DYNAMIC PERFORMANCE SIMULATION OF ALGAN/GAN HIGH ELECTRON MOBILITY TRANSISTORS

By

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<td>2DEG</td>
<td>Two-dimensional electron gas</td>
</tr>
<tr>
<td>AlGaN</td>
<td>Aluminium Gallium Nitride</td>
</tr>
<tr>
<td>DFT</td>
<td>Density Functional Theory</td>
</tr>
<tr>
<td>DiVA</td>
<td>Dynamic I-V Analysis</td>
</tr>
<tr>
<td>$f_{\text{max}}$</td>
<td>Maximum oscillation frequency</td>
</tr>
<tr>
<td>$f_{\text{r}}$</td>
<td>Cut-off frequency</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full-width at half maximum</td>
</tr>
<tr>
<td>GaN</td>
<td>Gallium Nitride</td>
</tr>
<tr>
<td>HEMT</td>
<td>High Electron Mobility Transistor</td>
</tr>
<tr>
<td>HFET</td>
<td>Heterostructure Field-Effect Transistor</td>
</tr>
<tr>
<td>HR</td>
<td>High Resistance</td>
</tr>
<tr>
<td>MBE</td>
<td>Molecular Beam Epitaxy</td>
</tr>
<tr>
<td>MESFET</td>
<td>Metal Semiconductor Field-Effect Transistor</td>
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<tr>
<td>MOCVD</td>
<td>Metalorganic Chemical Vapor Deposition</td>
</tr>
<tr>
<td>MOSFET</td>
<td>Metal Oxide Semiconductor Field-Effect Transistor</td>
</tr>
<tr>
<td>S3A</td>
<td>Sinusoidal Steady State Analysis</td>
</tr>
<tr>
<td>SI</td>
<td>Semi-Insulating</td>
</tr>
<tr>
<td>SRIM</td>
<td>Stopping and Range of Ions in Matter</td>
</tr>
<tr>
<td>TAT</td>
<td>Trap-assisted Tunneling</td>
</tr>
<tr>
<td>TCAD</td>
<td>Technology Computer Aided Design</td>
</tr>
<tr>
<td>TRIM</td>
<td>Transport of Ions in Matter</td>
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<tr>
<td>TMGa</td>
<td>Trimethyl Gallium</td>
</tr>
<tr>
<td>UID</td>
<td>Unintentionally Doped</td>
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GaN based devices have reached a point in terms of processing maturity where the favorable wide-band gap related properties can be implemented in several commercial and military applications. However, long term reliability continues to affect large scale integration of such devices, specifically the potential of AlGaN/GaN High Electron Mobility Transistors (HEMTs), due to the indefinite nature of defects in the structure and mechanisms of performance degradation relevant to such defects.

Recent efforts have begun to concentrate more on the bulk properties of the GaN buffer on which the heterostructure is grown, and how defects distributed in the buffer can affect the performance under various operating schemes. This dissertation discusses numerical simulator based investigation of the numerous possibilities by which such point defects can affect electrical behavior. For HEMTs designed for satellite communication systems, proton irradiation results indicate changes in the device parasitics resulting in degradation of RF parameters. Assumption of such radiation damage introducing fast traps indicate severe degradation far exceeding experimental observation. For power switching applications, the necessity of accurately capturing as-grown defects was realized when modeling current relaxation during bias switching.
Ability to introduce multiple trap levels in the material bulk aided in achieving simulation results replicating experimental results more accurately than published previously. Impact of factors associated with such traps, either associated with discrete energy levels or band-like distribution in energy, on the nature of current relaxation characterized by its derivative has been presented.
CHAPTER 1
GALLIUM NITRIDE TECHNOLOGY

Gallium Nitride (GaN) is a III-V semiconductor which first caught attention of the scientific community because of its direct band which potentially made it attractive for its electroluminescent properties. Grimmeiss and Koelmans [1] were the first to investigate the luminescence properties on GaN samples fabricated by heating gallium in an ammonia (NH₃) stream. However, these samples synthesized were in the form of needles and platelets. Maruska and Tietjen [2] recognized that the wide bandgap of III-Nitrides placing them in the colored to UV spectrum, along with potentially other high temperature applications, mandated further investigation. They carried out vapor-phase growth of GaN on sapphire substrate to form samples on which both electrical and optical characterization could be carried out. With further investigation into obtaining high quality GaN films and understanding compensation of Mg doping to obtain low resistivity p-type GaN, the GaN based blue and green LED was realized [3]-[10].

The improvement in the growth techniques were then taken advantage of by those looking into possible alternatives to GaAs based microwave devices. Material properties of GaN made it suitable for making transistors meant for high-power, high-frequency and high-temperature applications. Binari [11] analyzed a number of device architectures based on GaN and concluded that a heterostructure field effect transistor (HFET), similar to AlGaAs/GaAs devices, exhibited excellent dc and microwave performance parameters due to the presence of the 2-dimensional electron gas (2DEG) at the heterointerface. Khan et al. [12] concluded that the higher effective mass of GaN meant the 2DEG mobility was less affected by impurity scattering, allowing the introduction of donors which further increased sheet carrier density. Similar to optical
applications, these early transistor designs were based on GaN grown on sapphire substrates for lattice mismatch concerns. For high-temperature applications, 4H-SiC was introduced as a substrate for its excellent thermal conductivity [13], once better understanding of the buffer layer at the substrate interface was gained.

Applications

The material properties of GaN and its application in the form of AlGaN/GaN heterostructure based power devices thus make it the ideal candidate for use in various high power, RF communication and microwave electronics. However, it also faces competition from SiC, and potentially from diamond. In terms of process maturity, SiC holds the upper hand at the moment, with GaN slowly catching up. Several research programs have been set up in recent years to help select the right material and device architecture for some of these applications (Table 1-1). In particular, the potential growth of electric vehicles could spur investment in the development and enablement of large scale incorporation of wide-bandgap semiconductors into commercial power switching applications such as power supplies and motor drives [14], [15].

Table 1-1. Comparison of material properties and figures of merit of wide-band-gap semiconductors

<table>
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<tr>
<th>Parameter</th>
<th>4H-SiC</th>
<th>GaN</th>
<th>Diamond</th>
</tr>
</thead>
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<tr>
<td>( E_g ) (eV)</td>
<td>3.26</td>
<td>3.39</td>
<td>5.47</td>
</tr>
<tr>
<td>( E_{crit} ) (MV/cm)</td>
<td>2.2</td>
<td>3.3</td>
<td>5.6</td>
</tr>
<tr>
<td>( \epsilon_r )</td>
<td>9.7</td>
<td>9.0</td>
<td>5.7</td>
</tr>
<tr>
<td>( \mu_n ) (cm(^2)/V.s)</td>
<td>950</td>
<td>1700</td>
<td>1800</td>
</tr>
<tr>
<td>BFoM (w.r.t Si)</td>
<td>500</td>
<td>2700</td>
<td>9000</td>
</tr>
<tr>
<td>( \lambda ) (W/cm.K)</td>
<td>3.8</td>
<td>1.3</td>
<td>20</td>
</tr>
</tbody>
</table>
Modules and components composed of these devices have already found their application in several domains, particularly in the military sector, limited not just to terrestrial but could potentially be expanded to space environments as well.

Military

The figures of merit discussed above motivated the technology development for GaN processing over the last 20 years, and the current state of the art has allowed the deployment of GaN based systems for military operations. First such application is the missile defense system RADARs which till date have employed numerous different components to deal with scanning, tracking and electronic attack. For eg. during scanning phase, potential threats are determined by sending out long wavelength radio waves which fall in the S-band, whereas once the target has been detected, accurate tracking requires shorter wavelengths in the X-band. Vendors have indicated that GaN based systems have allowed compact integration of several such systems and fast switching between the different modes in real-time [16].

Microwave based directed-energy weapon systems are also currently under development. Impractical bulky gyrotron-based systems have been demonstrated in the past, but a GaN monolithic microwave integrated circuit (MMIC) based solid state alternative appears to be currently under development which will allow a smaller form factor, and thus expected to provide faster deployment through multiple platforms [17], [18].

Commercial

Adoption of GaN as an alternative in the commercial sector has been limited up to this point, for both RF and power switching applications. Products that are currently being developed and marketed to be taking advantage of GaN include wireless
charging, Light Detection and Ranging (LiDAR) and augmented reality applications [19]-[21].

LiDAR has played a prominent role in development phase of autonomous vehicles and robotics. But vehicles currently in the market that come closest to implementing autonomous driving capability favor RADAR due to superior performance under inclement weather conditions and computationally lighter operation.

**High Electron Mobility Transistor**

High Electron Mobility Transistor device architecture can be described according to the vertical and lateral features (Figure 1-1). The vertical stack of materials generally starts with a substrate such as sapphire, SiC or lately even Silicon and approximately 2-3 μm of GaN buffer layer grown on top of this substrate. Epitaxially grown material quality concerns dictate the presence of a roughly 25 nm thin layer of AlN at the GaN and substrate interface. An AlGaN layer of typically 20 to 30 nm in thickness is grown on top of the GaN to form the heterostructure which serves as the active region of the device. Aluminum mole fraction of 0.25-0.3 is generally favored for the AlGaN layer. A metal alloy Schottky gate generally comprised of Ni/Au/Ti is formed with nitride passivation on either side. The Schottky gate is expected to present a barrier height of 0.6-1eV. Ohmic type contacts on either side of the Schottky gate form source and drain contacts.

HEMT structures having different lateral dimensions will be discussed as per specific operation regimes depending on their applications. For example, HEMTs required for RF applications with high operating frequencies need shorter gate lengths [22], [23]. On the other hand, HEMTs meant for power conversion applications need to be able to handle large voltages at the drain. Such devices have an asymmetric
appearance due to a larger gate to drain spacing, also called the drain access region. Details about the lateral dimensions will thus be specified in the respective chapters.

Forbidden band-gap of GaN with temperature dependence can be described by:

\[ E_{g,GaN}(T) = 3.51 - 7.7 \times 10^{-4} \frac{T^2}{(T+600)} \text{ eV} \]  

(1-1)

which gives a band-gap of 3.43 eV at 300 K. Like other alloys, for AlGaN, parabolic dependence of band-gap on its composition is described by the following expression:

\[ E_g(x) = E_{g,AlN}x + E_{g,GaN}(1-x) - b.x(1-x) \]  

(1-2)

where band-gap of AlN is taken as 6.13 eV, \( x \) is the Al mole fraction and bowing parameter \( b \) which defines the parabolic relation with composition is assumed to be 1. At 300 K, with an Al mole fraction of 0.25 results in an AlGaN band-gap of 3.92 eV.

The resulting heterointerface has a net charge at its interface due to polarization effect. The polarization charge has two components, i.e., instantaneous polarization due to the polar nature of the III-N group, and the piezoelectric polarization due to the stress at the interface [24]. This interface charge is dependent on the thickness and composition of the AlGaN layer, and for the above-mentioned values results in a net positive charge of approximately \( 10^{13} \text{ cm}^{-2} \). Formation of the two-dimensional electron gas at the heterointerface thus takes place (Figure 1-2). Even though charges distributed throughout the bulk will also affect the 2DEG, the polarization charge happens to be the most critical component in determining the HEMTs characteristics.

While the 2DEG controls the electrical characteristics through both the threshold voltage and conductance in the access regions, mobility of the 2DEG electrons is
another important factor. Calibration of on-state conductance requires selection of the right parameters described by the mobility model, role of charge distributed in the structure and their effect on device behavior have been detailed with reference to steady state simulation in Chapter 4.

Owing to the presence of the 2DEG, a typical AlGaN/GaN HEMT with Schottky gate operates as a depletion mode device (Figure 1-3). Development of normally-off HEMTs has been successful in recent years by taking two approaches. First is a 2-chip solution in which a depletion mode HEMT is in cascode connection with a Si MOSFET [25]. The other solution is a single chip approach that uses p-doped GaN or AlGaN between the gate and heterostructure AlGaN layer [26].

**Motivation**

The adoption of GaN technology has been spurred by the numerous advantages the material properties of GaN, and in the form of heterostructure based transistors. Most of the discussion above has been limited to fundamental properties which typically define ideal electrical characteristics. However, when it comes to applications which expose hardware to harsher environments, long term reliability is to be taken into consideration. For satellite communication, the electronics requires to be immune to performance degrading space radiation, such as high energy electron and proton bombardment.

For GaN, it has been observed that the extent of damage is worse for proton strikes leading to displacement damage to the host lattice [27]. Empirical relation between lattice constant and displacement threshold necessary to cause damage place GaN at the same level as SiC, and much higher threshold than GaAs [28]. Subsequent investigation of proton irradiation studies of AlGaN/GaN HEMTs have exhibited a
positive shift in threshold, reduction in saturation current, degradation of RF performance parameters such as cut-off frequency, as well increased dynamic on-resistance.

Exposure to proton irradiation is assessed in the form of total dose the device has been exposed to, also termed as fluence, which can also be correlated to number of years in low-earth orbit. For most AlGaN/GaN HEMTs discussed in literature, critical steady state performance degradation is observed beyond fluence values of $10^{14}$ cm$^{-2}$. This corresponds to roughly 50-100 years in low earth orbit, which has established it as an ideal candidate [29].

However, a better understanding of the exact mechanisms that contribute to the observed degradation is necessary. With the aid of TCAD numerical simulations, it has now been established that vacancies resulting from displacement damage contribute to the observed degradation in steady state performance. Yet, further work is still required to get a better understanding of how the dynamic performance parameters in RF/microwave regime as well as power switching amplifiers get affected by such proton strikes. What makes this exercise even more tortuous is the process dependence of dynamic performance and higher sensitivity of bias switching transients to as-grown defects.

**Organization**

This dissertation will help provide a fundamental understanding of as to how point defects in the GaN buffer region can affect the electrical characteristics of an AlGaN/GaN HEMT. This insight will help support the ability to comprehensively model the behavior of such devices with the aid of TCAD numerical device simulators, under
various operating regimes, examining variations in their characteristics in the presence of the above-mentioned defects and identifying the causes for such non-idealities.

Chapter 2 will introduce several point defects that can be expected in the GaN buffer. More specifically, the trap levels introduced in the GaN band-gap by these defect centers in the form of isolated point defects or complexes will be presented. Chapter 3 will introduce the FLOODS TCAD numerical device simulation framework that has been utilized to carry out all the results discussed in this dissertation. The finite-element based FLOODS solves for the partial differential equations which describe the physics, and the argument for focusing on certain aspects of semiconductor physics in terms of AlGaN/GaN HEMTs will be put forward.

Chapter 4 reviews already published results of TCAD simulation of steady state behavior of proton irradiated HEMTs, elaborating further on the procedure that was followed to calibrate simulation and model parameters to fit simulation to experimental data. Chapter 5 discusses the possible mechanisms that can affect RF performance parameters of HEMTs post proton irradiation, building on conclusions made from investigation of steady state performance degradation. For Chapters 6 and 7, focus will shift from proton irradiation damage to as-grown defects, as their role in the lag observed in switching transients is investigated.
Figure 1-1. Normally-on AlGaN/GaN HEMT structure with 2DEG. Inset shows AlGaN layer grown on top of GaN to induce 2DEG at the heterointerface.

