properties. The plasma N\textsubscript{2} and NH\textsubscript{3} serve as nitridation sources and form thin nitridation layers on the AlGaN surface, and the nitrided film prevents GaO\textsubscript{x} growth at the initial of the ALD process.

Table 2-7 Binding energy and Ga-O/Ga-N ratio of AlGaN, PEALD Al\textsubscript{2}O\textsubscript{3} thin films on AlGaN with and without surface plasma treatment.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Ga-N</th>
<th>Ga-O</th>
<th>Al-O</th>
<th>Al-N</th>
<th>GaO\textsubscript{x}/GaN</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlGaN</td>
<td>20.02</td>
<td>20.84</td>
<td>74.33</td>
<td>73.67</td>
<td>0.057</td>
</tr>
<tr>
<td>PEALD</td>
<td>19.69</td>
<td>20.37</td>
<td>74.41</td>
<td>73.68</td>
<td>0.196</td>
</tr>
<tr>
<td>NH\textsubscript{3}</td>
<td>19.57</td>
<td>20.28</td>
<td>74.33</td>
<td>73.5</td>
<td>0.096</td>
</tr>
<tr>
<td>N\textsubscript{2}</td>
<td>19.62</td>
<td>20.47</td>
<td>74.29</td>
<td>73.52</td>
<td>0.059</td>
</tr>
</tbody>
</table>
2.3.4 Post-deposition annealing

The post ALD annealing of Al$_2$O$_3$ films is also considered as a critical step to improve film quality and interfacial properties. As suggested above, the crystal structure change of the Al$_2$O$_3$ film is subject to the post annealing temperature. Different annealing temperatures and gaseous species were investigated to acquire the best film quality and device performance.

The post annealing temperature study was conducted in N$_2$ ambient. It was reported that the annealing process can effectively reduce dielectric/semiconductor interface state density. We performed our annealing temperature lower than the Al$_2$O$_3$ phase transition point, since the polycrystalline dielectric film results in high leakage current. From previous section, we have already found that the phase transition for amorphous Al$_2$O$_3$ films to polycrystalline films occurs around 900°C. Therefore, the annealing temperatures were varied from 400°C to 700°C in our investigation to avoid this phase transformation [18].

Nitrous oxide (N$_2$O) plasma treatment is another widely used technique in silicon industry to form oxynitride films and improve interfacial properties. The incorporation of nitrogen in this annealing step can both increase dielectric constant and lead to a more robust oxide resistive to impurity diffusion. It was also found that a higher breakdown field and a lower interface state density were achieved after exposing Si/SiO$_2$ films to a N$_2$O plasma [19]. The N$_2$O surface pre-treatment on GaN surface was also investigated on GaN MIS diodes and a better dielectric/semiconductor interface was observed [20]. In our experiment, we performed a low temperature plasma N$_2$O annealing to observe if the dielectric transport behavior was improved.
2.4 References


Chapter 3 Defect state characterization

3.1 Background

Since metal-insulator-semiconductor transistors were invented, the dielectric/semiconductor interfacial property has always been the first issue to concern in terms of device performance and reliability. Traps and defect states at the dielectric/semiconductor interface not only affect an effective gate control to the conduction channel by shifting electrostatic potential, but also degrade device parameters such as current and transconductance. In addition, trapped holes and electrons may interact with carriers and damage interface or even bulk insulator by breaking local bonds. The dangling bonds create new traps and trap more holes and electrons. The entire process brings reliability problems in long term transistor operations.

Fortunately, our nature creates a nearly perfect silicon-silicon dioxide interface for us. The low state density at Si/SiO$_2$ interface allows the invention of silicon base MOSFETs, which enable tremendous advancement and breakthrough in modern electronic industry in the past half century. In the meanwhile, various theories, techniques and tools have been developed to characterize silicon based devices and Si/SiO$_2$ interface. These methods are mature and now being applied to other semiconductor material and device systems. In our work, we take the advantage and modify these characterization techniques to fit our own application.

Different from Si/SiO$_2$ interface, interfaces between dielectric and III-V based semiconductors have been facing serious issues due to lack of reliable native oxide and the binary characteristic of the materials themselves. The gallium arsenide (GaAs) society has been struggling with these problems for thirty years, and now same situation occurs in nitride based semiconductors. Usually, the density of defect states at a dielectric/III-V interface is around $10^{12}$/cm$^2$eV to $10^{13}$/cm$^2$eV, two
to three magnitudes higher than the number at Si/SiO$_2$ interface. In GaN MISH system, the dielectric/AlGaN interface plays an important role on realization of MIS-HEMT. In the following section, we characterized Al$_2$O$_3$/AlGaN interface and investigated the impact on Al$_2$O$_3$/AlGaN interface state density due to different processes and treatments.

### 3.2 Characterization setups

The capacitance voltage (C-V) technique is the most popular method for interface states characterization. This technique allows a fast test and facilitates the fabrication process for the test device since it can be performed on a simple diode structure. The MISH structure we introduced in chapter two was designed for the C-V characterization. Besides the interface state density, C-V curves can provide other information such as carrier density profiles and dielectric constant. A detail theory and interpretation of C-V curves in MISH system is explained in next section.

Agilent 4284A LCR meter and Boonton 72B capacitance meter were both used in our C-V characterization. The sweeping rate was set at 100 mV/s. The test frequency was varied from 100 Hz to 1MHz. Multi-frequency C-V was used to extract interface state densities. Samples were tested on MMR probe station.
3.3 Capacitance-voltage characterization

3.3.1 Theory and interpretation

Because there exist Al₂O₃/AlGaN and AlGaN/GaN two interfaces in the MISH diode, the C-V curves are significantly different from conventional C-V curves in silicon MOS caps. Figure 3-1 shows a general voltage sweep of the MISH diode from negative bias to positive bias. It can be noticed that there are three stages presenting in this curve. At the beginning of the sweep, almost no capacitance can be measured. At this stage 1, the 2DEG is depleted below the threshold voltage. As the gate voltage swept above the threshold condition, the 2DEG starts to accumulate at AlGaN/GaN interface. Then we obtain a constant capacitance which equals to the capacitance of the AlGaN layer in series with the Al₂O₃ layer. The capacitance curve keeps flat at stage 2 until the sweep reaches a high positive gate bias at which electrons at AlGaN/GaN interface partially transfer to Al₂O₃/AlGaN interface. The slope during this transition looks less steep than the one from stage 1 to stage 2, which indicates a higher density of states at Al₂O₃/AlGaN interface. At stage 3, electrons accumulate at Al₂O₃/AlGaN interface and the capacitance value corresponds to the capacitance of the Al₂O₃ layer.
3.3.2 Dielectric constant

