Nitin Goyal

Design and Modeling of High-Power Semiconductor Devices with Emphasis on AlGaN/GaN HEMTs

Thesis for the degree of Philosophiae Doctor

Trondheim, October 2013

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Preface

This thesis has been submitted to the Faculty of Information Technology, Mathematics and Electrical Engineering in partial fulfillment of the requirements for the degree *Philosophiae Doctor* at Norwegian University of Science and Technology. The work was carried out at UNIK-University Graduate Center, Kjeller under the supervision of Prof. Tor A. Fjeldly. This work was supported in part by the European Commission under Grant Agreement 218255 (COMON) and the Norwegian Research Council under contract 970141669 (MUSIC).

The main work presented in this thesis can be summarized as follows:

1. Development of an analytical model of the surface barrier height for the AlGaN/GaN hetero-structures.
2. Development of an analytical model of the two dimensional electron gas density for the AlGaN/GaN hetero-structures.
3. Proposal of a new method to calculate the critical thickness for strain relaxation in thick layer AlGaN/GaN hetero-structures.
4. Modeling of the effect of strain relaxation on the surface barrier height and the two-dimensional electron density at the AlGaN/GaN hetero-interface.
5. Modeling of the effect of a gate metal on the surface state properties of the AlGaN barrier layer and the resultant impact on the barrier height and the two-dimensional electron gas.
6. Proposal of a new design of LDMOS in combination with a Zener diode for performance enhancement in the on-state characteristics.

Dedicated to my Ph.D. supervisor Prof. Tor A. Fjeldly, whose confidence in me inspired me to do this work.

"(...) your work is going to fill a large part of your life,
and the only way to be truly satisfied is to do what you believe is great work.
And the only way to do great work is to love what you do.

(...) don`t be trapped by dogma.
Don`t let the noise of others` opinions drown out your own inner voice.
And most important, have the courage to follow your hearth and intuition. They somehow already know what you truly want to become."

Steve Jobs, Stanford 2005

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My stay in Norway is probably the most fruitful experience of my life. This was only possible because of the very nice administration at UNIK. They are wonderful people, and I owe all of them “tusen takk” for the very good working environment they offer in the comparatively boring (but equally beautiful) Kjeller. I had the opportunity to talk to many scientists and other nice people from different places. I also would like to thank all the masters students I met during these years for having me be part of the table tennis team and other activities. I thank my friend Arild

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I am always thankful to NTNU, UNIK, the Norwegian Research Council project MUSIC, and the EU project COMON for the financial support without which it would not have been possible to do this work.

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Last but not least, I thank God for bringing me to this beautiful and peaceful country, which has such nice and friendly people. I will miss these beautiful landscapes which I see every day from my window and on the way to UNIK.

Nitin Goyal

05 June, 2013

Abstract

AlGaN/GaN based HEMTs are becoming one among the favorite choices for future high-frequency, high-power, high temperature electronics applications. This can be attributed to the excellent physical properties such as a wide band gap (more than 3.4 eV), a high critical field for breakdown, and a good thermal conductivity of these nitride based heterostructures. The most interesting feature of these devices is the presence of a high mobility, two-dimensional electron gas (2DEG) with a sheet density of the order of 10^{13} cm^{-2} at the AlGaN/GaN interface, even in the absence of both an AlGaN barrier layer doping and a gate metal (bare surface). This phenomenon is attributed to the strong piezoelectric as well as spontaneous polarization effects in these nitride based devices, allowing an efficient, gate-controlled charge transport between the source and drain electrodes of the device.

To design these devices, it is very important to understand their fundamental properties, including the mechanism responsible for the formation of the 2DEG, and how this is influenced by the formation of defects in the AlGaN layer at large thicknesses and Al contents in the layer. Another important issue is to derive modeling tools suitable for device characterization and for reliability analyses. In this thesis, a comprehensive mathematical framework to address these issues is presented. A main focus has been on the fundamental surface properties of the AlGaN layer, especially those related to the surface donor density and the surface donor level, the effect of gate metal deposition on the donor states, and the effects of defect formation in the AlGaN layer at high strain levels. The present analysis allows important design parameters to be described mathematically in terms of these properties. The present modeling is verified by comparisons with experimental results for all practical ranges of AlGaN thicknesses and Al concentrations in the AlGaN layer.

Traditionally, silicon based LDMOS devices have been an important work horse in less demanding commercial high-frequency electronics for RF applications. As part of the present investigations, a new design is proposed for LDMOSFETs where the incorporation a Zener diode in the drift region of the device is shown to improve the on-state performance characteristics of the device.

List of Publications

Journal Publications

1. Nitin Goyal and T. A. Fjeldly, "Effects of Strain Relaxation on Bare Surface Barrier Height and Two-Dimensional Electron Gas in AlxGa1−xN/GaN Heterostructures", *J. Appl. Phys.*, vol. 113, 014505 (2013).