Figure 1-2. Band bending as a result of the net positive polarization charge at the heterointerface resulting in the formation of the 2DEG.
Figure 1-3. Typical transfer characteristics of a normally-on depletion mode HEMT at low drain bias ($V_{DS}=1\text{V}$).
For the simulation of defects present in the AlGaN/GaN heterostructure system, it is important to understand the origin of such imperfections from a process development perspective. With major breakthroughs having taken place in the last 20 years motivated by tremendous interest in employing GaN based devices to optical applications, the power electronics sector has sought to leverage this advancement in developing GaN as a viable alternative to other wide-bandgap materials. Better understanding of the process kinetics and stoichiometry have helped in achieving crystallinity that guarantee improved reliability.

The relative impact on device performance due to surface states at the AlGaN surface, resulting in 2DEG depletion in the drain-access region, is no longer as pronounced as during the nascent stages of development [30]-[38]. Instead, various processing techniques that have been adopted in fabrication of GaN based devices, have been recognized to introduce a multitude of point defects, which can be classified as not only intrinsic or native, but also originate from ambient sources. In this chapter, different aspects responsible for contributing to the defects leading to trap states in the forbidden band-gap of GaN will be discussed.

In section I, point defects expected to be present in a crystalline material will be defined together typical examples found in GaN. In section II, the two most prominent heteroepitaxial growth techniques, MBE and MOCVD, will be introduced. The ambient conditions, precursors, and other possible sources of contaminants will be presented together with variants of these growth techniques that can help in improving crystallinity.
The parameters responsible for selection of a suitable substrate will also be put forward together with the role of the nucleation layer in reducing extended defects. In section III, some of the fundamental point defects often detected in epitaxially grown GaN films will be described. These constitute of unintentional doping such as native defects and contaminants, or intentional doping such as Fe and C necessary to form high-resistance buffer layers. Their necessity from a device operation perspective as well as impact on reliability will also be presented.

**Point Defects**

Before going into the details of the various sources and trap parameters of the numerous defects that one encounters when carrying out defect characterization of GaN, a brief introduction to the isolated point defects that can be present in a crystalline material is necessary [39], [40].

**Vacancy**

A vacancy is formed when a host lattice atom is missing from its expected position in the lattice. These are encountered in the GaN lattice in the form of nitrogen and gallium vacancies, typically represented by \( V_N \) and \( V_{Ga} \) respectively. Theoretical studies, whose details will be discussed in Section III, show that quantity of such vacancies is dependent on the prevailing doping of the sample, with the vacancy that favors the compensation of the sample doping being more abundant. This is known as self-compensation. For eg, in an n-type GaN, \( V_{Ga} \) which acts as an acceptor is more likely to be present. Figure 2-1 shows the atomic structure of a nitrogen vacancy.

**Interstitials**

Interstitial defects comprise of numerous possible configurations where either host lattice atoms or impurity atoms are not at an expected lattice site. For eg, one can
have split-interstitials where two atoms can share a single lattice site, with centre of mass. Alternatively, atoms can occupy the open interstitial spaces, where the configuration is termed based on the symmetry and position of nearest lattice points.

**Substitutional**

When an impurity atom occupies the vacancy left behind by a host atom, a substitutional defect is formed. They are just as likely to be discovered in the GaN lattice due to the abundance of impurity sources in the growth ambience. Silicon occupying a gallium vacancy, denoted as $\text{Si}_{\text{Ga}}$, is the most likely cause for intrinsic GaN becoming n-type for it acts like a donor impurity. Figure 2-2 shows an interstitial oxygen atom transitioning to a occupy a nitrogen vacancy to form the $\text{O}_\text{N}$, a known donor impurity.

**Antisites**

Antisites are formed when a host lattice atom ends up occupying the vacancy associated with the other host atom. For eg., a Nitrogen atom occupying a gallium vacancy is denoted by $\text{N}_{\text{Ga}}$ shown in Figure 2-3. Theoretical studies show such point defects are less likely to be encountered.

**Complexes**

A combination of the three isolated point defects discussed above can result in what is known as a defect complex. Their likelihood of formation is dependent on the availability of the participating defects, which in GaN, is most likely to be vacancies, substitutionals or additionally passivation by Hydrogen. Figure 2-4 presents one such example.
Heteroepitaxial Growth Techniques

Molecular Beam Epitaxy

Molecular Beam Epitaxy (MBE) involves evaporating pure solid elemental sources onto a heated substrate to form the required film. Evaporation of these sources is carried out in effusion cells under ultra-high vacuum (UHV) conditions which can then be directed towards the substrate as molecular flux. MBE setups are generally equipped with in-situ growth monitoring.

GaN growth utilizes a gallium source in an effusion cell as described. Initially ammonia was employed as Nitrogen source which required higher temperatures, but currently rf plasma generated ionized N$_2^+$ gas serves as the source for active Nitrogen to help maintain lower growth temperature [41]. UHV conditions result in Nitrogen loss if abundant supply of activated Nitrogen is not supplied [42]. As will be discussed in more detail, Nitrogen vacancies in intrinsic GaN films can act like shallow donor-like point defects, resulting in higher background electron concentration and lower mobility. This has motivated development of different variants of MBE, specifically for high quality GaN film growth, that are capable of maintaining ample supply of N$_2$.

More commonly used rf discharged MBE is one of such techniques and has been utilized for intentional incorporation of Carbon for high-resistance buffer growth [43], [44]. In using active effusion sources such as rf or microwave discharged, care must be taken to optimize the kinetic energy imparted to the ionic species and the total flux of the gas. If not controlled, resulting structural defects in the films such as stacking faults can degrade device behavior.
**Metalorganic Chemical Vapor Deposition**

Metalorganic Chemical Vapor Deposition (MOCVD) is one of the most important compound semiconductor growth techniques in which co-pyrolysis of organometallic compounds of the film constituents are carried out. The organometallic compounds in their vapor phase, also known as precursor gases, undergo thermal decomposition at the substrate which is maintained at high temperature and at around 0.1-1 atm pressure.

In the case of GaN, these precursors are trimethyl gallium (TMGa) and ammonia \((\text{NH}_3)\). A controlled flow ratio of the precursors is maintained, often represented by III/V ratio. Typical values for this ratio are very small indicating abundant availability of ammonia. Vapor phase precursor gases are transported using hydrogen as carrier gas which also serves to flush away reaction by-product gases such as methane.

The necessity for high temperatures in promoting efficient decomposition can indirectly result in the formation of dislocations when growing on substrates that are not thermally compatible due to difference in thermal expansion coefficient. However, this problem can be solved to a certain extent by employing a low temperature grown nucleation layer. MOCVD growth under low pressure can be a work around for such cases where low temperatures are necessary. At low pressure, decomposition is most likely to occur at the surface, generating heat and consequently mobility at the surface without the need for a hot substrate [45].

Owing to difference in the growth process, MOCVD is inherently much faster than MBE growth. Maintaining the same III/V ratio, higher TMGa flow rate will result in higher growth rate. Also, compared to MBE, MOCVD is carried out at higher pressures which further helps in curtailing Nitrogen loss, resulting in fewer Nitrogen vacancies.
This is also evident in lower background electron concentration and higher mobility. Growth temperatures are however much lower for MBE, which is advantageous when growing heterostructures on lattice mismatched and temperature sensitive substrates.

**Substrate**

Crystal growth of pure GaN or any other III-N is extremely difficult using conventional techniques such as Czochralski process because of very high melting temperatures and decomposition pressure requirement. Because of such unfavorable conditions, pure GaN crystal wafers generally have small diameters which are not commercially viable. Selection of an optimum substrate upon which heteroepitaxial growth using MBE, MOCVD or HVPE can be carried out is vital.

The two most important parameters to be considered are the extent of lattice mismatch and thermal compatibility of GaN with the substrate. Among various options available, Sapphire offers the best alternative in terms of lattice matching. For high power and high temperature applications, SiC happens to be the substrate of choice due to its high thermal conductivity. Another advantage of SiC over Sapphire is the latter often tends to be a source of oxygen as donor contamination (O\textsubscript{N} substitutional) which can result in higher background electron concentration. Silicon has also been gaining attention as a viable substrate as this will help take advantage of Silicon processing breakthroughs and maturity and eventually help incorporate GaN based device production with existing IC fabrication facilities.

In order to reduce the stress due to mismatch at the interface, small crystallite-like structures of AlN are deposited on the substrate which serves as a buffer. The amorphous-like structure helps reduce strain on the epitaxially grown GaN layer, and serving as a nucleation center promotes lateral growth reducing dislocation density.
**Doping in GaN**

Even though degradation of dynamic behavior has been traditionally attributed to surface states at the Nitride/AlGaN interface, with improved passivation techniques, introduction of doping schemes and subsequent degradation in device behavior, attention has now shifted more towards the potential impact of defects in the GaN buffer. Different GaN based device structures, not just limited to HEMTs, have displayed degradation in dynamic performance [46]. Often dependent on the extent of doping of the buffer, the magnitude of current collapse worsened once it became necessary to introduce compensating traps in the buffer to improve current confinement in the active region[47]-[54].

In this section, some of the primary defect centers and their possible origin will be discussed in detail. First, some fundamental native defects expected to be found in the unintentionally doped (UID) GaN bulk will be presented, analyzing their expected trap levels in the band-gap and concentrations concluded from first-principles ab initio Density Functional Theory (DFT) calculations. UID-GaN is generally n-type but most commonly observed impurities include both donor and acceptor-like, and their potential source in the epitaxial growth process will be reviewed. The need for intentional doping to obtain high-resistance buffer and changes to existing process steps to achieve the same will be discussed.

**Unintentionally Doped GaN (UID-GaN)**

Fundamental native defects that can be present in an intrinsic semiconductor include vacancies, interstitials and antisites. As discussed in the section on epitaxial growth techniques, growth conditions and availability of precursors will play an
important role in determining formation of Nitrogen vacancies, which are known to act as shallow donors. In a wurtzite GaN crystal, where each Nitrogen atom is surrounded by four gallium atoms, a Nitrogen vacancy can lead to excess of 3 electrons at the site and thus act as a triple donor [39], [40].

Similarly, gallium vacancies are expected to be triple acceptors. From energetics and molecular dynamics, among other isolated native defects, gallium interstitial is a multiple donor which is most likely to be encountered, whereas antisites are least favorable. However, almost all native defects discussed here can be highly mobile in nature and result in formation of complexes with other native defects or impurities.

These defect levels can be of multiple charge states and correlated energy level and concentrations of such traps are extracted using first principles approach. Figure 2-5 shows the formation energy of a trap that is extracted by such first principles calculations and can be correlated to the availability of such defects. An interesting aspect of GaN introduced in the section on vacancies, is its tendency to self-compensate and render the film semi-insulating, despite intentional doping efforts. It has been concluded after several theoretical studies that formation of certain common native defects such as vacancies are favored depending on the position of the Fermi-level, i.e., how the GaN film is intended to be doped. Defects which compensate the effect of the introduced dopant are favored energetically, and hence the phenomenon is termed as self-compensation.

Theoretical computational techniques based on first principles ab-initio Density Functional Theory can be taken advantage of as a predictive tool in scenarios like these where multiple charge nature of isolated defects together with complexes and impurities
can form a complicated picture if relying solely on defect spectroscopy and characterization tools. By using pseudopotentials and plane wave basis set \[55\] to represent the system being studied, simultaneous determination of atomic geometries, electronic and dynamic properties can be carried out through evaluation of forces. The most widely followed approach, Local Density Approximation, based on the work of Kohn and Sham \[56\], approximates the many-body electronic ground state in terms of single particle interaction with an effective potential. The effective potential in such an approximation consists of ionic potential for atomic cores, Hartree potential for electron-electron interactions, and exchange correlation for many-body effects.

For an isolated point defect, a single defect is introduced in an infinite lattice known as supercell. The infinite lattice is replicated by placing periodic boundary conditions on the supercell. Defect formation energy is obtained from self-consistent determination of Fermi-level and formation energy from charge neutrality condition. Under thermodynamic equilibrium, for a given number of sites and configuration (which is 1 for native point defects being investigated here), defect formation energy can be used to determine concentration. Thermodynamic equilibrium represents growth conditions, which more accurately correlates to MOCVD grown samples due to the higher temperatures.

TCAD simulations for AlGaN/GaN HEMT, in replicating the defect states of UID-GaN bulk, implement what is known as the three-level compensation model \[57\], \[58\]. This model is grounded on photoionization spectrum studies of defects responsible for current collapse in GaN MESFETs in which two prominent deep levels were detected \[47\]. Point defects responsible for current collapse are expected to trap hot electrons
injected from the 2DEG deeper into the substrate. For a high resistance buffer region, deep traps at high concentration are expected to capture substantial number of electrons, particularly underneath the gate and drain-access region. Increased trapping and consequent depletion of 2DEG can be induced with higher drain voltage.

In photoionization spectroscopy, an initial high drain bias is followed by extraction of pulsed output characteristics under varying conditions of illumination. The procedure is explained schematically in Figure 2-6. Such drain bias stress induced current lag is commonly encountered and characterized by degradation of dynamic parameters, and will be discussed in more detail in Chapter 6. The current is observed in the linear regime as illumination is varied with different wavelengths helping probe traps at different energy levels. Comparison with the current under dark conditions yields the spectral response function:

\[ S(\lambda) = \frac{1}{\phi(\lambda).t} \frac{\Delta I(\lambda)}{I_{dark}} \]  \hspace{1cm} (2-1)

where \( \phi(\lambda) \) is the incident photon flux over time \( t \).

The observed spectral dependence of current collapse indicates presence of two deep traps (Figure 2-7). Strong coupling to the lattice is suspected owing to the broad nature of the spectrum. For such a scenario, photoionization threshold differs from thermally extracted trap depths by lattice relaxation energy. In implementing three-level compensation model, the two deep levels are assumed to be donor and acceptor-like respectively.

In three-level compensation model, in addition to the above two deep levels, shallow donor-like defects are included, most likely due to the presence of residual Oxygen and Silicon from ambient sources. These ambient sources can include carrier
gases, precursors and the growth setup [59]. Hydrogen and Carbon are other ambient impurities contributed by the above-mentioned sources. However, their contribution is more relevant from a p-type doping perspective. To obtain p-type sample in a pn-junction LED, GaN is intentionally doped with Mg acceptors which can get passivated by hydrogen and the sample rendered highly resistive. Carbon can get incorporated as acceptor-like deep level traps. More details on the control of C doping and control of electrical properties by intentional introduction of compensating defects will be discussed in the following section.

**Intentional Doping**

GaN based power devices were originally based on as-grown intrinsic samples, which in general tend to be n-type due to the presence of various native defects and impurities as discussed in the previous segment. The extent of incorporation of such impurities during processing will vary based on the nature of growth technique and conditions as well as vendor, and as a consequence lead to significant variation in device to device electrical performance. As the understanding of the process kinetics, ambience and source material improved over time, the extent of variation introduced could be controlled to such an extent that intentional introduction of doping could be utilized to accurately control the electrical behavior of the device as intended.