This simple curve also provides us other information of the materials and capacitors. From figure 3-2, the dielectric constant of the Al$_2$O$_3$ film and AlGaN film can be calculated using the following equations:

**Al$_2$O$_3$ dielectric constant is:**

\[
\epsilon_r = \frac{C_{\text{dielectric}} \cdot t}{\epsilon_0}
\]

where \( t \) is the film thickness, and \( C_{\text{dielectric}} \) is the dielectric capacitance per unit area and can be read from the C-V curve in stage 3.
Then according to the equation of parallel capacitor:

\[
C_{\text{total}} = \frac{C_{\text{AlGaN}} \cdot C_{\text{dielectric}}}{C_{\text{AlGaN}} + C_{\text{dielectric}}}
\]

where the total capacitance \( C_{\text{total}} \) is shown in stage 2.

The capacitance of AlGaN is

\[
C_{\text{AlGaN}} = \frac{C_{\text{total}} \cdot C_{\text{dielectric}}}{C_{\text{dielectric}} - C_{\text{total}}}
\]

AlGaN dielectric constant can be calculated by:

\[
\varepsilon_{r\text{AlGaN}} = \frac{C_{\text{AlGaN}} \cdot t_{\text{AlGaN}}}{\varepsilon_0}
\]

### 3.3.3 Carrier profile

We also need the C-V profile to study electrons confinement at AlGaN/GaN heterointerface. The distribution of electrons can be extracted from C-V curve at stage 2.
Figure 3-2 C-V curve of MISH diodes at negative bias.

Figure 3-3 Carrier density profile of MISH diodes along the vertical direction.
The depth is the distance from the deposited Al$_2$O$_3$ surface.
By applying the equation:

\[ N = \frac{C^3}{q\varepsilon_r\varepsilon_0} \frac{dV}{dC} \]

We can acquire the number of carrier concentration. And the depth can be calculated by

\[ x = \frac{\varepsilon_r\varepsilon_0}{C} \]

By plotting the carrier concentration as a function of depth, we can obtain figure 3-3. This figure shows a good confinement of 2DEG within ~5 nm near the heterointerface.

If we want to know the sheet carrier density, we can integrate the carrier concentration along z direction by:

\[ n_s = \int_0^\infty N(x)dx \]

This technique is very simple and useful to determine sheet carrier density at the interface [1]. Comparing the calculated value with sheet density value obtained from Hall effect measurement, we found them in a good consistency.

<table>
<thead>
<tr>
<th>Dielectric</th>
<th>Hall (cm(^2))</th>
<th>C-V (cm(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al(_2)O(_3)</td>
<td>1.06\times10^{13}</td>
<td>1.07\times10^{13}</td>
</tr>
</tbody>
</table>

Table 3-1 Comparison of 2DEG density measured from Hall system and calculated from C-V curve.
3.4 C-V characterization of interface states density

One of the most important application for C-V measurements is to extract the interface state density information. We first start with a single measurement. Figure 3-4 shows a typical C-V curve of Al$_2$O$_3$/AlGaN/GaN MISH capacitors in which the Al$_2$O$_3$ film is grown by PEALD. The gate bias was swept from -4 to 4V at 10 KHz. The 2DEG is first depleted as the capacitance is close to zero. At $V_g = -3$V, electrons start to accumulate at AlGaN/GaN 2DEG channel, and the capacitance increases until reaching a constant value equal to the capacitance of the dielectric layer in series with the AlGaN layer. As the sweeping voltage increases to 2V, the capacitance increases again, as electrons gradually transfer to dielectric/AlGaN interface. We can divide interface states at Al$_2$O$_3$/AlGaN into three categories: fixed charges, slow traps and fast traps. Fixed charges are located in deep energy states. They shift 2DEG threshold voltage. Fast traps can follow the C-V sweep. Their energy levels are much closer to conduction band. Slow traps stay in between the fixed charges and fast traps. They cannot follow AC signal but can respond to DC signal in the C-V. By applying different C-V techniques, we can distinguish these three types of interface states [2], [3].

The fixed charge at Al$_2$O$_3$/AlGaN interface shifts the threshold voltage of 2DEG accumulation. The equation is shown below,

$$ n = \frac{C_{Al_2O_3}}{q\Delta E}(V_{th} - V_{th(ideal)}) $$

where

$$ V_{th(ideal)} = \frac{q\eta_{Hall}}{C_{total}} $$
The fixed charge density is calculated by the difference between the real $V_{th}$ and the ideal $V_{th}$, which can be calculated from the measured 2DEG density at AlGaN/GaN interface. We substitute the sheet charge density measured in Hall measurement and the capacitance in accumulation stage in figure 3-4, and obtained a $V_{th(ideal)} \sim -6$V. The real $V_{th}$ is defined as the voltage at the capacitance equal to 90% of total capacitance can be read from the C-V curve. Here we choose ΔE as the energy range that cannot respond to either AC or DC C-V signal, which is from the valence band to the lowest energy level in slow traps. The energy level will be discussed below in multi-frequency measurements. Therefore, fixed charge density can be estimated ~ $7 \times 10^{12}$/cm$^2$eV.

![C-V characteristic of MISH diodes at 10 KHz.](image)

The C-V hysteresis measurement was used to study slow trap densities. As stated before, electrons at these states cannot follow AC signal but can follow DC bias voltage change. In figure 3-5, a forward sweep from -4 V to 4 V was performed and followed by a reverse sweep back to -4 V.
The entire C-V curve is shifted after a reverse sweep. The interface state density can be calculated from equation

\[ D_{it} = \frac{C_{Al_2O_3} \Delta V}{q \Delta E} \]

where

\[ \Delta E = kT \ln\left(\frac{f_1}{f_2}\right) \]

and the corresponding signal period is between DC sweep rate and the entire sweep time, from 0.1s to 100s. The detail calculation of \( \Delta E \) is given in next section. And the slow trap density is found around \( 2.2 \times 10^{13}/\text{cm}^2\text{eV} \) at the band range from \( E_c-0.6\text{eV} \) to \( E_c-0.42\text{eV} \).