2. Nitin Goyal, Raghvendra Saxena, "A New LDMOSFET with Tunneling Junction for Improved ON-State Performance", *IEEE Electron Device Letters*, vol.34, no.1, pp. 90-92, (2013).

3. Nitin Goyal, Benjamin Iniguez, Tor A. Fjeldly, "Analytical Modeling of Bare Surface Barrier Height and Charge Density in AlGaN/GaN Heterostructures", *Appl. Phys. Lett.* 101, 103505 (2012).

4. Sourabh Khandelwal, Nitin Goyal, and Tor A. Fjeldly, "A Physics Based Analytical Model for 2DEG Charge Density in AlGaN/GaN HEMT devices", *IEEE Trans. Electron Devices*, vol.58, no.10, pp. 3622-3625, (2011).

5. Sourabh Khandelwal, Nitin Goyal, and Tor A. Fjeldly, "A precise physics-based compact model for 2-DEG charge density in GaAs HEMTs applicable in all regions of device operation", *Solid State Electronics*, vol.79, pp. 22-25, (2013).

6. Nitin Goyal and Tor A. Fjeldly, "Bare Surface Barrier Height: A New Assessment of Structural Reliability in AlGaN/GaN Heterostructures", *Physica status solidi (c)* (submitted for publication) 2013.

Conference Publications

1. Nitin Goyal and Tor A. Fjeldly, "Bare Surface Barrier Height: A New Assessment of Structural Reliability in AlGaN/GaN Heterostructures", *Int. Sym. on Compound Semiconductor,* Kobe, Japan, May, 2013.

2. Nitin Goyal and Tor A. Fjeldly, "Impact of gate metal on surface states distribution and effective surface barrier height in AlGaN/GaN heterostructures", *Material Research Society, Spring Meeting,* San Francisco, Vol 1538, USA, April 2013.

3. Nitin Goyal, Benjamin Iniguez, and Tor A. Fjeldly, "Surface Barrier Height for Different Al Composition and Barrier Layer Thickness in AlGaN/GaN HEMTs", *Int. Conf. on Physics of Semiconductors,* Zurich, Switzerland, July 2012.

Table of Contents

Preface……………………………………………………………………………………III

Acknowledgements……………………………………………………………………………VI

Abstract……………………………………………………………………………………..IX

List of publications…………………………………………………………………………X

Table of contents……………………………………………………………………………XI

Abbreviations and Symbols …………………………………………………………….XIII

Part I. Introduction 1

Performance characteristics required for high voltage switching devices 2

Comparison of GaN with conventional semiconductors 5

Comparison of AlGaN/GaN HEMTs with other semiconductors devices 6

Applications of AlGaN/GaN HEMTs 8

Basic Crystal Structure of GaN 9

Piezoelectric and spontaneous polarization 10

Spontaneous Polarization 10

Piezoelectric Polarization 11

AlGaN/GaN HEMT structure 12

Mechanism of 2DEG formation in AlGaN/GaN and effect of surface states 13

Analytical modeling of the 2DEG carrier density and the surface barrier height for bare and metallized surfaces 15

Strain relaxation in AlGaN layers and its effects on device properties and behavior 16

Variation of surface states with Al composition in the AlGaN barrier layer and Implications on device design 18

LDMOSFET Design with a Zener diode in the drift region (Tunneling LDMOSFET) 19

Part I-References 21

Part II. Papers included in the thesis 24

Paper-A: Analytical Modeling of Bare Surface Barrier Height and Charge Density in AlGaN/GaN Heterostructures 25

Paper-B: Effects of Strain Relaxation on Bare Surface Barrier Height and Two-Dimensional Electron Gas in AlxGa1−xN/GaN Heterostructures 29

Paper-C: Impact of gate metal on surface states distribution and effective surface barrier height in AlGaN/GaN heterostructures 35

Paper-D: Bare Surface Barrier Height: A New Assessment of Structural Reliability in AlGaN/GaN Heterostructures 43

Paper-E: A New LDMOSFET with Tunneling Junction for Improved ON-State Performance 47

Part III. Conclusions and future work 49

Part III-References 53

Part IV. Errata 55

Abbreviations and Symbols

2DEG	Two Dimensional Electron Gas
FET	Field Effect Transistor
GaN	Gallium Nitride
HEMT	High Electron Mobility Transistor
LDMOS	Laterally diffused metal oxide semiconductor
MOCVD	Metal-Organic Chemical Vapor Deposition
PAE	Power Added Efficiency
SBH	Schottky Barrier Height
Si	Silicon
SiC	Silicon Carbide
WBG	Wide Bandgap
C_g	Gate Capacitance
C_{gd}	Gate-Drain Capacitance
L_g	Gate Length
μ_n	Electron Mobility
n_s	Charge Density at AlGaN/GaN Interface
C_g	Gate Capacitance
R_{on}	On-state Resistance
r_o	Output Impedance

Part I. Introduction

AlGaN/GaN high electron mobility transistors (HEMTs) have emerged as promising candidates for future radio-frequency (RF)/microwave power amplifiers and high-temperature electronics for hostile environments [1,2]. This has happened due to endless efforts made by researchers around the world for the last 20 years. The AlGaN/GaN material system is now regarded a backbone of both optical and microwave high-power electronics applications. This has led to a new market worth billions of dollars. The industry estimates that the worldwide GaN market will be 20 billion USD in 2014.