**Silicon**

Silicon has been an omnipresent donor-like impurity in GaN films, the source of which is suspected to be leaching from quartz lining of deposition furnaces [5]. Intentional doping was motivated by the need for the development of pn-junction blue LED. Undoped GaN being intrinsically n-type is expected to have electron concentration on the order of $10^{16} \text{ cm}^{-3}$, which is why high n-type doping is necessary for high
emission efficiency in LEDs. Nakamura et al. [60] presented the first studies of doping of high-quality GaN films with Silicon. Using a variant of MOCVD at atmospheric pressure, Silicon was introduced using monosilane as a precursor. Carrier concentration in the examined films showed good linearity with silane flow rate. One concern with introducing high concentrations of Silicon donors was the degradation of crystallinity through cracks, pits and non-uniform surface. It was avoided by using a novel MOCVD technique and GaN instead of AlN as buffer layer on a Sapphire substrate.

Silicon doped GaN based transistor was first reported as part of multiple GaN based devices being investigated for potential microwave applications [46]. The Si doped devices were of MESFET structure, with the doped active layer on top of a semi-insulating GaN buffer. These were fabricated using MOVPE and disilane as Silicon source. Current collapse was prominent when a drain bias was applied prior to drain sweeps. Photoexcited drain sweeps, similar to photoionization spectroscopy results discussed in terms of UID-GaN, showed uniform increase in current with wavelength, indicating uniform distribution of defects states in the band-gap.

First-principles theoretical calculations predict that Silicon is most likely to form a shallow-donor level by occupying a gallium substitutional site. Nitrogen substitutional sites are less favorable as Silicon atomic radius is closer to that of gallium. Experimental determination of intentional doping was carried out using variable temperature Hall-effect measurements [61]. This technique applies to samples which have been doped uniformly throughout the sample with high enough concentrations so that other unintentional impurities can be neglected. The sheet resistance and Hall coefficients can be utilized to extract carrier concentration and mobility in a uniform sample.
\[
n = \frac{r_H}{eR_H(n)} \tag{2-2}
\]
\[
\mu_n = \frac{R_H(n)}{r_{sq} d} \tag{2-3}
\]

where \(r_{sq}\) is sheet resistance, \(R_H\) is Hall coefficient and \(r_H\) is Hall scattering factor. With the intentional dopant species being the only dominant contributor to the carrier concentration, temperature dependence can be associated to the ionization of the donors and hence the defect level can be extracted.

\[
n(T) = \sum_{i=1}^{m} \frac{N_{D,i} n(T) g_i}{N_{C,\text{eff}}(T) \exp \left( \frac{\Delta E_{D,i}}{kT} \right)} - N_{\text{comp}} \tag{2-3}
\]

where \(m\) is number of distinct donor species, \(N_{D,i}\) and \(\Delta E_{D,i}\) are doping concentration and activation of respective donor species, \(N_{C,\text{eff}}\) is effective density of states and \(N_{\text{comp}}\) is concentration of compensating acceptors.

Samples were grown using MOCVD on Sapphire substrate and monosilane as Silicon source. Accurate control of growth stoichiometry is necessary as compensating acceptor in the form of gallium vacancy are expected in an intentional n-type sample. It was assumed that compensating acceptors were an order less than observed carrier concentrations in analytically extracting the donor-level. Energy level for Si and O doping was 0.017 eV and 0.029 eV respectively.

Unlike the MESFETs discussed in this section, HEMTs and HFETs do no rely on an intentionally doped n-type active region since high conductance is achieved by the presence of a 2DEG. However, an n-type active region, even if not doped intentionally, can be difficult to deplete completely in pinch-off. Short channel effects were thus a
major concern as drain bias in pinched-off regime resulted in conduction as electrons can flow through the bulk akin to punch-through phenomena observed in short-channel MOSFETs [48]. In this phenomenon, for a MOSFET, depletion region from the drain side can extend through the buffer underneath the gate region, reaching the source side, thus providing a leakage path. In an n–channel MOSFET, the substrate being p-type is utilized to make it difficult for the depletion to occur by making the substrate more p-type. Hence it became necessary to introduce a highly-resistive bulk GaN below the active region. Incorporation of high levels of p-type dopants that would compensate for the intrinsic n-type defects would result in a highly-resistive semi-insulating bulk that would avoid short-channel effects.

**Acceptor Compensation**

Mg is the most widely researched acceptor dopant in GaN motivated by the need for obtaining p-type GaN in a pn-junction blue LED. While introduction of activated Mg dopants presents several technological challenges, obtaining a purely p-type GaN sample is not the final goal when it comes to power devices. What is necessary from a HEMT perspective is the need to compensate the n-type GaN bulk underneath the active epitaxial region. Intrinsic native defects such as Ga vacancy and several process related impurities have been known to act as acceptor-like, compensating intentional and unintentional doping in n-type GaN samples. Carbon is one such acceptor like impurity, most commonly observed after Oxygen and Silicon. Another impurity known to behave as acceptor-like is Fe. Efforts put into better understanding the intentional incorporation of these two best understood acceptor dopants will be now discussed.

**Carbon:** Similar to Oxygen, Carbon contamination of GaN samples is attributed to unintended exposure to ambience, impurities in carrier gases, but most importantly
the metalorganic precursors. SIMS investigation of GaN films and other test structures showed varying levels of Carbon using different growth techniques [62]-[64]. Specifically, for MOCVD, the role played by reactant precursors gases was clear as correlation was observed in the level of incorporation of both Oxygen and Carbon with different growth conditions. This included lower Carbon contamination under increasing growth temperature, increasing growth pressure and higher V/III precursor ratios. Other impurities, including Silicon and Oxygen, did not exhibit significant variation with changes in the growth conditions.

A systematic study was carried out by Parish et al. [65] in both GaN and AlGaN to confirm these observations. Multiple layers of GaN was grown on a Sapphire substrate by MOCVD under different conditions. Growth conditions were systematically controlled through different temperatures, and varying precursor gas flow rate to control growth rate and V/III ratio. Similar to previous observations, lower Carbon incorporation was observed at higher temperatures, attributed to increased removal from the growth surface of methyl groups contributed by TMGa. Higher V/III precursor ratio, i.e. increased ammonia flow ensures fewer nitrogen vacancies which are expected to be preferred substitutional sites for C. As one might expect, contribution of methyl group by increasing TMGa flow also contributes to increasing Carbon concentration, but this increase was not as dramatic.

Using the same photoionization spectroscopy technique employed to probe deep-traps in UID-GaN based MESFETs, Klein et al. [66] studied current collapse phenomenon in an AlGaN/GaN HEMT incorporated with different levels of Carbon in the GaN buffer layer (Figure 2-8). MOCVD grown GaN buffer was grown on Sapphire
substrates, under different growth pressures. Growth under lower pressures results in increased incorporation of Carbon from ambient sources, resulting in High Resistance (HR) GaN buffer with increasing compensation. Identically to the analysis performed on MESFET device discussed in the UID-GaN segment [47], an initial drain bias was applied, promoting trapping of electrons in the HR buffer, followed by drain voltage sweeps under varying conditions of illumination. The spectral response, which is proportional to photoionization cross section under the chosen experimental conditions, is qualitatively similar to the MESFET device. Trap1 in HEMT with HR buffer exhibits lower cross-section, while Trap2 does show variation in spectral response for different HR buffers, indicating severe increase in current collapse with higher Carbon incorporation. Extraction of Carbon concentration contributing to current collapse can be obtained by analyzing the relative current increase with increasing photon dose. Trap2 once again exhibits clear increase with lower pressure, specifically for 65 Torr. Trap1 at mid-gap were speculated to be structural defect such as extended defects expected to form at lower pressures.

With knowledge of the role of growth conditions in the incorporation of Carbon in GaN, most of the initial work was focused on using MOCVD under different growth conditions. To carry out controlled doping, a dopant source will be necessary instead of relying on other precursor gases independent of growth parameters. Green et al. [44] presented an MBE based technique that utilized a carbon tetrabromide sublimation system. MBE growth was carried out on MOCVD-grown GaN on Sapphire templates. Other sources such as carbon tetrachloride, graphite and methane have also shown to successfully incorporate high concentrations of carbon into GaN but were not favorable
due to other processing challenges. These included introduction of undesirable contaminants, lack of control as well poor crystallinity of the carbon doped film [67]-[69].

**Iron:** Before being introduced as a compensation center in GaN, Iron was a known acceptor like dopant capable of leaving III-V materials like GaAs and InP highly resistive [70], [71]. Fe contamination of GaN samples prepared by HVPE was initially attributed to reactor equipment [72]. One of the first intentional doping of GaN with Fe for achieving high-resistance semi-insulating samples was carried out by Heikman et al. [73]. Samples were grown using MOCVD and ferrocene was used as precursor for Fe doping. Doping in different samples were carried out at different ferrocene partial pressures and displayed linear relation of Fe concentration with partial pressure.

One crucial characteristic of Fe doping is the decay of Fe concentration from the highly-doped region even if ferrocene flow is cut-off. Figure 2-9 shows a typical SIMS profile of a Fe doped semi-insulating (SI) GaN buffer doped with Fe close to the substrate [49], [74]. This effect was attributed to possible memory effects, a major drawback of MOCVD where precursor gases and species persist in the growth chamber. Other SIMS measurements carried out on AlGaN/GaN HEMTs have also shown the decay of Fe from the highly-doped buffer into the undoped region, attributed to diffusive redistribution from the buffer. Pile-up near the AlGaN/GaN interface is also consistently observed.

Polyakov et al. [75] carried out electrical and optical characterization for ohmic and Schottky diode like structures grown by MOCVD on Sapphire substrate to determine the exact condition that leads to donor compensating behavior with Fe doping. Thermal dependence of dark current in both devices displayed an activation
energy of 0.5 eV. Other major traps determined to be present in the samples were at 0.9eV, both below the conduction band edge, and above valence-band edge (Figure 2-10). The major trap at 0.5eV below conduction band was attributed to electrons traps responsible for Fermi-level pinning.

However, above results don’t necessarily point to formation of 0.5eV traps as direct result of Fe-doping. Other results from different sources such as low pressure MOCVD and HVPE with heavy Fe doping have shown Fermi-level pinning at $E_c-1.4eV$ and $E_c-0.95eV$ respectively [76]. MBE grown HEMTs and differing levels of Fe doping also exhibited that Fermi-level pinning traps near 0.5eV were not directly correlated to Fe doping [77], [78]. A number of experimental studies have suggested that these deep donor-like electron traps are most likely point defects or complexes decorating dislocations [79]-[81].

**Conclusion**

The point defects encountered in electrical and optical characterization of GaN buffer in devices have been introduced based on their trap signatures and origin (Figure 2-10). Native defects in the form of vacancies and interstitials are the dominant defects levels in proton irradiation damaged devices. As-grown defects in the form of substitutionals and complexes result from unintentional introduction of elements from the growth ambience. Intentional incorporation of acceptor doping to form HR and SI-GaN have helped shed light on some of these as-grown defects which may or may not be directly correlated to the introduced dopants. Variation in the growth parameters based on different vendors and facilities makes the process of attributing different trap signatures to specific sources extremely difficult. Steady-state behavior modeling which will be discussed in Chapter 3 will introduce the role of vacancies in electrical behavior
degradation. Chapters 6 and 7 will present how as-grown trap levels distributed throughout the GaN band-gap, based on the three-level compensation model, can affect the transient switching behavior.

Figure 2-1. Atomic structure of a Nitrogen vacancy indicated by the red circle [82] 2015 IEEE

Figure 2-2. Representation of transition of an interstitial Oxygen atom (position B) to a gallium vacancy to form SiGa (position A) [82] 2015 IEEE
Figure 2-3. Atomic configuration of a Nitrogen atom occupying a gallium vacancy to form an $N_{Ga}$ antisite [82] 2015 IEEE

Figure 2-4. Atomic configuration of a $O_N$ (red sphere) substitutional complex with a hydrogen (white sphere) passivated gallium vacancy [82] 2015 IEEE

Figure 2-6. Drain stress induced trapping (Quiescent stress) and 2DEG depletion in pulsed I-V measurement. Illumination aids detrapping of electrons in the pulsing transient phase.

Figure 2-9. SIMS profile and incorporation model of Fe doping in GaN buffers of different thicknesses [49] 2006 IEEE.

Figure 2-10. Expected native defects levels, detected trap levels in UID-GaN, GaN:C and GaN:Fe buffers and the three-level compensation model.
CHAPTER 3
SIMULATION METHODOLOGY

The Florida Object Oriented Device Simulator (FLOODS) has been employed for simulating the semiconductor device physics necessary to recognize the various mechanisms that can drive observed characteristics of AlGaN/GaN High Electron Mobility Transistors. FLOODS is a finite-element based technology CAD (TCAD) tool capable of solving coupled partial differential equations in a defined structure using Newton-iteration techniques. Limited not just to electrical behavior, applications requiring solutions for mechanical and thermal physics, in a coupled implementation have been published using this framework [84], [85]. The work presented here is however exclusively based on electrical behavior, described by Poisson’s equation for charge distribution and drift-diffusion model based continuity equations for carrier flow.

\[
\nabla^2 \psi = -\frac{q}{\epsilon} \left[ p - n + N_B^+ - N_A^- \right] \tag{3-1}
\]

\[
\frac{\partial n}{\partial t} = \frac{1}{q} \nabla J_n, \quad \frac{\partial p}{\partial t} = \frac{1}{q} \nabla J_p \tag{3-2}
\]

\[
J_n = -q\mu_n n \nabla \phi_{fn}, \quad J_p = q\mu_p p \nabla \phi_{fp} \tag{3-3}
\]

**Steady-State Simulation**

Poisson’s equation is the differential form of Gauss’s law (3-1), where \( \psi \) is the electrostatic potential and total charge concentration includes carriers, partially ionized traps, and fixed background charges, both in the device bulk and at the interfaces. Dielectric constant \( \epsilon \) has been implemented spatially constant for a given material. Continuity equation for the carriers is defined in terms of divergence of current, for electron and hole components separately (3-2). As per isothermal assumptions for the
drift-diffusion model, electron and hole current have been described in terms of their quasi-Fermi levels (3-3). For simulating the fundamental physics of a semiconductor device, the above equations are sufficient, as the solver solves for three unknowns: electrostatic potential, and quasi-Fermi levels for electrons and holes. Instead of quasi-Fermi-levels, electron and hole concentrations can also be solved for, and that is the preferred solution variable-set for simpler devices composed of a single contiguous material. However, quasi-Fermi levels are necessary for abrupt band-structure discontinuities in heterostructures as carrier concentrations will fluctuate drastically between the adjacent materials resulting in instability in the Newton-iteration procedure.