![C-V hysteresis characteristic of the MISH diode swept from -4V to 4V, and back to -4V at 10KHz. The voltage difference is also extracted to calculate the deep level interface state density.](image)

Figure 3-5 C-V hysteresis characteristic of the MISH diode swept from -4V to 4V, and back to -4V at 10KHz. The voltage difference is also extracted to calculate the deep level interface state density.
3.5 Multi-frequency C-V for interface states

The multi-frequency C-V characterization was carried to investigate fast traps located near the conduction band. C-V curves with three different frequencies (1KHz, 10KHz and 100KHz) are plotted in Figure 3-6. A frequency dispersion is observed at positive voltage since traps with a certain emission constant can only respond to a slow test signal. We may use Shockley Read Hall model to explain this behavior. The emission constant \( \tau \) can be expressed by

\[
\tau = \frac{1}{\frac{1}{\sigma v_{th}N_t} \exp\left(\frac{E_t}{kT}\right)}
\]

assuming \( E_t \) is the energy difference from the defect state to the conduction band. The emission constant has to be smaller than the test signal so that electrons at traps can follow the small signal and therefore can contribute to capacitance increase at positive bias.

![Figure 3-6 Multi-frequency C-V characteristic of the MISH capacitor with forward sweep from -4V to 4V at 1KHz, 10KHz and 100KHz. The solid lines are plotted to extract the onset voltage for the charge transfer process.](image)
In figure 3-6, low frequency C-V and high frequency C-V correspond to high and low test signals, since \( f \sim \frac{1}{\tau} \). Relating them to \( \tau \) expression, we can find \( f \sim \exp \left( -\frac{E_t}{k\tau} \right) \). It means that traps in deep states with larger activation energy (larger \( E_t \)) can only follow low frequency while not high frequency. In figure 3-7, \( E_t \) difference at two measurement frequency can be written as:

\[
\Delta E = kT \ln \left( \frac{f_1}{f_2} \right)
\]

and the trap density can be obtained by:

\[
D_{it} = \frac{C_{Al_2O_3} \Delta V}{q \Delta E}
\]

where \( \Delta V \) is the difference between voltages at the onset of capacitance increase and can be read from figure 3-6. It corresponds to the voltage at which electrons at traps start to communicate with the conduction band. Then an average trap density of \( 4.6 \times 10^{13} \text{cm}^{-2}\text{eV} \) can be acquired within the energy level from \( E_c-0.3\text{eV} \) to \( E_c-0.18\text{eV} \).

![Figure 3-7 Schematic band diagram of the Al₂O₃/AlGaN/GaN MISH capacitor that illustrates \( \Delta E \) and \( \Delta V \) at different C-V test frequencies.](image)

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Table 3-2 summarizes the density of three types of defects at Al₂O₃/AlGaN interface. As the defect energy level approaches to midgap, the density of the defect reduces.

Table 3-2 Al₂O₃/AlGaN interface defect densities in the PEALD MISH diode.

<table>
<thead>
<tr>
<th>Defect type</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed charge</td>
<td>7×10¹²</td>
</tr>
<tr>
<td>Slow trap</td>
<td>2.2×10¹³</td>
</tr>
<tr>
<td>Fast trap</td>
<td>4.6×10¹³</td>
</tr>
</tbody>
</table>

3.6 Effects of thermal ALD and PEALD Al₂O₃ thin films

Multiple ALD growth techniques have been developed to deposit Al₂O₃ films. Among them, two of the most frequently used methods are thermal ALD and plasma enhanced ALD. Both of them involve TMA as aluminum precursor, but the oxidizing agent are different. Thermal ALD uses H₂O vapor while PEALD uses plasma O₂. We have already compared their film qualities from the material perspective. When we fabricate our device structures with these films, it is also necessary to investigate their electrical properties and understand the difference of interfacial properties resulting from these dielectrics.

Some reports have already studied the influences from different technique grown films on silicon MOS capacitors [4]. The films were grown by O₃, H₂O and O₂ oxidants and all the samples were annealed at three different temperature conditions. The C-V curves of the three films show obvious discrepancy, indicating the enormous difference in interface state densities. The annealing treatments after three types of growth techniques also had different impacts on interfacial properties. In this section we discusses influences of thermal ALD and PEALD growth techniques.
on Al$_2$O$_3$/AlGaN/GaN MISH C-V curves and Al$_2$O$_3$/AlGaN interface states, and in following sections we focuses on various effects of pre-treatments and post annealing treatments on MISH devices.

Two samples with similar Al$_2$O$_3$/AlGaN/GaN MISH structure and processes were fabricated in this study except that Al$_2$O$_3$ films were deposited by thermal ALD and PEALD, respectively. These samples went through a same testing procedure and C-V measurements were performed on them.

Figure 3-8 shows C-V curves of these two ALD grown samples at 10KHz frequency. From this graph a clear discrepancy of these two curves can be observed. The 2DEG threshold voltage of the thermal ALD sample is much more negative. Also the capacitance at stage 2 of the thermal ALD sample is slightly lower than the one in the PEALD sample. In addition, even though the measurements were performed at same frequency, the C-V curve for the thermal ALD sample is less steep at the transition from stage 2 to stage 3 and the capacitance is much lower. The sweep for the thermal ALD sample has to stop at 3.5V since the sample shows the early breakdown behavior at less than 4V.
Figure 3-8 C-V profiles of MISH diodes with thermal ALD Al₂O₃ thin film and PEALD Al₂O₃ thin film.

Figure 3-9 (a) shows a close look of the C-V curves from stage 1 to stage 2 and figure 3-9 (b) shows the C-V from stage 2 to stage 3. According to previous analysis and equation, the fixed charge densities of these two films have a significant difference. Still using equations below:

\[ n = \frac{C_{Al_2O_3}}{q\Delta E} (V_{th} - V_{th(ideal)}) \]

where

\[ V_{th(ideal)} = \frac{qn_{Hall}}{C_{Al_2O_3/AlGaN}} \]
Then we can obtain the fixed charge density at thermal Al₂O₃/AlGaN interface. Notice that the negative fixed charge in the PEALD sample is larger than the one in the thermal ALD sample with same Al₂O₃ film thickness. Since the Al₂O₃ film itself exhibits negative interfacial fixed charges and positive bulk fixed charges as its intrinsic property, the larger density of fixed charges in the PEALD sample indicates the denser and better quality film with low positive fixed charges. The explanation can probably be that the use of thermal energy in thermal ALD does not fully activate the oxidant so that the precursor is not completely reacted, and therefore unreacted precursor may still exist in the thermal ALD film. On the other hand, PEALD provides plasma O₂ with enough energy to thoroughly oxidized TMA precursor, and a purer Al₂O₃ film is obtained. The number of fixed charges also plays a critical role on determining the threshold voltage of the device. The negative fixed charge results in a positive shift of the threshold voltage. The PEALD sample enables a threshold voltage that closer to the positive, and that might be beneficial to the development of the enhancement mode transistor that currently is still a big challenge.