The huge success of this material system is attributed to the unique properties, which separates it from the conventional semiconductor systems widely used in semiconductor devices, including Si and GaAs. This includes the unique capabilities of achieving high breakdown voltage, high current density, high cut-off frequencies, highly linear characteristics, and high operating temperatures [1,2].

Nonetheless, the traditional devices, including the LDMOS devices, still have a domineering market share in the less demanding applications.

Performance characteristics required for high voltage switching devices

In the field of electric power conversion, transistors are assumed to behave as ideal switches. In reality, transistors are not ideal switches but exhibit some delay while turning on and off and exhibit finite breakdown voltage. Therefore high breakdown voltage and low energy losses are the most important requirements for a semiconductor high power switch. The energy losses of a switching device are divided into static losses and dynamic losses. The static losses are the ones when the transistor is in the on-state or in the off-state. In the on-state, the transistor should demonstrate very low on-resistance (ideally zero) in order to decrease the conduction losses. In the off-state the transistor should behave as a perfect open circuit but, inevitably, some residual leakage current will flow. This leakage current should be very low in order to reduce the standby power consumption. The switching losses are due to the finite capacitance and resistance, the switching from the on-state to the off-state and vice versa, which should be fast. Another requirement for the switching transistors is related to passive elements such as capacitances, inductances, and filters, which form the power conversion system. By increasing the operation frequency, it is possible to reduce the size of the passive elements used, which results in a size

reduction of the power conversion system. Therefore, higher operational frequencies are often required as an important specification of a switching device. Finally, the requirements for an electric power switching device can be summarized as follows:

• High blocking voltage, which expands the utilization field
• Low specific on-resistance, which reduces the device conduction losses
• Low capacitance, which reduces the switching losses and increases the operation frequency
• High operation frequency, which reduces the apparatus size

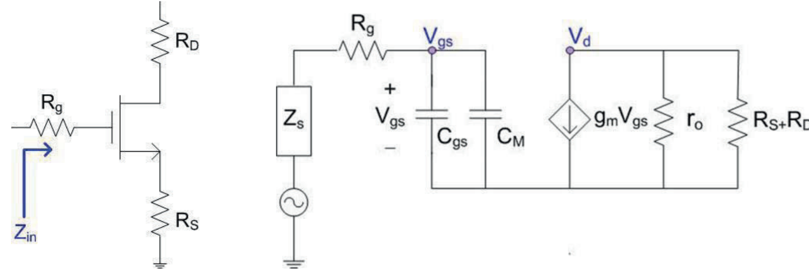

Figure 1. Terminal impedences of a transistors in the amplifier configuration and equivalent circuit [3,4].

If we look at the figure above representing terminal impedances of a transistor, which can be found in many standard text books/web links on RF circuit design [3,4], key electronic parameter such as the cutoff frequency f_T, the maximum oscillation frequency f_{max}, and the on-resistance R_{on} are given by the following expressions,

$$f_T = \frac{g_m}{2\pi C_g} \quad (1)$$

$$f_T = \frac{v_{sat}}{2\pi L_g} \quad (2)$$

$$f_{max} = \frac{1}{2}\frac{f_T}{\sqrt{2\pi \times f_T \times C_{gd}(R_g + R_s) + \frac{R_g + R_s}{r_o}}} \quad (3)$$

$$R_{on} = \frac{V_{BD}^2}{q\mu_n n_s (E_{crit}^2 - E_p^2)} \quad (4)$$

where g_m is the transconductance which is defined as $g_m = \frac{dI_d}{dV_g}$, v_{sat} is defined as saturation velocity, f_T and f_{max} are, respectively, the unity current gain frequency (cut-off frequency) and the maximum oscillation frequency (frequency at which the maximum power gain=1). $R_{d,}$ $R_{g,}$ and R_s

are the drain, gate, and source impedances, respectively. E_{crit} and E_p are the critical electrical field for breakdown and the built in electric field due to polarization, respectively.

For the GaN HEMTs, all of the above translate into the following attributes,

- High electron mobility
- Small source and drain resistance
- High f_T due to high electron velocity in large electrical fields
- High transconductance due to small gate-to-channel separation
- High output resistance

The main silicon power switching devices, such as the gate turn-off thyristor (GTO) and the insulated gate bipolar transistor (IGBT) have operation frequencies only in the range from a few Hz to the kHz range, while power GaN HEMTs and Si MOSFET devices can handle several MHz [1]. The GaN technology not only exceeds the operational frequency of silicon GTO and IGBT but also, very importantly, exceeds the switching capacity of the MOSFET devices [1,2]. If we look at above equations, we can observe why GaN technology is so important, namely because the GaN HEMTs possess a superior v_{sat}, and very low R_s and R_d which is basically the resistance of the un-gated part of the channel where the 2DEG density is quite large. Similar argument can be presented for R_{on}. Figure 2 shows R_{on} versus the breakdown voltage for a range of commercial devices, indicating the superior properties of the GaN devices, particularly for high voltage, high power applications [2].