In order to model steady state behavior accurately, partial ionization of deep traps have been considered [86]. Such traps can be as a result of radiation damage or as-grown defects (see Chapter 2). Carrier occupancy of such defects, and thus charge, is obtained based on their energy-level in the forbidden band-gap with reference to respective carrier Fermi-level (3-4).

\[
\begin{align*}
\frac{N_D^+}{N_D} &= \frac{1}{1 + 2\exp \left( \frac{E_F - E_T}{kT} \right)} \quad (3-4) \\
N(E) &= \frac{N_{tot}}{\nabla E \sqrt{2\pi}} \exp \left( -\frac{(E - E_T)^2}{2\nabla E^2} \right) \quad (3-5)
\end{align*}
\]

Computational issues need to be considered here as well, as the introduction of a discrete level can result in oscillations during Newton iteration. Newton’s method attempts at determining the derivative of the impulse-function like distribution in energy with respect to the quasi-Fermi level which makes the solution process unstable. To implement a broader distribution, traps \( N_{tot} \) are distributed in a Gaussian manner.
symmetrically around the intended trap level $E_T$ with a spread of $\nabla E$ (3-5). The full width half maximum of the distribution, given by $2\sqrt{2\ln 2}\nabla E$ as per definition, is generally on the order of 50meV, so significant variation in results from a discrete level implementation is not expected.

**Transient Simulation**

With the right material parameters and mobility model, steady-state behavior of an AlGaN/GaN HEMT can be accurately modeled through calibration of charge and trap distribution, Schottky barrier and contact resistances. Detailed steps to extract these factors and achieve good fit to experimental data will be discussed in Chapter 4. To get a comprehensive understanding of as to how traps introduced in the GaN bulk can affect dynamic device performance, in addition to the fundamental governing semiconductor equations (3-1 to 3-3), reaction-rate equations are included to simulate the effect of charge trapping and de-trapping mechanism:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla J_n - K_f n N_D^+ + K_r (N_D - N_D^+)$$  \hspace{1cm} (3-6)

$$\frac{\partial N_D^+}{\partial t} = -K_f n N_D^+ + K_r (N_D - N_D^+)$$  \hspace{1cm} (3-7)

where $N_D$ and $N_D^+$ are total and ionized donor-like traps respectively. Capture and emission rates, $K_f$ and $K_r$ respectively, are determined by the energy-level of the trap and time-constant associated with the defect, as per Shockley-Read-Hall statistics. Alternately, capture cross section can also be set to specify the responsiveness of the trap. Multiple acceptor and donor like traps can then be defined with independent energy-levels and capture cross-sections. Energy-level specified through reaction rate equations are discrete and result in exponential transients. Experimental results for
pulsed transient measurements on AlGaN/GaN HEMTs, however, tend to be of stretched exponential nature [31], [36], [51], [87], which has been attributed in the past to point defect decorated dislocations. More recent works have suggested that a band-like broadened distribution in energy instead of discrete level can just as well produce the observed spread in the relaxation spectra [88]. For simulating the latter case, reaction-rate equations with a Gaussian-like distribution of traps in energy, analogous to the implementation for static partially ionized traps, has also been employed.

At high drain-voltages, lattice self-heating is known to reduce current [89], which can be included through heat flow equation described for bulk material. Considering only steady state behavior, it can be observed that the resulting spatial variation of lattice temperature is contributed by the heat generation term, while the heat generation term itself is dependent on electric field and current. Consequently, high lattice temperature is expected near the drain edge in on-state, which impacts current through both carrier distribution and mobility. In all the simulations carried out, drain voltage applied to HEMT in the on-state have been limited to 5V, under which lattice-self heating is not expected to degrade current values significantly. Simulation and results discussed herein have been carried out without lattice self-heating at a constant temperature of 300 K.

Another aspect of carrier dynamics that can affect results if not considered is hot electron effects. In the presence of high electric field, electrons can gain excess energy without sufficient scattering events resulting in electron velocities exceeding saturation velocity. While such energetic “hot” electrons are more of a concern in terms of reliability under prolonged electrical stress, trapping simulations have shown hot
electron effects to produce more dramatic changes in current collapse simulations [90]-[92]. Hot electrons from the 2DEG, predominantly underneath the gate region get injected deeper into the substrate and get trapped. Simulation of hot electron effects requires inclusion of energy balance equations, also known as the hydrodynamic transport model.

**Small-Signal Analysis**

Development of small-signal analysis capability for FLOODS was motivated by the need to understand the impact of proton radiation damage on AlGaN/GaN HEMTs. Very few studies have tried to recognize the physics of RF performance degradation under ionizing radiation damage, some claiming the extent of degradation being comparatively more severe at higher frequencies [93]. For radiation induced defects to cause further degradation for RF application, it has been speculated that fast traps might also be present, in addition to the slow traps which had already been suspected to cause current collapse. To that end, the sinusoidal steady state analysis technique has been incorporated into FLOODS [94].

In general, a device simulator TCAD tool solves for the coupled partial differential equations that define the physics in a described device structure. These non-linear equations are discretized into linear form as per the grid definition of the structure. The resulting linear representation in most device simulation literature is:

\[ J \cdot X = B \]  

(3-8)

where J is the Jacobian matrix, B is a vector defining the boundary conditions such as contacts, and X is a solution variable vector. Jacobian matrix is the derivative of the vector representation of the defined discretized equations. For a steady-state solve, the
linear form described above is solved iteratively, with an update to the solution variable after each iteration, which continues till acceptable convergence criteria is met.

The sinusoidal steady state analysis technique assumes the system is subjected to a small-signal perturbation at a selected bias point. Assuming the symbolic representation of the governing semiconductor device equations at chosen DC bias point is represented by [95]:

\[
\begin{align*}
F_{vl}(V, n, p) &= 0 \quad (3-9a) \\
F_{nl}(V, n, p) &= \hat{G}_{nl}(n) \quad (3-9b) \\
F_{pl}(V, n, p) &= \hat{G}_{pl}(n) \quad (3-9c)
\end{align*}
\]

where \( F \) and \( G \) are non-linear functions of the solutions \( V, n \) and \( p \), equation (3-9a) represents Poisson’s equation, and equations (3-9b) and (3-9c) represent electron and hole continuity equations respectively with the dot term representing time derivative component. For an AC system, the solution vector arguments can be represented as:

\[
\xi(t) = \xi_0 + \xi e^{j\omega t} \quad (3-10)
\]

where \( \xi = V, n \) or \( p \), \( \xi_0 \) denoting the steady state solution corresponding to solutions for equations 3-9a to 3-9c.

A Taylor series expansion of the frequency domain solution of the system perturbed by the infinitesimal sinusoidal input \( \xi e^{j\omega t} \), neglecting higher order components is given by:

\[
\sum_j \left[ \begin{array}{ccc}
\frac{\partial F_{vl}}{\partial V_j} & \frac{\partial F_{vl}}{\partial n_j} & \frac{\partial F_{vl}}{\partial p_j} \\
\frac{\partial F_{nl}}{\partial V_j} & \frac{\partial F_{nl}}{\partial n_j} & -j\omega \frac{\partial G_{nl}}{\partial n_j} \\
\frac{\partial F_{pl}}{\partial V_j} & \frac{\partial F_{pl}}{\partial n_j} & \frac{\partial F_{pl}}{\partial p_j} - j\omega \frac{\partial G_{pl}}{\partial p_j}
\end{array} \right] \left[ \begin{array}{c}
V_j \\
\hat{n}_j \\
\hat{p}_j
\end{array} \right] = 0_{dc}
\]
The above expression is equivalent to the steady state Jacobian except for frequency dependent components associated with the time dependent variables $n$ and $p$. The expressions being discussed are relevant to electron and hole continuity equations which impart the frequency dependence. Similar expressions can be obtained when simulating SRH reaction rate equations involving trap concentrations as time dependent variables.

After assembly of the global AC matrix using equation 3-11, the frequency dependent and independent components are separated and AC boundary condition imposed through the following expression:

$$[J + jD]\bar{X} = B$$

which takes the following form for computational reasons:

$$\begin{bmatrix} I & -D \\ D & J \end{bmatrix} \begin{bmatrix} X_R \\ X_I \end{bmatrix} = \begin{bmatrix} B \\ 0 \end{bmatrix}$$

where $J$ is the Jacobian at the DC bias point. $B$ is boundary condition vector where elements corresponding to the contact potential are used to perturb the system with rest of the rows set to zero, as per Dirichlet boundary conditions. $D$ is a diagonal matrix in which just the diagonal elements corresponding to reaction rate equation solution variables are set to $j\omega$. This will include electron, hole and trap concentration. $X_R$ and $X_I$ are the real and imaginary solutions respectively.

At a given steady state bias, application of an AC signal will give an in-phase resistive output and an out-of-phase capacitive or imaginary component. Depending on whether the current is extracted at the same or different terminal as the sinusoidal input,
the conductance (and capacitance) or transconductance (and transcapacitance) can be obtained respectively. These results can then be used to further extract current-gain and cut-off frequencies, which will be demonstrated in Chapter 5.

**Hurkx Trap-Assisted Tunneling**

In the investigation of trapping mechanisms in AlGaN/GaN HEMTs, current transient analysis under different biasing and temperature conditions have consistently exhibited thermally independent processes [96], [97]. Taking into account the high electric fields, particularly in off and semi-ON state, electrons from the 2DEG can reach deeper into the bulk by tunneling (Figure 3-1). As no semi-empirical model simulating such a non-local trapping by deep traps in the bulk has been presented till date, a Shockley-Read-Hall based field-enhancement trapping formulation first presented by Hurkx et al. [98] has been implemented.

The Hurkx trap-assisted tunneling (TAT) model was originally proposed to simulate non-idealities and reduced temperature dependence of current in diodes under low forward biased conditions [99], [100]. It was determined that defect-states enhanced tunneling through the depletion region which resulted in higher current than that predicted by ideal diode equation. This effect of TAT is predominantly a heavy-doping effect in diodes as higher potential barrier suppresses thermionic emission much more significantly compared to tunneling.

Unlike other semi-empirical approaches to TAT which introduce this effect as a change to current directly, the Hurkx TAT model alters the recombination term which it makes it suitable for implementation in a bulk trapping mechanism (3-11). The model presents a field-effect function $\Gamma_n$ which enhances the capture-emission rate. The model
successfully captures such a non-local trapping effect by expressing the function in terms of local variables, making it suitable for numerical device simulator.

\[ \tau = \frac{\tau_0}{1 + \Gamma_n} \quad \text{or} \quad \sigma = \sigma_0(1 + \Gamma_n) \quad (3-11) \]

In a situation where tunneling is expected to contribute to the result, such as the electron concentration in the depletion region, or the GaN bulk for a HEMT, the net carrier density is a sum of conventional density in the conduction band and the tunneling component (3-12a), where the tunneling probability is calculated assuming a triangular potential well. Such a linearly varying potential barrier assumption of a triangular well can be justifiably applied to the band bending in the GaN if tunneling to defects close to the heterointerface. Tunneling is expected to take place from all locations and is taken into consideration by the limits of integration in deriving \( \Gamma_n \).

Conversely, emission is not limited to local release of electrons, and instead described by a partial thermal excitation followed by tunneling through the potential barrier into the conduction band (Figure 3-2). The resulting expression for enhancement of emission rate (3-12b) is based on work in which the effect of electric-field on emission-rate was captured through electron-phonon coupling in GaAs diodes.

\[ n_t(x) = n(x)(1 + \Gamma_n) \quad (3-12a) \]
\[ e_{n_t}(x) = e_{n_0}(x)(1 + \Gamma_n) \quad (3-12b) \]

In its original form, the limits of integration are determined by the range over which thermal emission can take place, \( \Delta E_n \), and with the local electric-field, can be correlated to the tunneling distance. Consequently, and conveniently, for implementation in a numerical device simulator, both electron concentration and
emission rate get enhanced by the same factor termed as field-effect function (3-12).

The function still requires an analytical form, which is dependent on the limits of integration $\Delta E_n$ dependent on the position of trap $E_T(x)$ with respect to the neutral side conduction band minimum $E_{cn}$.

$$\Delta E_n(x) = E_c(x) - E_{cn}, \quad E_T(x) \leq E_{cn}$$

$$\Delta E_n(x) = E_c(x) - E_T(x), \quad E_T(x) > E_{cn}$$  \hspace{1cm} (3-13)

In a diode, comparison with the neutral side conduction band is inconvenient because as it is a non-local variable. Assuming a heavily doped diode, the non-local neutral conduction band minimum $E_{cn}$ is replaced by the local quasi-Fermi level $\phi_{fn}(x)$. Such an assumption may not be applicable to an AlGaN/GaN HEMT, the position of the quasi-Fermi level with respect to the conduction band minimum at the interface will be dependent on the gate bias. Considering the bias point of interest, the reference level to determine the integration limits is set as the cross-over point of the Fermi-level and conduction band, i.e. $\Gamma_n$ is calculated only if $E_c(x) > \phi_{fn}(x)$. Such an assumption will result in the model being more accurate in the semi-ON state.

The analytical form of the field-effect function integral is dependent on the local electric-field, as it determines the lowest energy-level from which tunneling can occur. First form represents the condition of low electric-field and thus tunneling can occur from all possible conduction band levels:

$$\Gamma_n = 2\sqrt{3\pi} \frac{|F|}{F_{\Gamma}} \exp \left[ \left( \frac{F}{F_{\Gamma}} \right)^2 \right]$$  \hspace{1cm} (3-14)

where $F$ is local electric-field and $F_{\Gamma} = \frac{\sqrt{24m^*(kT)^3}}{q\hbar}$. 

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The second form represents the condition of high-electric-field when the tunneling is limited to a certain number of energy-levels $\Delta E_n$ at higher energies in reference to the trap-level:

$$
\Gamma_n = \frac{1}{2} \frac{kT}{\Delta E_n} \sqrt{\frac{\pi}{a}} \exp \left( \frac{b^2 - ac}{a} \right) \text{erfc} \left( \frac{b}{\sqrt{a}} \right)
$$

(3-15)

Figure 3-1. Injection of electrons from 2DEG to deeper into the buffer and subsequent trapping.

Figure 3-2. Capture and emission processes under low electric field (Left) and high electric field (Right) conditions in the depletion region.
Figure 3-3. Tunneling processes under semi-ON (Left) and ON (Right) gate bias with defined trap-assisted tunneling parameters.

Figure 3-4. Trap-assisted tunneling resulting in higher leakage current for higher defect density at low forward bias.
In Chapter 1, the importance of evaluation of the impact of proton radiation on AlGaN/GaN HEMTs was established. With GaN being more radiation tolerant than GaAs, a number of studies came to the conclusion that AlGaN/GaN heterostructure based devices exposed to proton radiation exhibited exceptional immunity to displacement damage than was anticipated [92], [101], [102]. Much of the degradation that is observed in terms of DC performance parameters include shift in threshold voltage and reduction in saturation drain current (Figure 4-1). Most commonly cited mechanism that has been considered involves introduction of deep traps in the active region capable of trapping electrons from the 2DEG and ionized impurities limiting the 2DEG mobility.