At stage 2, dielectric constant of the Al₂O₃ film can be calculated through the capacitance. The lower K value of the thermal ALD Al₂O₃ film also confirms the less dense film compared to the PEALD film.

From the previous interpretation of the C-V curve, we can estimate the interface state density through the slope and voltage difference at the transition from stage 2 to 3. The steeper curve for the PEALD sample indicates a better interface and a lower density. Since we have obtained the fast trap density for PEALD grown samples from previous calculation, the Al₂O₃/AlGaN fast trap density for thermal ALD samples can be also calculated by the same equation using multi-frequency C-V:
\[ \Delta E = kT \ln \left( \frac{f_1}{f_2} \right) \]

\[ D_{it} = \frac{C_{Al_2O_3} \Delta V}{q \Delta E} \]

We further carried out a C-V hysteresis measurement for the thermal ALD sample. Using the same calculation as shown in previous section, we can get the slow trap density. Combining all three types of defects, table 3-3 summarizes a comparison of the interface state density for the thermal ALD and PEALD Al_2O_3/AlGaN/GaN MISH structures. From this table, we can conclude that the PEALD sample has less traps but more fixed charges than the thermal ALD sample. Since normal transistor operation is mainly affected by the number interface states and traps, the PEALD Al_2O_3/AlGaN/GaN structure might offer a better device performance and reliability.

Figure 3-9 C-V profile of (a) 2DEG depletion to accumulation region and (b) 2DEG transfer from AlGaN/GaN to Al_2O_3/AlGaN interface region.
Table 3-3 Comparison of Al₂O₃/AlGaN interface defect densities in thermal ALD and PEALD MISH diodes.

<table>
<thead>
<tr>
<th>Defect type</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PEALD</td>
<td>Thermal ALD</td>
</tr>
<tr>
<td>Fixed charge</td>
<td>7×10¹²</td>
<td>4.1×10¹²</td>
</tr>
<tr>
<td>Slow trap</td>
<td>2.2×10¹³</td>
<td>3.6×10¹³</td>
</tr>
<tr>
<td>Fast trap</td>
<td>4.6×10¹³</td>
<td>6.8×10¹³</td>
</tr>
</tbody>
</table>

Another interesting point can be raised if we plot the capacitance in a logarithm scale versus the voltage bias in figure 3-10. Notice that the thermal ALD curve has a larger capacitance tail at stage 1 that corresponds to the off channel and 2DEG depletion. This is an indication that more electrons and leakage exist in this region for the thermal ALD sample. In terms of the device performance, we can probably translate this phenomenon into a larger subthreshold leakage and worse off-state behavior in thermal ALD grown transistors.
3.7 Effects of pre-deposition surface treatments

It is believed that the surface treatment prior to dielectric deposition might have a positive effect on dielectric/semiconductor interfacial properties. The plasma technology has been extensively utilized in semiconductor industry. The implementation of the plasma process into surface treatment results from its various functions. First, energetic plasma species either chemically react with surface contaminants or physically break impurity bonds so that organic and other impurity contents reduce due to their dissociation with surface. The plasma may also react with surface atoms and form a thin interfacial layer. This layer may change the surface functional group and therefore benefit subsequent growth. Either usage can provide a cleaner surface and improve interfacial properties [5]. In our research, several plasma surface treatment methods were
investigated and improvements of Al₂O₃/AlGaN interface were observed. Figure 3-11 compares the C-V profiles of three types of MISH diodes with plasma N₂, plasma NH₃ treatment and without treatment. The sample under N₂ treatment has the steepest slope at the transition region. The NH₃ treatment sample is also slightly better than the one without surface treatment. The detail analysis is given below.

![C-V profiles comparison of MISH diodes with NH₃ pre-deposition treatment, N₂ pre-deposition treatment and without treatment.](image)

3.7.1 Plasma N₂

The MISH diode was fabricated using standard process, except that a 10 minutes plasma nitrogen treatment was applied to AlGaN surface prior to Al₂O₃ deposition. C-V techniques described above were performed on samples with and without treatments to compare the treatment effects.
Table 3-4 shows the defect state densities with 50W, 100W plasma N\textsubscript{2} treatment and without any treatment.

Table 3-4 Comparison of Al\textsubscript{2}O\textsubscript{3}/AlGaN interface defect densities in MISH diodes with different N\textsubscript{2} plasma power.

<table>
<thead>
<tr>
<th>Defect type</th>
<th>Defect density (cm\textsuperscript{-2}eV\textsuperscript{-1})</th>
<th>Defect density (cm\textsuperscript{-2}eV\textsuperscript{-1})</th>
<th>Defect density (cm\textsuperscript{-2}eV\textsuperscript{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-treatment</td>
<td>7×10\textsuperscript{12}</td>
<td>50W</td>
<td>100W</td>
</tr>
<tr>
<td>Fixed charge</td>
<td>4.5×10\textsuperscript{12}</td>
<td>5.6×10\textsuperscript{12}</td>
<td></td>
</tr>
<tr>
<td>Slow trap</td>
<td>2.2×10\textsuperscript{13}</td>
<td>5.2×10\textsuperscript{12}</td>
<td>9.1×10\textsuperscript{12}</td>
</tr>
<tr>
<td>Fast trap</td>
<td>4.6×10\textsuperscript{13}</td>
<td>8.6×10\textsuperscript{12}</td>
<td>1.6×10\textsuperscript{13}</td>
</tr>
</tbody>
</table>

From the table above it can be summarized that the diodes with 50W and 100W plasma N\textsubscript{2} surface treatments both have better interfacial properties than the one without treatment. The explanation for these results can be described as following: The plasma nitrogen radicals can react with surface impurities such as native oxides and carbon so the number of defects can be reduced. In addition, by replacing these impurities on the surface, nitrogen atoms can be bonding with underneath gallium atoms, and therefore form a surface nitridation layer on AlGaN. The nitridation layer can prevent Ga-O bonds formation during the ALD growth. The XPS characterization in last chapter also suggests less Ga-O bonds existing after surface treatment. The reduction of Ga-O bonds minimizes the interface state density and improves the Al\textsubscript{2}O\textsubscript{3}/AlGaN interfacial properties.