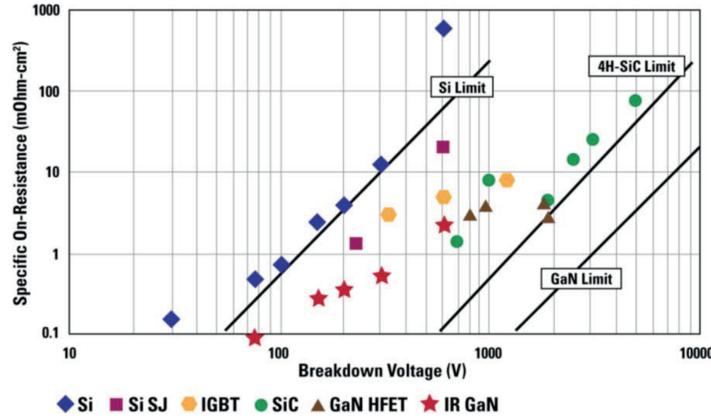

Figure 2. Comparison of R_{on} for Si, SiC and GaN versus breakdown voltage. (SiSJ: Silicon Super Junction devices, IR GaN: International Rectifier GaN devices) [2].

Comparison of GaN with conventional semiconductors

Large bandgap energies (E_g) result in high electric breakdown fields (E_{crit}), which enable high voltage applications. Furthermore, such materials withstand high operating temperatures and provide for improved radiation hardness. GaN and SiC have bandgap energies about two to three times those of conventional semiconductors such as Si, GaAs, and InP. The electric breakdown fields for the wide band gap (WBG) materials are excellent and very high, typically one order of magnitude larger than for the conventional semiconductors [1].

As discussed in the previous section, to achieve high currents and high frequency operation, high charge carrier mobility (μ_n) and high saturation velocity (v_{sat}) are desirable characteristics. Bulk GaN and SiC values for the electron mobilities, are about 900 cm^2/Vs for bulk GaN and, depending on the polytype, and approximately 700 cm^2/Vs for SiC. In general, WBG semiconductors have relatively low mobility but very high values for the saturation velocity, which is reached at high electric fields [1,2,5,6]. However, when the 2DEG forms at the interface AlGaN/GaN hetero-structures, the mobility values are much superior (higher) than for bulk GaN due to reduced scattering and the two-dimensional confinement effects. Hence, the mobility and saturation velocity of the 2DEG at the $Al_xGa_{1-x}N$/GaN hetero-junction is very suitable for high-power, high-frequency device applications. These values are sufficient for transistors specifically designed for high-power operation. The room temperature (RT) mobility of the 2DEG, which is typically between 1800 cm^2/Vs and 2000 cm^2/Vs, is significantly better

than that of bulk GaN and SiC. The 2DEG sheet charge density (n_s) of the $Al_xGa_{1-x}N/GaN$ structure is very high, with experimental values up to 1 x 10^{13} cm^{-2}, due to the piezoelectric and spontaneous polarization induced effects. This value of n_s is about a factor of 10 better than those of $Al_xGa_{1-x}As/In_xGa_{1-x}As$ and $In_xAl_{1-x}As/In_xGa_{1-x}As$ hetero-structures [1,2,5-11].

The thermal conductivity (k) of a semiconductor material is a measure for the ease with which dissipated power can be extracted from the device. This is a very important parameter for high-power device design. Poor thermal conductivity leads to degraded device operation at elevated temperatures. In general, conventional semiconductors are poor thermal conductors, particularly GaAs and InP. Conversely, SiC and especially diamond are excellent thermal conductors. GaN is comparable with Si, the best of the conventional semiconductors [1,2,5,6].

The relative permittivity ε_r is an indication of the capacitive loading of a transistor and affects the device terminal impedances. The values of ε_r for the WBG semiconductors are considerably lower than those for the conventional semiconductors. In the case of GaN and SiC, the values of ε_r are about 20% lower whereas for diamond the value is about 55 % lower. This permits, for example, a GaN device to be about 20% larger in area for a given impedance. As a consequence, this increased area enables the generation of larger currents and higher microwave output power [1,2,5,6].

From the above comparison it is clear that GaN offers much better high-power/high-frequency performance possibilities than GaAs and SiC.