First proton irradiation results were published by Cai et al. [103] who did observe degradation of saturation current and transconductance, correlating it to the reduction of sheet concentration of electrons in the 2DEG and Hall mobility. Both DC and RF parameter degradation was observed upon proton irradiation by Luo et al. [29] who subjected these devices to relatively low doses but proton energy of 40MeV, which is drastically higher compared to most proton irradiation studies. Both findings reported recovery in the observed parameters upon annealing at high temperatures and displacement damage from proton strikes introducing deep traps capable of depleting the 2DEG was identified as the primary mechanism.

Gaudreau et al. [104] noted degradation in Hall mobility in AlGaN/GaN heterostructure based resistive structures, as the device transitioned from metallic to
insulator like behavior upon exposure to proton fluence values exceeding $3 \times 10^{15} \text{ cm}^{-2}$.

Karmarkar et al. [102] first attempted to quantify the energy imparted by the incident protons to the host lattice, determining that the resulting displacement damage was fairly uniform around the active region (Figure 4-2). Among the various factors that can affect the 2DEG sheet density, defects in the AlGaN layer were considered to be more important as they directly affected the net polarization charge. Kalavagunta et al. [92] attempted to model post-irradiation behavior by introducing acceptor–like traps in the AlGaN.

More recent experimental and TCAD modeling results of proton-irradiation induced DC performance degradation have identified the dominant role of acceptor-like defects introduced in the GaN bulk. Several groups have presented different degradation models and mechanisms when investigating such irradiated devices from different vendors and academic sources. Experimental results have established that there is significant process dependence which then emphasizes the need to accurately model as-grown defects [105]-[109].

In this chapter, comprehensive steady-state simulation of unirradiated and proton-irradiated AlGaN/GaN HEMTs will be presented. In the first section, the simulation parameters discussed in Chapter 3 will be analyzed in greater detail to obtain qualitative agreement with commonly observed steady-state behavior. Particular attention will be on the factors affecting the threshold voltage and static on-resistance, through which one can calibrate simulation results to fit transfer and output characteristics. In section two, results obtained from radiation modeling effort using the
discussed simulation methodology will be presented and their implications will be considered.

Simulation Parameters

A simple AlGaN/GaN HEMT structure that is implemented in FLOODS was presented in Chapter 1. Steady-state simulations were carried out to model pre- and post-radiation characteristics of the HEMT described by Liu et al. [110]. The vertical material stack and dimensions are identical to the example described in Chapter 1. Gate is symmetric in position laterally between source and drain, with gate length of 1 \( \mu \text{m} \) and gate to contact spacing of 1.5 \( \mu \text{m} \). For steady-state simulation, the two most important factors determining drain current at a certain bias point are threshold voltage and on-state conductance.

Threshold Voltage

Threshold voltage for AlGaN/GaN HEMTs have been defined along the same lines of charge control model used for GaAs based HEMTs [101], [111]:

\[
V_{TH} = \Phi_B - \Delta E_c - \frac{q N_D d^2}{2\epsilon} - \frac{\sigma d}{\epsilon} + E_f 0 - \frac{q^2 N_B}{C_B} \tag{4-1}
\]

where \( \Phi_B \) is the barrier height of the Schottky gate, \( \Delta E_c \) is conduction band-offset at the interface, \( N_D \) and \( N_B \) are net donor-like trap concentration expected to be present in AlGaN and GaN respectively, \( d \) is the thickness of AlGaN layer, \( \sigma \) is the sheet charge at the heterointerface, \( C_B \) is the effective buffer-to-channel capacitance. The first component necessary for modeling of HEMTs is the incorporation of polarization sheet charge at the AlGaN/GaN heterointerface. The net polarization charge can be considered as an effective sheet charge representing not just the spontaneous and
piezoelectric polarization, but also the defects in the AlGaN bulk, represented by the third term on the right side of equation (4-1), as well as the charges at the nitride/AlGaN interface. Control of the channel is through a Schottky gate with barrier height generally reported between of 0.6 eV-1eV based on leakage current measurements [29]. Schottky diode leakage has not been realized in the discussed simulations since it is not expected to affect the on-state behavior significantly.

While the polarization charge and Schottky gate are the two key parameters in the charge control model based threshold voltage expression, another factor that has been essential to calibrate threshold behavior was the charge distributed in the GaN bulk. A typical intrinsic GaN sample is generally not perfectly semi-insulating. Instead it can be contaminated by several elements from ambient sources as discussed in Chapter 2, most often by Silicon, Oxygen and Carbon. In numerical simulations carried out using FLOODS, it was observed that device turn-off characteristics were rather poor than expected when as-grown defects were modeled through fixed donor-like charges exceeding concentrations of $10^{15}$ cm$^{-3}$. Figure 4-3 shows the subthreshold behavior of three HEMTs described with fixed densities of positive and negative charges, comparing their subthreshold slopes and off-current. Figure 4-4 provides a two-dimensional representation of electron distribution in the GaN substrate under subthreshold condition. It can be expected that an n-type substrate will be difficult to pinch-off, specially under stronger drain bias when punch-through like leakage is expected to be even more severe.
On-State Conductance

To accurately model the static-on resistance of the HEMT, experimentally observed 2DEG mobility can be utilized. The Farahmand model [112] for GaN bulk mobility is also often employed in several TCAD simulation studies:

\[
\mu_{\text{low}} = \mu_{\text{min}} \left( \frac{T}{300} \right)^{\beta_1} + \frac{\left( \mu_{\text{max}} - \mu_{\text{min}} \right) \left( \frac{T}{300} \right)^{\beta_2}}{1 + \left[ \frac{N}{N_{\text{ref}}} \left( \frac{T}{300} \right)^{\beta_3} \right]^\alpha} \\
\mu_{\text{high}} = \frac{\mu_{\text{low}}}{\left( 1 + \left\{ \mu_{\text{low}} \left( \frac{E}{E_{\text{Sat}}} \right) \right\}^{\beta_4} \right)^{1/\gamma}} \\
\alpha = 0.66, \beta_1 = -1.02, \beta_2 = -3.84, \beta_3 = 3.02, \beta_4 = 0.81, \beta = 0.85 \left( \frac{T}{300} \right)^{0.4}
\]

where \( \mu_{\text{min}}, \mu_{\text{max}} \) are fitting parameters, \( N \) is the total ionized impurity concentration with \( N_{\text{ref}} = 10^{17} \text{ cm}^{-3} \), saturation electric field \( E_{\text{Sat}} = 3.3 \times 10^7 - \left( 3 \times 10^6 \frac{T}{300} \right) \). Figure 4-5 shows Monte Carlo calculations for drift velocities for which the above model was proposed by the same authors. This model captures velocity saturation through a low electric field and high electric field dependence. Ionized impurity scattering as a result of point defects in the bulk is also captured by this model. In the results presented in this chapter, the impact of ionized impurity dependence of mobility will be discussed in more detail. Additionally, for more accurate calibration of on-resistance, contact resistance can be tuned to fit experimental results.
Results and Discussion

First application of FLOODS to simulate DC behavior of HEMTs was with the end goal of modeling proton radiation damage in the form of change in output characteristics and electric field distribution [86], [110]. The experimental results being modeled had shown that devices to be tolerant to radiation damage for low fluence values, and as fluence reached $2 \times 10^{14}$ cm$^{-2}$, degradation in parameters such as saturation drain current and transconductance were observed. Hall mobility measurements helped attribute these changes to reduction in 2DEG sheet density and mobility. A positive shift in threshold credited to the formation of deep traps in the GaN bulk was also correlated to an improvement in breakdown and critical voltage.

The devices thus simulated in FLOODS utilized a constant mobility of 1907 cm$^2$/Vs for unirradiated device and a 41% degradation for the device radiated at $2 \times 10^{14}$ cm$^{-2}$. Experimentally observed degradation of contact resistances was also implemented. However, these two factors were not sufficient in modeling the irradiated devices. As discussed in the previous section, the output characteristics, in the particular the threshold voltage, was determined to be highly sensitive to charge introduced in the GaN bulk. To determine an appropriate trap concentration corresponding to the proton fluence, TRIM (Transport of Ions in Matter) [27] was used, a Monte Carlo program capable of determining energy loss of proton irradiation to a material stack and calculate resulting vacancy concentrations (Figure 4-6). From the positive shift in threshold observed experimentally, negative charges were expected to be introduced in the bulk. However, negatively-charged traps introduced uniformly throughout the bulk overestimated the threshold voltage shift, while lower concentrations of traps failed to obtain the right transconductance. To get the exact fit,
concentrations in agreement with TRIM results of $10^{17}$ cm$^{-3}$ were limited to 30nm of the GaN bulk adjacent to the interface (Figure 4-7).

With the above study, the requirement to develop predictive capability of FLOODS in AlGaN/GaN HEMT design was realized. As the reason for confining radiation induced negative charges within 30nm from the heterointerface was not certain, a more detailed analysis of the impact of deep-traps on device behavior was necessary. While such deep-level traps in the GaN band-gap could be of as-grown origin as well as a result of displacement, primary focus was on deep-traps as result of proton irradiation.

Preliminary simulation studies helped conclude that as-grown defects were most likely not in equivalent quantity as vacancies due to displacement-damage. These studies simulated as-grown defects as fixed background charge calibrated to fit pre- and post-radiation results [113]. The number of factors to observe thus was limited to the role of nitrogen and gallium vacancies, their concentrations and location in the bulk of active region.

As discussed in Chapter 2, first-principles theoretical calculations have shown that among the native defects in GaN, Nitrogen vacancies are most likely donors, close to the conduction band, while gallium vacancies are deep acceptors. As per TRIM simulations, both the vacancies are expected to be in the same order for various fluence values. This results in strong compensation throughout most of the GaN bulk, hinting towards the tolerance observed in DC behavior for lower fluence values.

Near the heterointerface, even relatively shallow donor-like traps are expected to be occupied due to the abundance of electrons in the 2DEG. The resulting net charge is
due to uncompensated acceptor-like defects (Figure 4-8). At high fluence, the resulting high concentrations of charges, even if confined to a depth of 30nm, can significantly shift the threshold (Figure 4-9). Similar trap concentrations in AlGaN did not influence the overall electrostatics so as to affect the threshold by the same magnitude as was observed experimentally. Alternatively, the electrostatic contribution of charges in AlGaN bulk can be incorporated with the net sheet charge at the heterointerface, and a relative comparison with expected polarization sheet charge shows that AlGaN of thickness of 25nm will need charge concentrations to exceed $10^{18}$ cm$^{-3}$.

Effectively modeling the electrostatic influence of ionized trap charges resulting from displacement damage by proton irradiation is not sufficient in replicating output and transfer characteristics (Figure 4-10). Selection of the correct mobility model is required which will include velocity saturation effects under high electric field. In addition, post-radiation experimental results have shown degradation in Hall mobility, thus capturing ionized impurity scattering is also vital. The Farahmand mobility model includes both factors together with temperature dependence which is helpful during lattice self-heating simulations. An accurate bulk mobility model may not be necessarily suitable for all modeling efforts on 2DEG based conduction. Comparing pre-irradiated devices, in the Farahmand mobility model, peak mobility is 1406 cm$^2$/Vs as opposed to a constant mobility of 1907 cm$^2$/Vs discussed above.

**GaN Buffer Trap-Assisted Tunneling**

In Chapter 3, the potential non-local trapping mechanism that involves tunneling of electrons from the 2DEG into traps in the GaN buffer region was introduced. The Hurkx trap-assisted tunneling (TAT) scheme utilized to simulate this phenomenon was also described in detail with reference to a highly doped pn-junction diode in Chapter 3.
In this section, the results obtained upon application of the tunneling model to the HEMT structure will be discussed.

Two devices will be compared to observe how the Hurkx TAT model affects their behavior. Both devices are of the irradiated kind discussed in this chapter, with shallow donors and deep acceptors, and shallow donor traps in the GaN are most likely to trap 2DEG electrons. First device was expected to be irradiated by a proton fluence of $10^{14}$ cm$^{-2}$, hence vacancy defect levels of the order of $10^{17}$ cm$^{-3}$. The second device had lower vacancy defect densities of $10^{15}$ cm$^{-3}$, corresponding to fluence of $10^{12}$ cm$^{-2}$.

Figure 4-12 shows the band bending and position of the trap levels with respect to the heterointerface and Fermi-level under no bias at the gate or drain. Unoccupied traps closer to the interface in the case of higher defect densities are highly likely to be affected by the tunneling model, but the increasing energy barrier will limit the electrons from tunneling deeper into the substrate.

Figure 4-13 shows the difference in the trap occupancy between a simple SRH trapping model and the Hurkx TAT model, defined by $\Delta N_D = N_{D,SRH} - N_{D,TAT}$. For both devices, TAT has lower ionized traps, hence higher occupancy by electrons on account of tunneling, by approximately 10%. Also, the device providing lower energy barrier shows tunneling occurring deeper into the substrate.

Figure 4-14 shows the difference in the output characteristics when comparing local trapping SRH model with the TAT model. The right axis compares the absolute values $\Delta I_{DS} = I_{DS,SRH} - I_{DS,TAT}$ for the devices. The left axis presents $\Delta I_{DS}$ normalized to the current obtained from simple SRH model. From both examples, although a
difference is observed, it can be concluded that the effect is almost negligible in the on and semi-ON states.

**Conclusion**

The displacement damage as affecting the steady state behavior of AlGaN/GaN HEMTs was modeled through a two-level vacancy model. Monte Carlo simulation of proton irradiation results show equal likelihood of gallium and nitrogen vacancy formation in both AlGaN and GaN. DFT calculations indicate Nitrogen vacancy as a shallow donor-like defect while gallium vacancies are deep acceptor-like in nature, resulting in compensation and limiting the electrostatic contribution to ionized acceptors located in the GaN in close proximity to the heterointerface. Other proton-irradiation studies have seen larger threshold voltage shifts for similar proton fluence, attributed solely to deep acceptor-like traps in the GaN, and confirming a process dependence in the degradation process. Even though doses at which such degradation is observed are fairly large, corresponding to nearly 50-100 years in low Earth orbit, proposal of a consistent model will require better understanding of both displacement-damage induced and as-grown defects.

Figure 4-1. Id-Vg curve of MBE grown AlGaN/GaN HEMTs under Ga-rich conditions, irradiated with protons of 1.8MeV [105] 2010 IEEE.
Figure 4-2. TRIM simulation results showing energy transferred by 1.8MeV protons [102]. 2004 IEEE

Figure 4-3. Simulation results showing Id-Vg curves (Left), and subthreshold-behavior (Right) for different doping levels of GaN buffer.

Figure 4-4. Electron distribution in the GaN bulk near pinch-off (VGS=-3V).
Figure 4-5. Monte-Carlo simulation of electron drift velocity against electric field for GaN [112] 2001 IEEE

Figure 4-6. TRIM simulation of expected range of Ga and N vacancy concentration upon proton irradiation at 5MeV [86] 2013 IEEE

Figure 4-7. Experimental (symbols) and simulation (lines) pre and post-irradiation Id-Vg curves for VDS=5V [86] 2013 IEEE
Figure 4-8. (Left) Experimental (symbol) and simulation (lines) post-irradiation Id-Vg curves [113]. (Right) Representation of irradiation damage to GaN bulk.