Comparing with the 50W plasma treatment sample, the 100W plasma sample has a higher interface state density. The possible reason for the higher trap density can be due to stronger ion
bombardments at high power that lead to the damage of surface stoichiometry. Energetic nitrogen ions break Ga-N and Al-N bonds and create traps at AlGaN surface.

3.7.2 Plasma NH₃

The effects of plasma NH₃ treatment was also investigated. Similar processes were applied to MISH diodes fabrication and a 10 minutes NH₃ treatment was employed before ALD. Table 3-5 compares the interface state densities with different treatment power.

The NH₃ plasma treatment has similar effects as the N₂ plasma treatment. As other studies also suggested, the nitrogen based plasma treatments are able to recover N-vacancy related defects. NH₃ may bring particular benefits because the hydrogen inside can passivate not only surface dangling bonds but bulk defects in GaN as well [6]. In our study, the effectiveness of the NH₃ plasma treatment is not as good as the N₂ treatment, which confirms our XPS study on GaOₓ/GaN ratio. Other report shows that NH₃ is not sufficient to remove native oxides on GaN by nature [7].

<table>
<thead>
<tr>
<th>Defect type</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-treatment</td>
<td>50W</td>
<td>100W</td>
<td></td>
</tr>
<tr>
<td>Fixed charge</td>
<td>7×10¹²</td>
<td>6.4×10¹²</td>
<td>6.2×10¹²</td>
</tr>
<tr>
<td>Slow trap</td>
<td>2.2×10¹³</td>
<td>9.7×10¹²</td>
<td>1.1×10¹³</td>
</tr>
<tr>
<td>Fast trap</td>
<td>4.6×10¹³</td>
<td>2×10¹³</td>
<td>1.9×10¹³</td>
</tr>
</tbody>
</table>

Table 3-5 Comparison of Al₂O₃/AlGaN interface defect densities in MISH diodes with different NH₃ plasma power.
3.8 Effects of post-deposition annealing

We have studied and characterized the Al$_2$O$_3$/AlGaN interface and the post annealing effects on interface states to better understand the relative importance of these issues. The Al$_2$O$_3$ layer was deposited by atomic layer deposition in Savannah thermal ALD system. Trimethylaluminum and water vapor were used as the Al and O sources for the Al$_2$O$_3$ films. The samples then underwent post deposition annealing at 400 °C, 500 °C and 600 °C for 5 minute in nitrogen atmosphere, respectively. Non-annealed Al$_2$O$_3$/AlGaN/GaN structure was also fabricated for comparison.

![C-V curves comparison of MISH diodes with and without post-deposition annealing.](image)

C-V curves of non-annealed sample and annealed sample are compared. The threshold voltage of the annealed sample shifts toward the positive side, which shows a reduction of positive fixed charges. The positive fixed charge here represents the net fixed charge in both bulk Al$_2$O$_3$ film and
at Al₂O₃/AlGaN interface. The bulk Al₂O₃ fixed charge was found carrying positive charges [8]. In this ALD system, the number of the positive fixed charges in bulk films exceeds the negative charges at the interface so that the net fixed charge density is positive. We can also find the elimination of ledges at the 2DEG onset. This probably indicates the local defect reduction by the annealing and the recovery of dangling bonds. The higher capacitance at positive voltage shows more electrons accumulated at Al₂O₃/AlGaN interface due to less trapped electrons at interface states.

![C-V hysteresis curves](image)

Figure 3-13 Forward and backward C-V sweep of MISH diodes with 400°C, 500°C, 600°C 5 minutes post-deposition annealing and without post-deposition annealing.

C-V hysteresis curves (shown in figure 3-13) and multiple frequency C-V profile (not shown here) also suggest that the trap densities of annealed samples are much lower than non-annealed samples. The calculated defect densities of samples with different annealing conditions is listed in table 3-
6. It is approximately shown that the 600 °C 5 minutes annealed sample has the lowest defect density.

Table 3-6 Comparison of Al₂O₃/AlGaN interface defect densities in MISH diodes with different post annealing temperature.

<table>
<thead>
<tr>
<th>Defect type</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
<th>Defect density (cm⁻²eV⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>As-deposited</td>
<td>400°C</td>
<td>500°C</td>
<td>600°C</td>
</tr>
<tr>
<td>Fixed charge</td>
<td>4.2×10¹²</td>
<td>3.2×10¹²</td>
<td>3.4×10¹²</td>
<td>3.4×10¹²</td>
</tr>
<tr>
<td>Slow trap</td>
<td>4.9×10¹³</td>
<td>3.5×10¹³</td>
<td>3.8×10¹³</td>
<td>2.7×10¹³</td>
</tr>
<tr>
<td>Fast trap</td>
<td>1×10¹⁴</td>
<td>7.3×10¹³</td>
<td>7.2×10¹³</td>
<td>5.3×10¹³</td>
</tr>
</tbody>
</table>

3.9 References


Chapter 4 Dielectric conduction and reliability

One of the most important reasons for introducing dielectric layer into GaN heterostructure is to suppress gate leakage current during device operation. The dielectric material should have good insulating properties so that electrons in the channel cannot transport to gate terminal. Therefore, it is necessary to study carrier transport properties for our Al₂O₃ films. In this chapter, current voltage (I-V) tests were carried out on the MISH diodes and the temperature dependence of I-V curves were analyzed.

4.1 Dielectric conduction mechanisms

Dielectric conduction properties have been well studied in silicon industry due to the need of thinner dielectric films and the development of high K dielectric materials in both logic and memory application. In Table 4-1, several common current transport mechanisms are summarized [1]. It should be noticed that most of these processes involve the temperature and voltage variables.
As dielectric thickness reduces, quantum mechanical tunneling becomes more and more significant. This quantum process involves the penetration of electron wave through dielectric potential barrier and shows a strong field dependence. The tunneling behavior can be separated into three categories: direct tunneling, Fowler-Nordheim tunneling and trap assisted tunneling.