Comparison of AlGaN/GaN HEMTs with other semiconductors devices

GaAs devices were the backbone of the high frequency semiconductor devices in the last two decades but they are not always suitable for high-power switching and RF applications due to several drawbacks like high substrate costs, narrow band gap and low thermal conductivity. SiC technology has emerged in the past 10 years as the best choice to overcome the limitations of the Si technology for power switching applications in the low frequency range for power converter and smart grid applications [1,2]. SiC devices benefit from the excellent thermal conductivity of the substrate. However, their electron mobility is significantly lower than that of GaN devices, and also, the SiC material lacks a hetero-junction technology.. Moreover, SiC technology suffers from very high intrinsic material costs and is not highly scalable in substrate size, epitaxial deposition equipment throughput, material supply, and device-fabrication manufacturing

platforms. Another disadvantage is the complexity of the processing. The cost of the GaN technology, on the other hand, can be lowered by growing the III-nitride materials on Si substrates, which are available in large diameters up to 300 mm. From a processing point of view, GaN-on-Si devices can be processed in the Si high volume foundries using the same high throughput and high yielding process technologies as used for Si-based devices [1,2].

In RF mobile telephony and data applications, Si LDMOS transistors are the backbone of today's base-station power amplifiers (PAs) owing to their excellent price-to-performance ratio compared with other commercially available technologies, such as GaAs HFETs and Si bipolar junction transistors (BJTs) [1,2,9,10]. Emerging wireless cellular networks are designed to provide high data rate services beyond traditional voice transmission. To support these higher data rates, wide-band code-division multiple access (W-CDMA) place severe demands on the linearity of the base station power amplifiers and thereby on the power transistors. The transistor linearity specification, commonly expressed in terms of the adjacent channel power ratio (ACPR), also known as the adjacent channel leakage ratio (ACLR), can be as stringent as -65 dBc. ACPR is a measure for the amount of power spilling into the adjacent channels referenced to the power in the transmit channel [1].

To achieve the required linearity, W-CDMA transistors must operate with the power backed off to well below their peak capability. As LDMOS technology is capable of providing only moderate power density, it is necessary to use devices with very large gate peripheries and correspondingly very low die impedances to realize the required large powers. As a consequence, the bandwidth of the matching circuit is reduced. All these issues can be circumvented by using a technology that enables higher total output power and increased bandwidth resulting from a more compact layout, as in the case of GaN based HFETs [1]. As GaN HFETs show much higher linearity than Si LDMOS devices, it is now possible on the system level to reduce the complexity of the linearization circuitry necessary for high bandwidth wireless systems. In this way, a same-sized device can handle higher power that results in lower costs per Watt of power and lower system costs. The higher impedance levels of these smaller devices also ease the input matching and high-bandwidth design considerably. Recent GaN commercial devices clearly show that AlGaN/GaN HEMTs are capable of delivering a favorable breakdown voltage and on-resistance beyond the material limits of Si and SiC semiconductors used today for high-power switching applications as was shown in the Figure 2. Likewise, the comparison of different technologies in

terms for power and frequency handling capabilities shown in Figure 3 [6] clearly indicates that the AlGaN/GaN HEMTs are a prime contender in a wide and important range of power-frequency combinations.

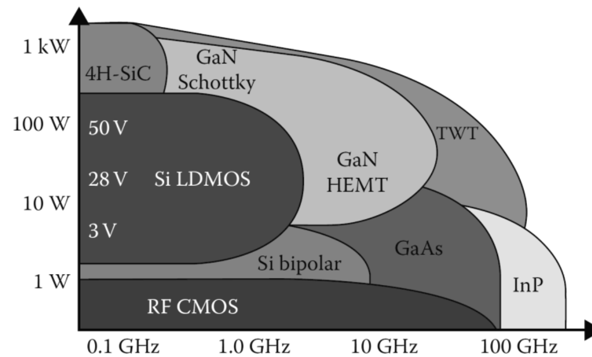

Figure 3. Power-frequency diagram showing various commercial semiconductor devices in their respective region of operation. Important to note is that GaN is rapidly expanding into the Si LDMOS and TWT region of operation [6]

Applications of AlGaN/GaN HEMTs

High-efficiency and high-linearity power amplifiers for base-stations, which power 4G wireless broadband cellular networks were among the first commercial GaN-based applications. US and Japanese companies like Fujitsu, Matsushita Electric, OKI Electric, Triquint, RFMD, and IR are now major players in this field. Other high-volume commercial applications of GaN-based electronics are high-frequency MMICs (wireless broadband communication links), hybrid electric vehicles (DC-AC conversion), high temperature electronics (automotive, energy production), switches (plasma display panels, low-frequency high-power switching), high-voltage power rectifiers (inverter modules), micro electro-mechanical systems, MEMS (pressure sensors), and Hall sensors (automotive applications), hybrid electric vehicle (HEV) platforms, and military and commercial aircraft engine electronics [1,2,5,6].

Oil well logging represents another highly developed industry where high temperature electronics technology is being applied. The use of high temperature electronics in this market actually exceeds that of other application sectors like automotive or aerospace [12,13]. Since

GaN junctions allow rectification with low reverse leakage current at junction temperatures as high as 600°C, they permit power-device operation at the high temperatures experienced in these applications. This, in combination with the superior power switching properties at room temperature make GaN technology a likely contender in realizing high-power electronics beyond the capability of Si at all temperatures.