Figure 4-9. Simulated positive threshold shift as a function of concentration of V$_{Ga}$ and V$_N$ [113].

Figure 4-10. Simulated reduction in saturation drain current due to ionized impurity scattering as a function of concentration of V$_{Ga}$ and V$_N$ [113].
Figure 4-11. Comparison of 2DEG mobility data in literature for different fluence and proton energy values (symbols) and mobility model (line) [113].

Figure 4-12. Relative position of shallow donor trap level ($E_C-0.15$ eV) with respect to Fermi-level under no bias for irradiation at different fluence values.
Figure 4-13. Difference in shallow donor trap ionization between simple SRH and Hurkx TAT model for the different trap concentrations.

Figure 4-14. Difference in transfer characteristics current between simple SRH and Hurkx TAT model.
CHAPTER 5
RF PERFORMANCE SIMULATION

With considerable effort being put into understanding degradation of DC performance of AlGaN/GaN HEMTs, it has been established that the GaN substrate makes it the best candidate for radiation-prone environments. However, with most practical applications of such HEMTs being in power switching and RF applications, investigation of the impact of radiation induced damage on dynamic performance under realistic operating conditions is extremely vital in establishing their suitability to aforementioned applications.

In Chapter 4, analysis of the degradation of DC parameters aided in establishing the location, energy levels and concentrations of such point defects. But to understand the time scales at which such defects affect the device behavior, simulation of carrier trapping dynamics from both large signal transient as well as small-signal response is essential.

In this chapter, the utilization of Sinusoidal Steady State Analysis (S3A) technique, implemented in FLOODS, in examining the potential impact of various defect parameters, and consequent influence on RF performance of AlGaN/GaN HEMTs will be presented. Specifically, focus will be on the role played by the electron capture cross-sections of donor-like defects, distributed in the GaN bulk, on transconductance, current-gain and cut-off frequency at various operating frequencies.

Background

Preliminary examination that brought attention to radiation reliability of AlGaN/GaN HEMTs from an RF standpoint was the excess degradation in high
frequency parameters compared to DC transfer characteristics. Most of the earlier studies observed radiation reliability under proton fluence values ranging from \((10^9 \text{ - } 10^{15} \text{ cm}^{-2})\) and proton energy in a wide range of 2MeV-40MeV. As was the case for DC characteristics, maximum degradation in transconductance was also observed for lower values of proton energy [29], [22], [93], [114]. For such lower values of proton energy in the range of 1MeV-5MeV and fluence values less than \(10^{14} \text{ cm}^{-2}\), transfer characteristics, including transconductance, exhibited a positive shift corresponding to change in pinch-off attributed to net positive charge in the GaN bulk near the interface [113]. Variation in peak transconductance is also observed, however the exact nature of such variations under low doses show dependence on the substrate itself. Beyond fluences of \(10^{14} \text{ cm}^{-2}\), degradation in transconductance is much more prominent with increased shift in pinch-off and severe reduction in peak transconductance (Figure 5-1).

High frequency performance parameters such as cut-off frequency \(f_T\) and maximum oscillation frequency \(f_{\text{max}}\) are not only dependent on transconductance, but also on resistive and capacitive components of the HEMT structure bound to be affected by radiation damage.

\[
f_T = \frac{g_m}{2\pi(C_{GS} + C_{GD})}
\]

\[
f_{\text{max}} = \frac{f_T}{\frac{R_i + R_s + R_g}{R_{ds}} + (2\pi f_T)R_g C_{GD}}
\]

Luo et al. [29] observed that the degradation in \(f_{\text{max}}\) was dependent on gate dimensions. Increased sensitivity of shorter gate lengths to radiation damage was attributed to pronounced changes in the capacitive and resistive components. HEMTs
utilized for RF applications generally employ shorter gate lengths which allow higher operation speeds, but as observed, can also suffer from higher sensitivity to radiation damage. It must be noted that the devices were exposed to proton energies of 40MeV. Recent proton radiation damage experiments utilize energies in the range of 1-5MeV. Liu et al. [22] observed equivalent degradation in both RF parameters, $f_{\text{max}}$ and $f_T$, with significantly more deterioration for 5MeV proton energy when compared higher proton energies. The decline in performance was correlated to reduction in mobility and 2DEG depletion. Chen et al. [93] observed similar trends for HEMTs in which AlGaN/GaN heterostructure growth was carried out by MBE under Ga-rich and NH$_3$-rich conditions.

The nature of transfer characteristics degradation showed slight variation between the two devices. This was attributed to defects at different energy levels in the band-gap. While Ga-rich device showed more degradation of peak transconductance, NH$_3$-rich device had significantly greater current-gain degradation. Both devices displayed approximately equal decrease in average $f_l$ and $f_{\text{max}}$ for different gate bias (Figure 5-2). The difference in the extent of degradation for DC and RF parameters was attributed to fast traps and surface states which would affect the capacitive and resistive components at GHz operating frequencies.

**Simulation Methodology**

To inspect the impact of proton irradiation on RF performance of AlGaN/GaN HEMTs, transconductance was first observed under varying gate biases using S3A technique. Acceptor and Donor defect levels, corresponding to the gallium and Nitrogen vacancies respectively, identified to be responsible for DC parameter degradation were introduced in the GaN substrate. Concentration of such defects were also varied corresponding to 2MeV of proton bombardment under different fluence values.
Simulated device structure utilized the same stack as that for steady state simulations. Two different gate lengths were implemented: 1 um and 0.2 um to confirm consistency of the simulation results.

Similar to steady state simulations, the partial differential equations employed to simulate fundamental semiconductor physics include Poisson’s equation and current continuity equations for electrons and holes. Similar rate equations were also implemented for hole capture and emission. The S3A technique is capable of obtaining frequency domain solutions of time dependent variables declared through the rate equations. This includes carrier and trap concentrations.

**Results and Discussion**

**Transconductance**

Simulation results showed a positive shift in transconductance, similar to that observed in DC transfer characteristics, with severe degradation in peak transconductance for proton fluence approaching and exceeding $10^{14}$ cm$^{-2}$ (Figure 5-3). The results of using shallow donor-like trap levels show reasonable match with those observed in Ga-rich substrate growth. Similar donor-like defect concentrations introduced deeper in the band-gap will cause larger shift in pinch-off, as the extent of compensation is less under same gate bias, whereas peak transconductance degradation should be identical for both shallow and deep-levels. The transconductance values were obtained by selecting a low operating frequency of 100Hz. Defects were specified as donors or acceptors, along with their concentrations, energy level in the band gap and a time constant corresponding to the trap capture cross-section [115].

The role of dynamic aspect of such point defects from a transient perspective is straight-forward. The transition rate of traps depends on an initial stress bias and
consequent on-pulse, where the defects transition from an initial state to a final state determined by the occupancy of such defects and the availability of respective carriers. For the case of AlGaN/GaN HEMTs having abundance of electrons near the interface, the process of electron trapping and detrapping from donor-like traps dominates. The general position of the Fermi-level in the GaN bulk renders most acceptor-like defects completely ionized. Hence, hole-trapping as well as recombination-generation kinetics can be ignored.

For small signal analysis, defects actively contributing to the AC performance parameters lie at the Fermi-level, assuming such defects are fast enough to respond to the analysis frequency. The contribution of such a single-level defect can be represented in a general quantitative form using an equivalent circuit which represents current continuity equations and Poisson’s equation [116]. This equivalent circuit technique can be extended to various equilibrium and non-equilibrium scenarios. However, the complexity of the analysis will increase manifold if applied to a complex structure with multiple defect-levels. From a small signal analysis perspective, understanding the impact on device performance by multiple slow and fast traps thus involves obtaining the spatial distribution of defects at the Fermi-level (Figure 5-4). Comprehending the extent to which such defects at half-occupancy can affect RF parameters such as transconductance and current-gain at various operating frequencies necessitates the use of sinusoidal steady state analysis in a TCAD simulation framework, as was made available through the implementation of S3A analysis technique in FLOODS.
In order to understand how time constants specified in the definition of the traps played a role in the simulation result, traps with slow ($\tau^{-1} << 100\text{Hz}$) and fast ($\tau^{-1} >> 100\text{Hz}$) time constants were selected. First, with comparison of impact on transconductance, it was observed that these time constants directly affected the involvement of defects close to the Fermi level, in agreement with the small signal nature of such frequency domain simulations. While in general not significant, the difference becomes relatively more prominent near pinch-off, as shallow donor levels coinciding with the Fermi level are closer to the 2DEG interface (Figure 5-5). The implications are much greater when investigating their impact on current-gain at higher frequencies and consequently cut-off frequency.

**Current Gain**

From equations 5-1 and 5-2, it can be concluded that, unlike $f_{\text{max}}$, cut-off frequency $f_T$ can be analytically extracted using only transcapacitive components, $C_{GS}$ and $C_{GD}$, which is a relatively straight forward process using S3A technique. Current gain thus obtained from analytical expression showed excellent agreement with gain obtained directly from currents at the respective input and output terminals. As the simple drift-diffusion model assumed does not apply accurately at high frequencies expected, above simulations were carried out in the range of 1Hz-1GHz.

With linear roll-off in current gain, cut-off frequency can be obtained by extrapolation, with the device biased at peak transconductance as is generally done experimentally (Figure 5-6). Selection of time constants was carried out such as a clear distinction between slow and fast traps can be made in the current-gain frequency sweep for the observed frequency range. Slow traps were defined with $\tau = 1$ sec and
fast traps with $\tau = 0.1$ ns. From equation 5-1, current gain and cut-off frequency are dependent on two factors. Transconductance, as discussed in the previous section, exhibited a distinction with faster traps, capable of responding to the small signal frequency, leading to marginally more degradation. However, being dependent on additional capacitive components, current gain was expected to be more sensitive.

Degradation of cut-off frequency under different gate bias was simulated (Figure 5-7). Difference can be observed between not only unirradiated and radiated devices, but also between fast and slow traps. Unlike the results of transconductance simulation, a different trend is observable when comparing radiated devices with traps of different time constants. The distribution of cut-off frequency around peak transconductance is in good agreement with experimental results, with 13% degradation when comparing unirradiated device with radiated device with slow traps.

Near pinch-off, dissimilarity between unirradiated and radiated devices is discernible, contrasting to that observed experimentally. While neither slow or fast traps provide an exact match, simulation results of fast traps lie further away from unirradiated device values. Examination of transcapacitive components $C_{GS}$ and $C_{GD}$ proved that the variation in cut-off frequency could indeed be attributed to the contribution of fast traps.

To confirm the role played by fast traps in determining the transcapacitive elements, donor-like traps at different energy levels were compared. Figure 5-8 illustrates the gate bias dependence of capacitive components responsible for affecting cut-off frequency, with shallow donor-like defects introduced in the GaN bulk. A shift in the capacitive response is observed indicative of the role played by the change in
energy-level of the defects. Since the shift in peak corresponded well with the change in energy-level, trap ionization was observed right underneath the gate. The transition in the ionization of donors with changing bias can be correlated to the change in capacitance. Capacitance appears to decrease as gate is biased more and more towards pinch-off, as one would expect with the region underneath the gate getting depleted. Since the traps are relatively shallow, the partially ionized traps begin to influence the capacitance as the device approaches pinch-off. A peak capacitance is observed, for donors at different energy-levels, as the partially ionized donors appear to be spatially distributed in close vicinity to the gate. Beyond this point, the capacitance decreases and the influence of traps is distinctly reduced, as the region underneath the gate becomes completely depleted, and the traps completely ionized. The width of the peak in capacitance can be correlated to the rate at which the traps get ionized with gate bias.

**Conclusion**

The effect of proton irradiation induced donor-like defects on RF performance of AlGaN/GaN HEMTs was studied using small signal analysis capability of FLOODS. In particular, the possible introduction of fast traps capable of affecting device behavior at RF frequencies was investigated. Current-gain frequency sweep simulations show that in the presence of such fast traps, the extent of variation of irradiated devices from virgin devices would be significantly larger than what has been observed experimentally. From the few experimental results available in literature, it can be concluded that degradation in RF parameters is most likely due to introduction of slower defect centers responsible for DC and transient switching performance degradation.
Process dependence observed also necessitates a closer inspection of as-grown defects using current transient methodologies.

**Figure 5-1.** (Left) Degradation of transconductance with increasing proton fluence [93] 2014 IEEE (Right) Process dependence of peak transconductance degradation [114] 2013 IEEE

**Figure 5-2.** Reduction in cut-off frequency with increasing proton fluence at 1.8MeV [93] 2014 IEEE
Figure 5-3. Degradation of transconductance with increasing proton fluence.

Figure 5-4. Ionization of shallow donors near peak transconductance. Inset shows partially ionized traps that will contribute to small signal behavior.

Figure 5-5. Degradation of transfer characteristics (Left) and comparison of transconductance for slow and fast defects.
Figure 5-6. Current gain compared between unirradiated, irradiated with slow and irradiated with fast defects as a function of frequency.

Figure 5-7. Cut-off frequency variation as a function of gate bias (left) and trans-capacitive components for slow and fast traps.
Figure 5-8. Two-dimensional illustration of ionized donors for different trap depths at different gate bias points.
The most incessant technological issue that has plagued GaN based device reliability has been the role played by slow traps in degrading switching speeds. The attractive properties of GaN making it the ideal candidate for microwave and RF applications have often been obscured by the various carrier trapping processes diminishing their efficiency. The slow nature of these trapping-detrapping events affect devices not just under long term electrical stress and harsh environments, but due to the presence of as-grown defects in virgin devices as well. These mechanisms manifest themselves in the form of slow recovery of current in time, what is termed in literature as gate-lag, drain-lag and current collapse under various pulsed I-V characterization techniques.

The purpose of this chapter is to introduce the impact of slow traps present in the GaN bulk on the dynamic switching behavior of AlGaN/GaN HEMTs. While considerable effort has been concentrated in establishing the role of surface traps at the Nitride/AlGaN interface, improved passivation techniques have revealed that poor switching characteristics can also be contributed by defects present in the GaN buffer. The complex nature of as-grown defects, their origin as well as their impact on device behavior was briefly highlighted in Chapter 2. To comprehend their role in degrading switching behavior will require a systematic approach discussed in the following sections, and extended further in Chapter 7.

In the first section, experimental techniques that have been developed to compare dynamic behavior and extract parameters of traps that are responsible will be presented briefly. In the second section, the role of numerical simulators employed in
literature in understanding some of the trapping mechanisms which contribute to the switching performance deterioration will be highlighted. In the third section, details necessary to be presented so as to provide adequate insight about the physics involved in the current transient will be discussed. This will be done by comparing two devices exhibiting behavior at different levels of physical complexity on account of their bulk properties.