Direct tunneling occurs in thin dielectric films (usually less than 5 nm). This type of tunneling does not require a high electric field. The tunneling current can increase exponentially when dielectric thickness decreases. As oxide thickness scales down, high K dielectric materials have to be developed to prevent excessive gate current leakage which affects the circuit operation. The expression of direct tunneling current is:

\[ J \propto \varepsilon_i^2 \exp \left( -\frac{4\sqrt{2m^*} (q \phi_B)^{3/2}}{3qh \varepsilon_i} \right) \propto V^2 \exp \left( -\frac{b}{V} \right) \]

<table>
<thead>
<tr>
<th>Process</th>
<th>Expression</th>
<th>Voltage &amp; temperature dependence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tunneling</td>
<td>( J \propto \varepsilon_i^2 \exp \left( -\frac{4\sqrt{2m^*} (q \phi_B)^{3/2}}{3qh \varepsilon_i} \right) )</td>
<td>( \propto V^2 \exp \left( -\frac{b}{V} \right) )</td>
</tr>
<tr>
<td>Thermionic emission</td>
<td>( J = A^{**} T^2 \exp \left[ -\frac{q (\phi_B - \sqrt{q \varepsilon_i / 4\pi\varepsilon_i}}{kT} \right] )</td>
<td>( \propto T^2 \exp \left[ \frac{q}{kT} (2a \sqrt{V} - \phi_B) \right] )</td>
</tr>
<tr>
<td>Frenkel-Poole emission</td>
<td>( J \propto \varepsilon_i \exp \left( -\frac{q (\phi_B - \sqrt{q \varepsilon_i / 4\pi\varepsilon_i}}{kT} \right] )</td>
<td>( \propto V \exp \left[ \frac{q}{kT} (2a \sqrt{V} - \phi_B) \right] )</td>
</tr>
<tr>
<td>Ohmic</td>
<td>( J \propto \varepsilon_i \exp \left( -\frac{q (\phi_B - \sqrt{q \varepsilon_i / 4\pi\varepsilon_i}}{kT} \right] )</td>
<td>( \propto V \exp \left( -\frac{c}{T} \right) )</td>
</tr>
<tr>
<td>Ionic conduction</td>
<td>( J \propto \varepsilon_i \exp \left( -\frac{q (\phi_B - \sqrt{q \varepsilon_i / 4\pi\varepsilon_i}}{kT} \right] )</td>
<td>( \propto V \exp \left( -\frac{d'}{T} \right) )</td>
</tr>
<tr>
<td>Space-charge-limited</td>
<td>( J = \frac{9 \varepsilon_i \mu V^2}{8d^3} )</td>
<td>( \propto V^2 )</td>
</tr>
</tbody>
</table>

\( A^{**} \) = effective Richardson constant. \( \phi_B \) = barrier height. \( \varepsilon_i \) = electric field in insulator. \( \varepsilon_i \) = insulator permittivity. \( m^* \) = effective mass. \( d \) = insulator thickens. \( \Delta E_{ac} \) = activation energy of electrons. \( \Delta E_{ai} \) = activation energy of ions. \( V \approx \varepsilon_i d \). \( a = \sqrt{q / 4\pi\varepsilon_i d} \). \( b \), \( c \), and \( d' \) are constants.
where $E_{ox}$ is the oxide electric field, $m_{ox}$ is the oxide average electron mass, $\Phi_B$ is the potential barrier height between metal and dielectric conduction band, $q$ is electron charge and $\hbar$ is Planck constant divided by $2\pi$.

Fowler-Nordheim tunneling is a special type of direct tunneling as electrons only tunnel through the top triangular potential barrier of the dielectric film. This type of tunneling usually occurs in thicker dielectric film and requires a high enough electric field in the dielectric. The Wentzel-Kramers-Brillouin (WKB) approximation is often involved during the tunneling current calculation. The equation is listed as below:

$$J \propto E_{ox}^2 \exp\left[-\frac{4\sqrt{2m_{ox}^*(q\phi_B)^2}}{3q\hbar E_{ox}}\left(1 - \left(1 - \frac{V_{ox}}{\Phi_B}\right)^{\frac{3}{2}}\right)\right]$$

Trap assisted tunneling is another tunneling process that electrons tunnel to semiconductor through assistance of trap states which result from pre-existing traps in the dielectric or bulk traps induced by electrical stress during device operation. This tunneling can happen at very low electrical field and the tunneling current will increase as more traps are created due to the stress. The equation for trap assisted tunneling is:

$$J \propto \exp\left[-\frac{4\sqrt{2m_{ox}^*(q\phi_t)^2}}{3q\hbar E_{ox}}\right]$$

Thermionic emission and Frenkel-Poole emission are two important transport mechanisms in dielectrics besides tunneling processes. Thermionic emission involves electrons jumping over the dielectric potential barrier and usually occurs at high temperature because of the need of enough
thermal energy. Frenkel-Poole emission, however, is strongly dependent of both temperature and electric field. This process requires thermal excitation of trapped electrons to dielectric conduction band.

Figure 4-1 describes four types of tunneling processes.

![Figure 4-1 Schematic band diagram illustrating conduction mechanisms of (a) direct tunneling, (b) F-N tunneling, (c) thermionic emission and (d) F-P emission.]

4.2 Gate conduction current of thermal ALD and PEALD Al$_2$O$_3$ thin films

MISH diodes with thermal ALD and PEALD grown Al$_2$O$_3$ films of 12 nm thickness were fabricated and characterized by I-V measurement. Schottky structure diodes without Al$_2$O$_3$ films were also fabricated and tested as comparison.

Figure 4-2 shows negative to positive I-V sweep on three diodes with thermal ALD, PEALD and without ALD process. We observe a significant reduction of gate leakage current in both thermal ALD and PEALD MISH structures compared to the schottky structure. It indicates that Al$_2$O$_3$ films can effectively suppress leakage current at a high voltage bias. Besides, PEALD Al$_2$O$_3$ film shows
better insulating property than thermal ALD Al₂O₃ film, since plasma process reacts with precursor more completely and provides a denser and better quality film [2].

![Figure 4-2 J-V characteristic of schottky diode and MISH diodes using thermal ALD and PEALD Al₂O₃ growth.](image)

### 4.3 Effects of post deposition treatment

MISH diodes fabricated by PEALD Al₂O₃ film with 5 minutes 500°C N₂ post deposition annealing were studied by I-V measurement and compared to diodes without any post treatment.

It is shown that the device after N₂ annealing has a slightly increased leakage current. This could possibly be explained by decrease of Al₂O₃ film thickness after annealing. Reduction of tunneling distance may exponentially enhance tunneling current.
4.4 Temperature dependent I-V characterization

Gate current transport properties were investigated by I-V measurement from room temperature to 200°C. The result is shown in figure 4-4. There is a clear temperature dependence for current density starting from gate voltage ~ 0.7V. After $V_g = 2.4V$, current densities measured at different temperatures begin to converge and become less temperature dependent.
To understand the actual gate current transport mechanism at different bias and temperature, we plot $J/E$ vs $1000/T$ with different bias conditions in figure 4-5. We can observe three straight curves at low to medium voltage (1.2V-2V) regime, which can be fitted into Frenkel-Poole hopping model [3]:

$$J \propto E_{ox} \exp\left[-\frac{q}{kT}(\Phi_t - \frac{qE_{ox}}{\pi\varepsilon_{ox}})\right]$$

where $\Phi_t = 0.905\text{V}$ is extracted as a trap level in the oxide and $\varepsilon_{rox} = 8.29$ is Al$_2$O$_3$ dielectric constant.