For low-power circuits, GaN-based electronics will likely be of interest in the temperature range beyond the reach of silicon-on-insulator (SOI) electronics, i.e., in the range above 300 ^{o}C. Another application of GaN-based electronics is in high-voltage power rectifiers used, for example, as key components of inverter modules in power flow control circuits. Lateral AlGaN-based Schottky rectifiers have shown reverse blocking voltages up to 9.7 kV.

AlGaN/GaN HEMTs also exhibit a promising potential for the construction of digital integrated circuits (ICs), especially for operations at high temperatures where silicon or GaAs-based technologies fail. High-temperature digital ICs can provide the enabling technology in intelligent control and sensing circuits for automotive engines, aviation systems, chemical reactors and well-logging for oil exploration systems. GaN-based power devices can operate with less cooling and fewer high-cost processing steps designed to maximize heat extraction.

Basic Crystal Structure of GaN

In general, the majority of group III-nitrides exist in two different types of crystal structures; Wurtzite (hexagonal) and zinc-blende (cubic) [1,5,6]. The Wurtzite structure shown in Figure 4 has a hexagonal unit cell having two lattice constants a and c, while the zinc-blende structure is formed from a group of cubic unit cells and has a higher degree of crystallographic symmetry as its lattice constants are equal in three perpendicular directions. The Wurtzite structure is the thermodynamically stable phase under ambient conditions. On the other hand, zinc blende is a metastable structure and mainly forms when a film is grown on a cubic substrate, e.g., GaAs and 3C-SiC under carefully controlled conditions. The group III nitrides normally crystallize in the hexagonal (Wurtzite) phase. A unique feature of the hexagonal III-nitrides grown along the c-axis is the existence of strong spontaneous and piezoelectric fields [5,6,8]. The three parameters that define the Wurtzite lattice are the edge length of the basal hexagon (a_0), the height of the hexagonal lattice cell (c_0), and the cation-anion bond length ratio (u_0) along the [0001] direction,

all in units of c_0. The subscript "0" indicates that these values are those of the equilibrium lattice. In an ideal Wurtzite crystal the c_0/a_0 ratio equals $\sqrt{8/3} = 1.633$ and the value for u_0 is 0.375 [1,6].

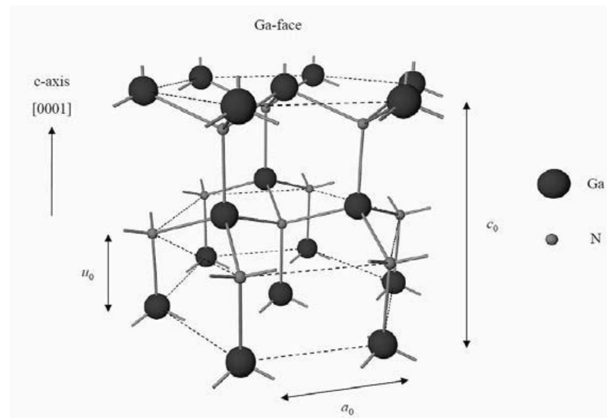

Figure 4. The wurtzite structure of GaN [1].

Piezoelectric and spontaneous polarization

The polarization field in the nitride-based hetero-structures comes from two parts, the spontaneous polarization and the piezoelectric polarization. Due to the non-central symmetry, nitrides exhibit a macroscopic spontaneous polarization field along the hexagonal c-axis in the Wurtzite lattice. In addition, lattice mismatch in AlGaN/GaN-type hetero-structures induces piezoelectric polarization.

Spontaneous polarization

The involvement of nitrogen, which is the smallest and the most electronegative Group V element, makes the III-nitrides special among the other III-V compounds as this has a strong effect on their properties. Because of the $1s^2 2s^2 2p^3$ electronic configuration of the N atom, or empty outer orbitals, the electrons involved in the gallium-nitrogen covalent bond will be strongly attracted by the Coulomb potential of the N atomic nucleus. This means that this covalent bond will have stronger ionicity compared to other III-V covalent bonds. This ionicity, which is a microscopic polarization, will result in a macroscopic polarization if the crystal lacks inversion symmetry. The Wurtzite III-nitrides do not have inversion symmetry along the [0001] direction. This fact, in combination with the strong ionicity of the metal-nitrogen bond, results in

a strong macroscopic polarization along the [0001] direction. Since this polarization effect occurs in the equilibrium lattice of III-nitrides at zero strain, it is called spontaneous polarization [1,6,8].