**Experimental Techniques**

In gate-lag experiments, a fixed drain bias is applied and the gate is pulsed from pinch-off to on-state (Figure 6-1) [31], [90]. The resulting transient generally shows a slow increase towards the final steady state value as the traps at the passivation/AlGaN interface as well as underneath the gate, in both the AlGaN barrier and GaN buffer layer, are expected to detrap.

For drain-lag experiments, a fixed gate bias is applied while the drain voltage is switched. Such a switching can be in the form of high-to-low voltage or low-to-high voltage. For a low-to-high drain bias switch, the transient exhibits an overshoot followed by a decay with time as it eventually reaches the steady-state value corresponding to the high drain bias. The high-to-low drain bias switch displays a drop in the drain current further below the steady state value corresponding to the low drain bias, as it gradually increases towards to the final steady-state current value. Such drain-lag transients happen to be sensitive to buffer traps in the drain-access region [117]-[119].

A more comprehensive dynamic performance characterization technique involves extracting output characteristics under pulsed biasing conditions. While the exact nature of such techniques can be varied as per the device structure and spatial location of interest, it usually comprises of applying a quiescent bias stress for a long
duration where the device may be biased in the off, semi-ON or completely-on states, followed by an on-pulse for a selected time period where the HEMT is expected to demonstrate lag. Figure 6-3 represents a single switching event during such an experiment where the HEMT is initially kept in pinch-off under high drain bias during quiescent stress. Unlike gate and drain-lag experiments, this setting happens to be a practical scenario for microwave power devices, and under which excessive 2DEG depletion from the drain-access region can result in significant current collapse with increasing quiescent drain bias [50], [58], [120].

By applying drain voltages of increasing magnitude during the on-pulse as shown in Figure 6-4, and sampling the current at the end of the on-pulse, a dynamic output characteristics is obtained. Such a characterization procedure is often termed as dynamic I-V analysis (DiVA) technique in literature [92], [118]. Using the DiVA procedure, the extracted dynamic I-V is typically compared to the static output characteristics to depict the extent of current collapse, while the slope of the dynamic I-V curve in the linear region can be used to extract dynamic ON-resistance.

Under strong pinch-off, trapping directly underneath the gate is associated with a transition in threshold voltage, and is expressed in the form of dynamic threshold as a parameter. It is observed in the dynamic I-V as a lower saturation current. With the application of a strong drain bias during stressing phase, depletion of the 2DEG in drain access region is associated with a collapse, manifesting in the form of higher resistance in the linear region of the dynamic I-V curve.

While analytical techniques have been applied to the various experimental results for understanding the nature of traps, the complexity presented by the multitude
of defects in the AlGaN/GaN heterostructure becomes unfeasible to examine without the aid of 2D TCAD simulations.

**TCAD in Literature**

Similar to experimental work, most researchers who initially leveraged TCAD to study switching performance of HEMTs directed their attention towards donor-like surface states expected at the unpassivated AlGaN surface. Gate-lag simulation results did support the hypothesis that such defects, which get negatively charged during quiescent stress, form a virtual gate adjacent to the drain side gate-edge, and consequently depleting the 2DEG. Surface traps have been neglected in the simulations discussed herein for two reasons. Firstly, the exact mechanisms are a topic of debate and cannot be captured effectively using a TCAD framework. Secondly, the primary aim is to identify the impact of buffer traps. There could be a possibility that even static charged surface traps can influence drain access region depletion in conjunction with buffer traps and will be discussed as a possible future work.

Unlike gate-lag, replicating drain-lag and pulsed I-V measurements however necessitate the introduction of traps in the GaN buffer in TCAD simulations. Under strongly pinched-off and high drain bias conditions, punch-through would lead to distribution of 2DEG electrons deeper into the buffer region. For simulating unintentionally doped GaN buffer, the three-level compensation model is commonly invoked [57], [58], [119]. In this model, shallow donor-like traps such as Silicon and Oxygen are included along with two deep traps detected by Klein et al. [47]. While the deeper of the two traps is confirmed to be due to incorporation of Carbon as an acceptor, the other deep trap whose origin is yet unknown is assumed to be a deep
donor. Also, the concentration of the deep donor is assumed to be higher than the acceptor trap, allowing the Fermi-level to be pinned at the deep donor level.

With the application of drain voltage, either under pinched-off, semi-ON or fully-ON state, hot electrons are expected to spill over deeper into the substrate, enhancing their trapping probability. Hence, to completely realize the extent to which buffer traps can lead to current collapse, employing the energy balance or hydrodynamic model, discussed in Chapter 3, is necessary, albeit at the cost of computational effort, which is why simulation results discussed herein have used the drift-diffusion model instead. Kalavagunta et al. [92] were able to model gate-lag effect in post-irradiated devices by introducing bulk traps in the GaN with the hydrodynamic model, in addition to surface states already present in the virgin devices.

While current collapse has always affected dynamic switching behavior of GaN based devices, the problem’s severity increased drastically as acceptor compensated high resistance buffer was introduced to combat punch-through like short-channel effects. Uren et al. [58] presented in-depth analysis of current collapse for intrinsic and compensated buffers using numerical simulations, including results for various acceptor concentrations and profiles. For intrinsic buffers, the three-level compensation model lead to same conclusion as before, that trapping of carriers injected into the buffer was the responsible mechanism. However, for high resistance buffers with acceptors, the more severe current collapse was brought about by negative space charge in the buffer leading to a strong back-gating effect induced dynamic threshold increase.

From the above discussion, it can be concluded that most of the literature based on numerical simulations have been able to qualitatively capture lag observed in
transient switching experiments. However, to get more quantitative accuracy requires accurate information regarding all trap parameters. Most spectroscopy techniques are unable to provide all the necessary information regarding the traps which can help replicate the transients in simulations. Moreover, the sampling of current over varied time scales presents a unique challenge for every device may present defects of varying signatures and spatial locations. Thus, considering the extent of non-idealities present in the GaN buffer which can affect transient behavior, instead of attempting accurate modeling of dynamic performance, the results discussed henceforth have used TCAD as an educational tool to enlighten on how to correlate variation of defect parameters, specifically related to trap energy-levels in the forbidden band-gap, to the myriad of transient behavior characteristics observed in literature.

**Simulation Parameters**

All simulations carried out were of the form of dynamic I-V analysis depicted in Figure 6-3, where the device is pinched off at $V_{th} - 2V$ and high drain voltage is applied during a quiescent phase. Most experimental quiescent bias pulse duration tend to vary depending on the observed time interval required for the HEMT under investigation to reach steady-state. In FLOODS simulations, the quiescent bias was established through a steady state solution followed by transient simulation of the on-pulse.

During the transient switching phase, bias at the gate is brought to zero, while the drain is dropped to a lower value in the linear regime of the dynamic I-V curve. If the current value is extracted at fixed time, resulting pulsed I-V can then be compared to the steady state I-V characteristics. However, the primary aim of these switching simulations is to observe transients in greater detail to grasp the role of different defect
parameters. Hence instead of extracting pulsed I-V like in DiVA, the HEMT is allowed to reach its final steady state in the transient phase.

Results of transient simulations are generally presented as current transients correlated to two-dimensional representation of trap ionization. However, such an illustration is generally not sufficient to reveal the extent of 2DEG depletion. Moreover, the two-dimensional nature of the representation cannot be quantified visually when comparing different devices. For this purpose, an approach based on extraction of substrate charge and its transition will be correlated to transition in current. The need to present and compare variation in ionized traps, specifically in the drain access region, will be highlighted and then utilized in the Chapter 7 where the impact of different parameters relevant to trap energy-level will be compared.

Results and Discussion

First, the commonly used approach in literature will be utilized with a relatively simple example. A single shallow donor level at concentration of $10^{16}$ cm$^{-3}$ has been introduced in the GaN buffer uniformly, with constant 2DEG mobility (Figure 6-5A) [121]. For a shallow donor, ionization can be observed under the gate upon pinch-off as expected, and the extent of ionization increases further with the application of a high drain bias (Figure 6-5B).

While an increase in ionization in the drain access region with increasing quiescent drain bias can be observed, the magnitude of current variation during the transient on-pulse is minimal (Figure 6-5C). During the transient phase, the ionized defects trap electrons from the 2DEG, resulting in the specified miniscule decrease in current. It was concluded that the effect of quiescent drain bias induced ionization, which was predominantly underneath the gate, was limited in its impact on both
dynamic threshold voltage and on the drain access region conductance. However, the above conclusion is difficult to comprehend from the illustrations provided, which has generally been the norm in presenting TCAD simulation results.

In the next example, a more complicated scenario is presented. The two-vacancy model observed in irradiated HEMTs, with shallow donors and deep acceptors, both at equally high densities of $10^{17} \text{ cm}^{-3}$ has been incorporated into the GaN bulk. Together with the Farahmand mobility model which includes ionized impurity scattering, a relatively complex transient behavior was observed. The Fermi-level is deeper and no longer pinned to the shallow donor-level, hence donors are now completely ionized except near the heterointerface (Figure 6-6A). Upon application of quiescent bias of $V_{GSQ}=-5\text{V}$ at the gate, occupied traps underneath the gate become ionized, while application of high drain bias of $V_{DSQ}=100\text{V}$ results in electron injection deeper into the bulk, which marginally reduces the ionization of the donors.

In the transient phase, current transient indicates a gradual increase in current throughout the on-pulse till steady state is reached (Figure 6-6B). It was anticipated that ionized impurities underneath the gate can affect the transient through increased scattering, and thus current variation may not be solely correlated to trapping and 2DEG depletion. Extracting the transition in substrate charge along the slice at the drain-side gate edge indicated two independent processes.

Figure 6-6C helps confirm that 2DEG electrons reoccupied the ionized donors underneath the gate at an earlier stage represented by process I, while trapped electrons deeper in the bulk are released gradually, denoted by process II. Figure 6-6B and 6-6C have been illustrated with colors correlating the current transient to the
substrate charge varying with time. It can be seen the faster response is from the donors at the heterointerface (process I), while the slower response is from deeper in the bulk (process II). With the ionized impurity scattering affecting the mobility, the trapping of electrons at the heterointerface is overcome by the improved mobility as the density of ionized impurity reduces, resulting in a net increase in current. The above mechanism would have been impossible to conclude had the transition in substrate charge was not made available.

**Conclusion**

The sensitivity of an AlGaN/GaN HEMT’s transient switching performance to as-grown defects has been presented. Even unstressed and unirradiated devices can exhibit slow response to bias switching which has been characterized through several experimental techniques. The role of TCAD simulation tools in understanding the mechanisms which lead to observed degradation has also been discussed. With more attention on GaN buffer, the impact of trap energy-level related parameters such as depth in the band-gap, presence defect bands as opposed to discrete levels and multiple trap levels will be presented in Chapter 7.
Figure 6-1. A) Gate bias during quiescent stress and on-state (Left) and drain current transient in on-state (Right). B) Electron trapping in off-state (Left) and detrapping in on-state (Right).
Figure 6-2. A) Drain bias during quiescent stress and transient phase (Left) and drain current decay transient. B) Negligible electron trapping during quiescent stress (Left) and increased trapping under high drain bias (Right).
Figure 6-3. A) Synchronous gate and drain bias switching (Left) and quiescent bias dependent transient. B) Electron trapping during quiescent stress (Left) and detrapping in the transient phase (Right).

Figure 6-4. Dynamic I-V Analysis (DiVA) technique with alternate quiescent and measurement pulses (Left) and extracted dynamic I-V (Right).
Figure 6-5. A) Shallow donor ionization and B) ionization with increasing quiescent drain stress. C) Current transients corresponding to quiescent stresses in B.
Figure 6-6. A) Shallow donor ionization for irradiated HEMT under quiescent stress. B) Current (Left) and substrate charge integrated along indicated line (Right) during transient. C) Donor trap ionization at different times corresponding to color notation of transients in part B shows two distinct mechanisms I. Trapping at the heterointerface, II. Detrapping from the substrate.
In Chapter 6, the crucial aspects related to experimental procedures resorted to when characterizing the switching behavior of AlGaN/GaN HEMTs were discussed, followed by a summary of the use numerical simulators in analyzing the impact of trapping centers on the dynamic performance of GaN based power devices. Also, the need to extract and present data involving ionized traps and their transition in a quantifiable form in addition to the generally favored two-dimensional illustration was established.

In this chapter, the understanding gained from the Chapter 6 that has been applied to carry out numerical simulations using FLOODS will be discussed in terms of deep traps present in the GaN forbidden band-gap. As it has been established, even an intrinsic GaN can be host to several deep-level traps in its band-gap which renders quantitatively replicating its transient behavior exceptionally challenging. The purpose of this chapter will therefore be focused on understanding how several parameters related to energy-level of the traps can affect the observed transients. The three-level compensation model utilized to simulate unintentionally doped GaN will be used.

The active trapping center in the three-level compensation model is the deep donor level where Fermi-level pinning is observed. The first parameter to be considered will be the trap energy-level and how its variation in the band-gap affects the transient. Almost all numerical simulations in literature on GaN buffer traps have presented results based on traps at discrete energy-levels [122]-[124], but more recent experimental findings have correlated the stretched exponential nature of transients to a Gaussian-
like broadening of the trap-level [88]. Yet another factor whose impact on transient behavior has not been investigated in great detail is the presence of multiple discrete energy-levels [125].

**Device Geometry**

From the two examples presented in Chapter 6, it can be concluded that the extent of current collapse observed is minute compared to what is generally observed in experiments. Even for irradiated device simulation, the extent of carrier trapping in the buffer was not sizeable enough to deplete the 2DEG, resulting in current collapse varying from 2-5% depending on off-state stress and on bias. Although experimental results show significant variation, even unirradiated UID-GaN samples have exhibited more than 20% increase in dynamic on-resistance under identical stress [126]. Numerical simulation results in literature which have exhibited noticeable current collapse tend to be of smaller geometry compared to the longer dimension devices discussed in Chapter 6.

Following the above observation, two devices were compared having different lateral dimensions. Both HEMTs share the same substrate, including identical defect parameters for the three-level compensation model and exhibit almost equal pinch-off voltage for low drain bias. The shorter HEMT has a gate length $L_G$ of 0.3 $\mu$m, gate to drain spacing $L_{GD}$ of 1 $\mu$m, and source to gate spacing $L_{GS}$ of 0.5 $\mu$m. The larger device has these dimensions scaled to ten times the shorter device. Figure 7-1 shows the distribution of potential under quiescent bias of $V_{GSQ}=5V$, $V_{DSQ}=30V$. The extent to which potential drop from the gate edge extends along the drain access region is a reliable indicator of 2DEG depletion.
Similarly, it can also be shown that, to produce equivalent current collapse in the two devices, the larger device will require quiescent drain bias scaled according to its lateral dimensions. Figure 7-2 shows the normalized transient response as the short-channel HEMT is subjected to quiescent bias of $V_{GSQ}=-5V$, $V_{DSQ}=1V$, while the long-channel HEMT is biased at $V_{GSQ}=-5V$, $V_{DSQ}=10V$ during quiescent stress. Both HEMTs are switched on under identical bias of $V_{GS}=0V$, $V_{DS}=5V$, and resulting transient shows a normalized collapse of approximately 1% for both devices. It is must be noted that dynamic I-V like simulations in literature for long-channel HEMTs have examined the possible role of novel mechanisms that can exacerbate current collapse [127], [128].