Figure 4-4 Forward J-V characteristics of MISH diodes from room temperature (25°C) to 200°C with a step temperature increase of 25°C.
In medium to high voltage bias range, J/E vs 1/T curves deviate from straight lines, and eventually become flat at low temperature when the bias is above 3.2V. It indicates that another transport mechanism dominates in this range [4]. Since the current density no longer depends on temperature, it is likely that tunneling mechanism may take place in this high oxide field region.

Trap assisted tunneling (TAT) and Fowler-Nordheim tunneling (FNT) are two possible tunneling mechanisms [5] since the oxide field is relatively high and the oxide thickness is not too thin. According to tunneling equations,

\[ J \propto \exp \left[ -\frac{4\sqrt{2m^*_{ox}(q\phi_t)^3}}{3q\hbar E_{ox}} \right] \]
and

\[ J \propto E_{ox}^2 \exp\left[-\frac{4\sqrt{2m^*_ox(q\Phi_B)^3}}{3\hbar E_{ox}}\right] \]

At low measurement temperatures (25°C and 50°C), we can fit our data with Fowler-Nordheim plot \((J/E^2 \text{ vs } 1/E)\), assuming \(m^*_ox\) is an averaged electron tunneling mass \(~0.23m_0\) [6]. In the F-N plot, the dielectric barrier height \(\Phi_B\) is extracted as \(~2.6-2.9\) eV, which is in agreement with our XPS data on Al₂O₃/AlGaN barrier height. At high temperatures, however, the F-N fitting is no longer valid since the extracted barrier height is substantially lower than previous value. At high temperatures, we can fit our curves with TAT plot \((J \text{ vs } 1/E)\), and trap states of \(~1.1-1.2\) eV can be extracted in our measurement temperature range. Therefore, we suggest that TAT may be dominant tunneling mechanism at high temperatures.
4.5 Dielectric reliability

Reliability of dielectric materials has become a more and more important issue as transistor dimensions and dielectric thickness scale down. When a gate voltage is applied to the dielectric, damage may happen in the dielectric and eventually an accumulative degradation leads to a dielectric breakdown [7]. The entire breakdown process can be separated to several stages. An early wearout is usually a long term event if the applied voltage is not high enough. In this stage, degradation increases slowly by trap generation and structural damage in the dielectric. If degradation induced defects are able to form a current conduction path along the dielectric, the current density suddenly increases by several order magnitude and short term breakdowns are triggered by local heating in the dielectric. The local temperature then reaches to dielectric melting point and permanent physical damage occurs in the dielectric.

![Figure 4-7 Dielectric breakdown processes after long term gate stress.](image)

Dielectric reliability of Al₂O₃/AlGaN/GaN MISH diode is essentially of great importance in GaN based high power transistors since devices might be operated in very critical conditions that need high voltage and high current levels. Unfortunately reliability studies of this system are very few up to now [8]. In our work, we absorbed several well developed reliability theories and evaluation methods from on Si/SiO₂ and Si/high K systems and implemented them to our MISH structures.
4.6 Reliability test

4.6.1 Stress test

Stress test is the most common dielectric reliability test. Usually a constant current or a constant voltage stress is applied to the sample and the voltage or current shift is recorded as a function of time. The density of traps generated by stress can be calculated by \( Q = C \cdot \Delta V \) in the constant current stress test.

In this work, the constant-current stress test was used to study Al\(_2\)O\(_3\) film reliability. We performed gate current stress tests at three different levels and observed gate voltage shifts under stress. Figure 4-8 illustrates \( V_g \) variation as a function of time in these stress conditions. At low stress level, the \( V_g \) remains unchanged after an initial trap filling process that results from electrons falling into traps at the interface and the bulk oxide. This small voltage shift indicates a good \( V_{th} \) stability in this MIS structure. When the stress is increased to a high current density that corresponds to a high oxide field, the gate voltage begins to drop and voltage signal becomes noisy. This could probably be explained by a hole trapping process in the oxide film. These holes may come from impact ionization due to heavily injected electrons under high oxide field. And trapped holes increase the oxide electric field near the oxide/semiconductor interface. According to the equation for tunneling, an increased electric field will result in a higher tunneling current. In the case of constant-current test, the gate voltage should decrease to keep the current unchanged. At high stress levels, defect and trap generation becomes so severe that significant voltage drops are observed.
4.6.2 Dielectric breakdown field distribution

The dielectric breakdown field is a good indicator of the dielectric material quality [9]. For a given dielectric, the breakdown field depends on traps, defects and the density of the material. Less pre-existing defects and denser films usually have higher breakdown fields. But even for films on the same sample with same process condition, breakdown fields may vary from one diode to another. It is necessary to investigate statistics of breakdown fields within a certain number of sample size. In addition, the degree of statistical variation of measured fields is also a good reflection of dielectric reliability. The less variation indicates the better deposition process.

Our study compared the breakdown field distribution for Al₂O₃ films with PEALD and thermal ALD growth in MISH diodes. N₂ and plasma N₂O post annealing effects on PEALD film
breakdown fields were also investigated. Post treatment process conditions were 5 minutes 500°C for N₂ post deposition annealing and 20 minutes 500°C for plasma N₂O post annealing, respectively.

Thermal ALD Al₂O₃ films have lowest breakdown fields among all samples. The calculation gives an average breakdown field of 7.4 MV/cm. This result is in agreement with our previous suggestion that thermal ALD Al₂O₃ films do not exhibit good insulating properties. PEALD Al₂O₃ films, however, show an average breakdown field of 8.6 MV/cm. In addition, more than 75% of test samples fall into the breakdown field range of 8-9 MV/cm. The small variation of samples indicates the reliable deposition process.