In addition to the ionicity of the covalent bond, the degree of non-ideality of the crystal lattice also affects the strength of spontaneous polarization. In III-nitrides, although the covalent bond parallel to the c-axis is strongly ionic and is primarily responsible for the spontaneous polarization, the other three covalent bonds in the tetrahedral structure are also equally ionic. The resultant polarization from these other three bonds is actually aligned in the opposite direction and serves to counteract the polarization of the other bond. As the c_0/a_0 ratio decreases, c_0 decreases and a_0 increases, these three covalent bonds will be at a wider angle from the c-axis and their resultant compensation polarization will decrease. As a result the macroscopic spontaneous polarization will increase. It can be seen that as the lattice non-ideality increases, c_0/a_0 ratio moves away from 1.633 of the ideal lattice, the value of spontaneous polarization (PSP) increases from GaN to AlN. The direction of the spontaneous polarization field in nitrides depends on the polarity of the crystal, that is, whether it's Ga-faced or N faced. Almost all MOCVD-grown nitrides are Ga-faced, while the nitrides grown in MBE system are usually N-faced. In addition, nitrides have a strain induced piezoelectric polarization, which is much higher than that in the traditional III-V semiconductors [1,6,8].

Piezoelectric Polarization

Strain is known to change the ideality of the crystal lattice. If stress is applied to the III-nitride lattice, the ideal lattice parameters c_0 and a_0 of the crystal structure will change accordingly to accommodate the stress. Hence, the polarization strength will be changed. This additional polarization in strained III-nitride crystals is called piezoelectric polarization. If the nitride crystal is under biaxial tensile stress, the in-plane lattice constant a_0 will increase and the vertical lattice constant c_0 will decrease. Hence, the c_0/a_0 ratio will decrease from 1.633 of the ideal lattice and the total polarization strength of the crystal will increase because the piezoelectric and spontaneous polarizations will act in the same direction [1,2,5,6].

AlGaN/GaN HEMT structure

The AlGaN/GaN hetero-structure is basically a stack consisting of a thin, strained, unintentionally doped AlGaN layer on top of an unintentionally doped GaN layer. This is shown in Figure 5, where also the corresponding energy band diagram is indicated.

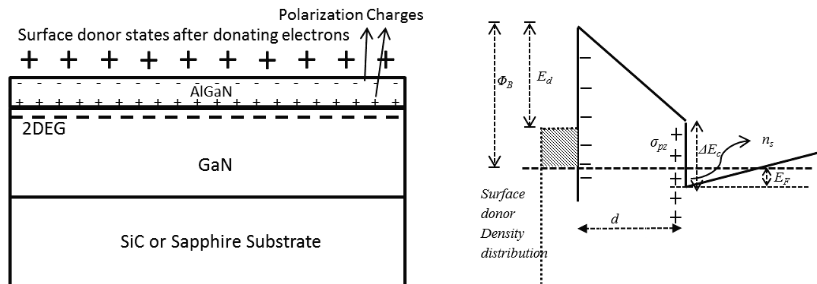

Figure 5. AlGaN/GaN HEMT stack structure showing polarization charge distributions at different interfaces (left) and the corresponding band diagram showing various charges at the different interfaces including the 2DEG at the AlGaN/GaN interface (right).

Due to the inherent polarization effects present in these materials, a thin sheet of charges is induced at the top and bottom of the interfaces of the AlGaN layer [1,2,7,9-20]. As a result of this, a high electric field is induced in the AlGaN barrier layer and surface donor states at the top interface donate electrons to form 2DEG at the AlGaN/GaN hetero-junction without the application of a gate bias [7]. Hence, these devices are normally *on* devices. The source and drain ohmic contacts are then formed to make transistors. The threshold voltage or V_{TH}, also called the or cutoff voltage V_{cutoff}, of the AlGaN/GaN HEMTs depends on the design of the epitaxial structure, namely, the Al composition and the thickness of the AlGaN barrier. However, the threshold voltage can be adjusted to become positive and enhancement-mode (E-mode) operation is realized. Compared to the D mode HEMTs, E-mode devices allow elimination of a negative-polarity voltage supply, and therefore, contributes to reducing the circuit complexity and system cost. A common fabrication technique of modifying the HEMTs' threshold voltage is so-called "gate-recess", whereby the thickness of the barrier layer under the gate metal is reduced and, with the help of the gate metal work function, the threshold voltage can be shifted to a positive value. A device with gate-recess is illustrated in Figure 6.

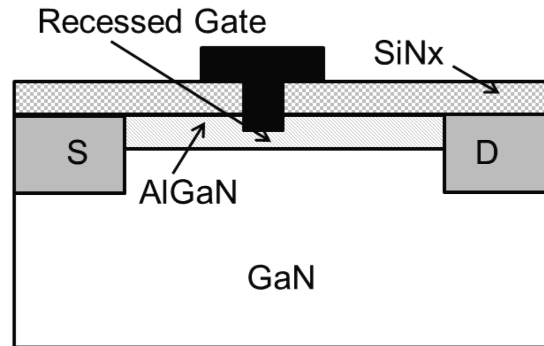

Figure 6. Recessed-gate AlGaN/GaN HEMT structure to realize a normally *off* device.