The primary objective of this chapter is to gain a fundamental understanding of as to how the variation of numerous factors associated with the deep-trap levels can affect the transient switching behavior. The results thus discussed in the following examples have been simulated using the short-channel HEMT using typical localized Shockley-Read-Hall trapping. The three-level compensation model was implemented in the GaN buffer for all devices with the deep-donor trap having an emission time constant defined as $\tau = 1$ sec.

As indicated by Figure 7-3, first the energy level of the deep donor level is varied. Second, the deep donor level is implemented as a band-like Gaussian distribution in energy, rather than a discrete level. Lastly, the deep donor traps are split up into multiple trap levels, to show how such a distribution differs in transient response from a band-like distribution. All transient simulations presented henceforth in this chapter were carried out in a dynamic I-V analysis-like switched biasing with quiescent stress bias point of ($V_{GSQ}=-5V$, $V_{DSQ}=10V$) and transient on phase bias of $V_{GS}=0V$, $V_{DS}=5V$. 

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Energy-Level Dependence

The deep donor level in the three-level compensation model is commonly introduced in the range of 1eV-1.8eV below the GaN conduction band minimum. Transient results for dynamic I-V like simulations with different deep donor-levels have been published before [57] but the comparison of the extent of current collapse and the exact mechanism was not the primary aim of the authors. In this exercise, transient current of three devices with deep donors at 0.4eV, 1eV and 2eV below the conduction band were compared by normalizing to the final steady state current.

Figure 7-3 shows that deeper traps are slowest to recover to steady-state as one might expect according to slower emission rates. However, the normalized magnitude of current collapse has a U-shaped dependence on the deep donor level, with the trap at $E_{DD}=E_C-1eV$ showing maximum current collapse. Figure 7-4 illustrates how the ionization of these defects transitions from quiescent stress bias to final steady-state condition under on-state. Figure 7-4 does provide a clue as to the extent of collapse expected from the deionization of the traps, but is difficult to support the observations made with regards to current collapse for different trap-levels.

Transition in substrate charge integrated vertically along a slice in the drain access region (50nm to the right of drain-side gate edge) was normalized and compared in Figure 7-5. Even though one-dimensional integration still cannot provide an accurate quantitative correlation with the current collapse, it can be used to compare scenarios like this in conjunction with the two-dimensional illustrations of Figure 7-4. A more accurate representation will require the extraction of a two-dimensional integration of charge in the GaN buffer and observing its subsequent transition, but such a feature has, as of now, not been implemented in FLOODS.
The U-shaped dependence of current collapse on trap-level can then be explained as follows. For a trap that is shallow, the tendency to trap electrons is too small to significantly deplete the 2DEG, as per SRH statistics. On the other hand, if the trap happens to be too deep in the band-gap, band-bending dictates that the partially ionized traps are now too far off from the interface. Application of even a strong drain bias cannot influence the occupation of these distant traps to an extent where they can influence the 2DEG.

Theoretically, an individual discrete trap level in a uniformly disturbed (either by carrier injection or illumination) sample is expected to display purely exponential change in current with time as the sample returns to equilibrium. Current relaxation and transient methodologies derive information about active trap levels in the HEMT by observing the current transients, which are often of stretched rather than pure exponential forms, in terms of time on a log scale [31]. While this presents several experimental setup challenges, it does provide insight into the nature of deep traps present in the HEMT structure which participate in electron trapping under regular biasing conditions.

The characteristics of the transient are studied by extracting their derivative in terms of the log scale of time i.e. $\partial I(t)/\partial [\ln(t)]$. A transient that would be purely exponential for time constant $\tau$ can be given by:

$$I(t) = I_0 - A \exp\left(-\frac{t}{\tau}\right)$$  \hspace{1cm} (7-1)

while its derivative in terms of $\ln(t) = \delta$ takes the form:

$$\frac{\partial I(t)}{\partial[\ln(t)]} = A \left(\frac{t}{\tau}\right) \exp\left(-\frac{t}{\tau}\right)$$  \hspace{1cm} (7-2a)

$$\frac{\partial I(t)}{\partial[\delta]} = A \exp(\delta) \exp(- \exp(\delta))$$  \hspace{1cm} (7-2b)
which is appears as an asymmetric peak with a slightly longer tail on the left or negative side.

However, transients observed experimentally are extended or stretched exponential:

\[ I(t) = I_0 - A \exp\left( -\left( \frac{t}{\tau} \right)^\beta \right) \] (7-3)

where \( \beta \) is the stretching factor, and derivative of equation (7-3) in terms of \( \ln(t) = \delta \) is:

\[ \frac{\partial I(t)}{\partial [\delta]} = A[\exp(\delta)]^{\beta} \exp(-[\exp(\delta)]^{\beta}) \] (7-4)

Compared to equation (7-2b), (7-4) represents a peak with amplitude scaled down by a factor \( \beta \), and full width at half maximum (FWHM) on either side widened by \( \beta \).

From Figure 7-4, the stretched exponential for the deep-level at Ec-1eV is discernible compared to its introduction at shallowest and deepest energy-levels. Figure 7-7 shows the derivative of the switching transient with respect to logarithm of time for deep-levels introduced at various levels in the upper-half of the band-gap. Similar to current collapse, an even more prominent U-shaped dependence is observable in the stretched exponential transition characterized by its derivate. The carrier detrapping kinetics that determines the stretching factor and factors responsible for the observed mechanism require further investigation.
Multi-level Traps

Results discussed above replicated a scenario were Fermi-level is expected to be pinned to a single dominant donor-like trap level. To examine how the relative energy of the Fermi-level with respect to the trap-level of interest can affect the details of the exponential transition, a multi-level donor scheme has been implemented. Identical to the three-level compensation model, instead of one discrete donor at $E_{DD}=E_C-1\text{eV}$ with density of $N_{DD}=10^{17}\text{cm}^{-3}$, two discrete donor levels have been introduced with identical densities of $N_{DD1}=N_{DD2}=5\times10^{16}\text{cm}^{-3}$. Device samples have been defined, with the shallower of the two levels at $E_{DD1}=E_C-1\text{eV}$, while the deeper trap has been introduced at $E_{DD2}$ varying from $E_C-1.01\text{eV}$ to $E_C-2.0\text{eV}$.

Figure 7-8 shows the switching current transient for the two samples. Transient observed in both samples can only be associated with the shallower trap as Fermi-level is expected to lie between the two deep donor levels, with the deeper donor completely occupied under the simulated bias conditions. Comparison of the transients will require comparison of their respective derivative with the logarithm of time. The transient for sample1 with separation of only 10 meV is expected to behave very similar to the single discrete trap level. On the other hand, transient for other samples exhibit slight shift in the relaxation time constant and a more gradual detrapping evident by a lower peak and wider stretching factor for the derivative.

Another illustration of implementing multiple-trap levels was carried by introducing three deep donor levels, with concentrations $N_{DD1}=N_{DD2}=N_{DD3}=2\times10^{16}\text{cm}^{-3}$, and $E_{DD1}=E_C-1\text{eV}$, $E_{DD2}=E_C-1.1\text{eV}$, $E_{DD3}=E_C-1.2\text{eV}$ (Figure 7-9). The purpose of a lower defect density and closed spacing in energy was to obtain transients associated with all
the donor levels. This was confirmed upon observing both the current transient and its derivative with three distinct peaks.

**Gaussian-Broadening**

Polyakov et al. [88] have recently proposed the possibility of band-like distribution of defect states in the band-gap that can contribute to stretched or extended exponentials in the current transients. Such a band of defect states are expected to be distributed in a symmetric Gaussian manner in energy around a specific energy level.

In Chapter 3, the implementation of Gaussian-like distribution of static defects in steady-state simulations was discussed. While the purpose of such a distribution is to avoid computational instability, a similar distribution can be implemented through FLOODS for transient simulations. Finite number of discrete trap levels distributed in energy and concentration to represent a Gaussian-like band have been defined through rate equations. For a simple comparison, examples discussed below involve three levels defining the Gaussian band.

In order to study the effect of a Gaussian spread in energy, four devices have been compared. All the devices implement the three-level compensation model, with deep donor at Ec-1eV participating in the trapping dynamics. The first device has a “discrete” deep-donor, hence identical results to the one discussed in the previous section (Figure 7-4) are expected. The other three HEMTs have the Gaussian broadening of the deep donor defined with a FWHM of 0.05 eV, 0.1 eV and 0.2 eV respectively.

Figure 7-10 shows the current transient response to dynamic switching for all the four samples. Closer inspection of the transition requires representation of its derivative (Figure 7-11). A clear shift in the current relaxation time constant peak is observed with
increasing FWHM. For FWHM of 0.05 eV and 0.1 eV, the derivative has a lower and considerably wider peak, indicating a more uniform detrapping process as compared to the discrete definition. For FWHM of 0.2 eV, the description of the Gaussian by finite energy levels has become evident with larger spacing in energy between the trap levels. A multi-level like transition is observed with sharper and multiple peaks.

The examples presented are very specific in the sense the Fermi-level is expected to be pinned at the mid-level of the defined deep donor distribution. The resulting transient after bias switching may not have identical exponential nature if the Fermi-level pinning is not observed, as was the case in the multi-level trap examples.

**Conclusion**

Transient simulations were carried out for HEMT structures with deep traps introduced in GaN buffer. Investigation involved understanding the impact of off-state drain stress on the electrostatics that lead to depletion of the 2DEG in the drain access region. Critical dependence on device dimensions were observed but further analysis on the effect of gate length and gate to drain spacing is necessary. The impact of variation of parameters related to deep traps introduced in the buffer was carried out on the shorter dimension HEMTs. The nature of transients was compared among devices with single discrete trap levels, multiple trap levels and band-like distribution in the upper half of the GaN buffer where Fermi-level is typically observed to be pinned.
Figure 7-1. Potential distribution under quiescent bias of $V_{GSQ}=-5V$, $V_{DSQ}=30V$ for short-channel HEMT (Left) and long-channel HEMT (Right).

Figure 7-2. Comparison of normalized transient phase current for short-channel (Black) and long-channel (Red) HEMT.
Figure 7-3. Schematic representation of trap-level distribution with three-level compensation (Left), Gaussian band-like distribution (Center) and multiple-trap levels (Right).

Figure 7-4. Comparison of normalized transient phase current for deep donor-like traps at different levels.
Figure 7-5. Deep donor-like trap ionization under quiescent stress (Left) and On-state final steady state (Right) for trap level at A) $E_{DD}=E_C-0.4\text{eV}$, B) $E_{DD}=E_C-1\text{eV}$, and C) $E_{DD}=E_C-2\text{eV}$. 
Figure 7-6. Transition in substrate charge normalized to final steady state value for each deep-trap.

Figure 7-7. Derivative of transient with respect to log of time for deep donor at different energy levels.
Figure 7-8. (Left) Current transient for two deep-levels with shallower trap at Ec-1eV and (Right) derivate of the transient.

Figure 7-9. (Left) Current transient and (Right) derivate with log of time for three discrete traps.

Figure 7-10. Comparison of transient phase current for deep donor-like traps at Ec-1eV with different extent of broadening.
Figure 7-11. Derivative of current with respect to logarithm of time shows a shift in peak, a narrower peak and a longer tail for broader Gaussian broadening in energy.
CHAPTER 8
CONCLUSION AND FUTURE WORK

Two-dimensional numerical simulations using FLOODS TCAD were carried out to get an in-depth understanding of the electrical behavior of AlGaN/GaN HEMTs.

Taking into consideration the range of application space over which GaN has been attracting attention, simulations were carried out to extract performance parameters characterizing steady-state, RF and high power switching behavior. First, the impact of proton irradiation damage to lattice and subsequent steady-state and RF performance deterioration of HEMTs designed for space communication applications was established. For power electronics applications, the role of as-grown defects in causing current lag and collapse in pulsed/dynamic characterization techniques was determined.

**Conclusion**

Steady-state simulation results have indicated the introduction of vacancies in the GaN lattice, with Gallium and Nitrogen vacancies forming deep acceptor and shallow donor respectively. Experimental results showing degradation of RF performance such as cut-off frequency upon proton irradiation have led to speculation that such lattice damage result in relatively fast traps. Using FLOODS small-signal analysis capability, the contribution of shallow donor-like traps akin to Nitrogen vacancies determined from steady state performance modeling effort was simulated assuming different trapping time constants. Even though more experimental results are necessary, comparison of simulation results have indicated that fast traps degrade current-gain through device parasitics, much more severely than experimentally observed.
Transient simulations to observe the effect of dynamic I-V like bias switching was carried out to understand how point defects in the GaN buffer lead to transients observed experimentally, with the eventual goal of simulating impact of proton irradiation on dynamic behavior. The necessity of accurately replicating as-grown defects was realized for reproduction of the exact magnitude and nature of current relaxation. This included extending the commonly used three-level compensation with multiple deep donor levels and band-like Gaussian distribution of trap levels to understand the exact impact on the nature of transients characterized by their derivative with the logarithm of time. For multi-level discrete traps, the relative magnitude of the derivative peak and width was correlated to the Fermi-level determined by the depth of other trap levels. For band-like distribution of traps in energy, the wider distribution correlated to shorter and wider peak indicative of a more gradual detrapping process.

**Future Work**

The results presented on transient switching simulations have led to the conclusion that buffer traps may not completely explain the lag observed experimentally for different device geometries. Although difficult to specify quantitatively because of variation in results found in literature, devices having larger lateral dimensions have also shown increased dynamic on-resistance with higher drain stress in quiescent phase. As per the numerical simulations discussed herein, the drift-diffusion model together with traps introduced only in the GaN cannot replicate the extent of current collapse in longer drain access region devices.

As has been discussed before, adopting the hydrodynamic model can inject hot electrons deeper into the bulk increasing the likelihood of severe 2DEG depletion even in larger devices. Additionally, the role of surface states on the AlGaN layer need
investigating as change in surface passivation techniques have shown to impact dynamic behavior [126]. Such charges if positive, and if comparable to the polarization charge at the AlGaN/GaN interface, could severely deplete the 2DEG.
LIST OF REFERENCES


[50] V. Desmaris et al., “Comparison of the DC and Microwave Performance of AlGaN/GaN HEMTs Grown on SiC by MOCVD With Fe-Doped or Unintentionally


BIOGRAPHICAL SKETCH

Shrijit Mukherjee was born in Mumbai, India in 1990. He completed his Bachelor of Engineering in Electronics Engineering from University of Mumbai in 2011. He received his Master of Science in Electrical and Computer Engineering from University of Florida in 2014. He is completing his doctoral dissertation under the guidance of Dr. Mark Law focusing on TCAD simulation of AlGaN/GaN High Electron Mobility Transistors.

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