The N₂ annealing treatment on PEALD Al₂O₃ films does not significantly change the dielectric breakdown field. An average number of 8.2 MV/cm is slight below the average field of samples without annealing. The increase of leakage current could be a factor that contributes to the reduction of the mean breakdown field. On the other hand, plasma N₂O annealed samples exhibit supreme insulating properties with an average breakdown field of 8.9 MV/cm. The plasma N₂O annealing allows both oxygen and nitrogen incorporation into Al₂O₃ film. Incorporated nitrogen atoms harden the dielectric film and improve the film resistance to dielectric breakdown.
Figure 4-9 Dielectric breakdown field distribution of MISH diodes with (a) PEALD Al$_2$O$_3$ films, (b) thermal ALD Al$_2$O$_3$ films, (c) PEALD Al$_2$O$_3$ films after N$_2$ post deposition annealing and (d) PEALD Al$_2$O$_3$ films after plasma N$_2$O post deposition annealing.
4.6.3 TDDB test

One of major concerns of dielectric thin film reliability in long term is time dependent dielectric breakdown. An empirical model was first introduced with the observation of logarithm time to failure versus electric field relation. Two theories were then developed to explain this model. One theory focused on the dipolar interaction with electric field (E-Model) while the other one was based on Fowler-Nordheim tunneling (1/E-Model). Both of them were found fit experimental results very well.

The E-Model can be expressed by the following equation:

\[ \ln t \propto \frac{Q_1}{K_b T} \gamma E_{ox} \]

where \( Q_1 \) stands for the activation energy required for breaking a bond and \( \gamma \) stands for a field acceleration factor.

The 1/E-Model can be expressed by the following equation:

\[ \ln t \propto \frac{Q_2}{K_b T} - \frac{G}{E_{ox}} \]

where \( Q_2 \) stands for the activation energy related to current induced hole injection and capture and \( G \) also stands for the field acceleration factor.

We employed this TDDB test in our work in order to study Al\(_2\)O\(_3\) dielectric lifetime and reliability. The test was performed on Al\(_2\)O\(_3\)/AlGaN/GaN MISH capacitors with three constant gate voltage stress (3.4V, 3.7V and 4.0V) and 10 devices at each voltage condition. The result is plotted through Weibull distribution in figure 4-10. A Weibull slope of 2.87 is extracted by fitting \( \ln(-\ln(1-F)) \) vs \( t_{BD} \) (time to breakdown) curves. The inset figure shows a lifetime plot of this structure. The time
to 63% breakdown plot shows a field dependence of $1/E$, which also indicates that the current-driven breakdown process is dominated by tunneling conduction. This result is also in agreement with the conclusion of tunneling transport mechanism in the previous analysis.

Figure 4-10 Weibull distribution in three TDDB tests at 3.4V, 3.7V and 4V gate voltage. A Weibull slope of 2.87 is extracted from the plot. Inset plot shows a field dependence of 63% time to breakdown.

4.7 References


Chapter 5 Summary and future work

Our research helps us understand the properties of nitride based materials and devices. Although the entire picture of achieving required interfaces and dielectrics has yet to be realized, part of the issues and problems has been revealed and solved in this work.

5.1 Materials and fabrication

Thermal ALD and PEALD Al$_2$O$_3$ thin films were successfully deposited on MBE grown AlGaN/GaN heterostructure epitaxial layers. Both Al$_2$O$_3$ thin films exhibit better surface morphology. The thin film crystal structure changes from amorphous to polycrystalline after annealing under 1000°C for 5 minutes. The XPS study reveals the band offset of Al$_2$O$_3$/AlGaN interface. The fabrication of Al$_2$O$_3$/AlGaN/GaN MISH diodes was also achieved using Ti/Al/Ni/Au stack as ohmic contact while Ni/Au as gate contact. The pre-deposition treatment shows a lower oxygen concentration at interface after ALD growth. The future work could be emphasizing on developing better dielectric materials. ALD growth and surface treatment conditions can also be optimized to pursue an even lower density of interface states.

5.2 Interface

Interface state characterization by C-V test were widely used in our work. C-V profiles provide us plenty of information on dielectric material properties and dielectric/semiconductor interfacial properties. The profound C-V technique and its derivative tools enrich our knowledge and understanding on electrical performance. Traps with different energy levels were differentiated by
C-V hysteresis curves and multi-frequency C-V. Effects of deposition methods on defect densities were studied. It suggests that PEALD provides better film quality with lower defect densities than thermal ALD. The use of NH\textsubscript{3} and N\textsubscript{2} pre-deposition surface plasma treatment and post-deposition annealing also improves the interfacial behavior. In the future, more work should be focused on deep level states characterization by photo assisted C-V or DLOS. The employment of light source enables the characterization of mid-gap defect states. Since the interfacial property depends on the intrinsic compatibility of the dielectric and semiconductor material, seeking another GaN matched dielectric other than Al\textsubscript{2}O\textsubscript{3} might be an alternative solution to achieve a lower interface state density. AlN makes itself almost perfect candidate for AlGaN/GaN gate dielectric material due to its nitride based nature and small lattice mismatch with GaN. However, the high quality and high conformity film deposition needs to be realized first.

5.3 Dielectric

Al\textsubscript{2}O\textsubscript{3} dielectric thin film leakage current and conduction mechanisms were investigated. PEALD Al\textsubscript{2}O\textsubscript{3} thin films exhibit better leakage current suppression compared to thermal ALD films. The result of temperature dependent I-V characterization suggests us that Poole-Frenkel emission dominates in dielectric current transport at medium electric fields, while at high electric fields, Fowler-Nordheim tunneling and trap-assisted tunneling dominate at low temperatures and high temperatures, respectively. In terms of dielectric reliability, we employed stress test, dielectric breakdown field distribution statistics and TDDB test on Al\textsubscript{2}O\textsubscript{3} thin films. It shows that PEALD Al\textsubscript{2}O\textsubscript{3} films have a larger average dielectric breakdown field than thermal ALD films, while the plasma N\textsubscript{2}O post deposition annealing can improve the average breakdown field. TDDB test
results can be fit with 1/E field dependent model and a Weibull slop of 2.87 is extracted on PEALD Al$_2$O$_3$ thin films.

5.4 Summary

To summarize, this work focused Al$_2$O$_3$/AlGaN/GaN MISH structure design, fabrication and characterization. We successfully designed our processes, deposited Al$_2$O$_3$ thin films on AlGaN/GaN epitaxial layers by thermal ALD and PEALD techniques and fabricated Al$_2$O$_3$/AlGaN/GaN MISH diodes. Several electrical characterization methods were modified and performed to evaluate dielectric/semiconductor interfacial properties, dielectric conduction mechanisms and reliability. By applying pre-deposition surface treatment and post-deposition annealing, we were able to significantly improve the interface and dielectric material with a reduction the interface state density and gate leakage current. These achievements might offer a better device performance and reliability in MIS-HEMTs, and enable the further progress and development of nitride based power electronics.