Mechanism of 2DEG formation in AlGaN/GaN and effect of surface states

The formation of the high mobility two-dimensional electron gas (2DEG) density at the AlGaN/GaN interface, even in the absence of both doping in the AlGaN barrier layer and gate metal (bare surface), can be attributed to the presence of strong piezoelectric and spontaneous polarization effects. In the last few years, considerable research has been performed to explain the mechanism and the source of electrons for the 2DEG formation [3-15]. It has been shown, using experiments as well numerical simulations, that the presence of donor states at the AlGaN surface is the main source of the electrons. Till now this is assumed to be the only valid theory to explain the behavior observed experimentally. Understanding the formation of the 2DEG is very important to explain the mechanism of current collapse and various other effects in ac and dc characteristics, and is thus very crucial to the device design [5, 21].

The bare surface donor model (SDM) by Ibbetson *et al.* was proposed to explain the behavior of 2DEG charge concentration with variation in the barrier layer thickness [7]. They assumed that a high density of surface donor states exists at a particular energy level E_{do} in the forbidden gap measured relative to the conduction band minimum of the AlGaN surface, as illustrated in Figure 7. With increasing barrier thickness d, this level moves higher due to the constant electric field in the barrier. Once this level reaches the Fermi level, the surface donor states start donating electrons to form the 2DEG at the AlGaN/GaN interface. According to this model, the Fermi level at the surface will remain essentially constant (Fermi level pinning) once

the barrier layer reaches the critical thickness d_{cr}, below which the 2DEG vanishes. Therefore, according to SDM, the surface barrier height $q\Phi_B$ remains almost constant (increases only in the range of kT/q) with increasing d once the donor level is reached. This model was justified by certain experimental data as well as by numerical simulations. However, this model could not be reconciled with experimental observations by Koley *et al*. that the $q\Phi_B$ of the bare surface increases with increasing d [16]. Instead, these observations were explained by assuming low-density surface donor states distributed over a range of energies below a particular donor energy level E_d in the forbidden gap, as indicated in Figure 7 [16-18] (see Paper A and Paper B, Part II of this thesis). Hence, with increasing d, the conduction band moves up and, simultaneously, lift E_d with respect to Fermi level. Thus, when E_d crosses the Fermi level, the surface donor states start donating electrons to form the 2DEG at the hetero-interface. Therefore, in this model, $q\Phi_B$ will increase with increasing d even in the active regime as shown in Figure 8 [18] (see Paper A and Paper B, Part II of this thesis). Experiments and numerical simulations show that both the 2DEG charge concentration qn_s and $q\Phi_B$ first increase linearly and eventually saturate with increasing barrier thickness [16-19].

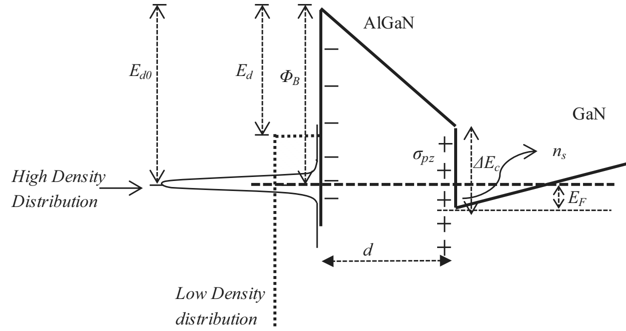

Figure 7. Band diagrams of a AlGaN/GaN HEMT showing the various charges at the interfaces and illustrating the formation of a 2DEG with electrons supplied by surface donor states. Two cases with different distributions of the surface donor states in the energy gap are shown: (a) single surface donor level with high density; (b) distributed surface donor states with low density. The shaded box illustrates the amount of electrons donated to the 2DEG by low-density surface donor states [18].

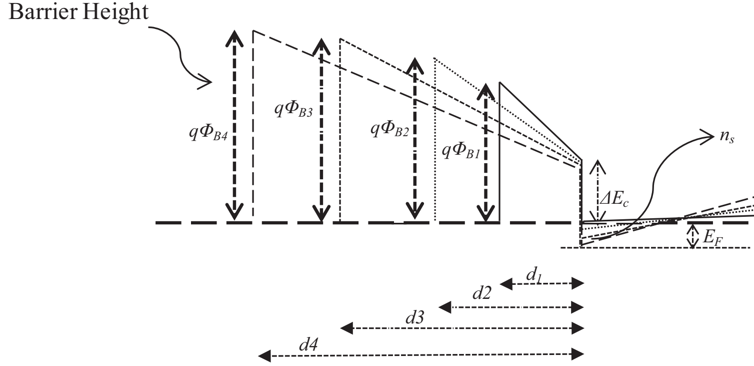

Figure 8. Schematic diagram depicting the increase in surface barrier height with increasing AlGaN thickness. Also shown is the simultaneous increase of the 2DEG density at the AlGaN/GaN interface [18].

Analytical modeling of the 2DEG carrier density and the surface barrier height for bare and metallized surfaces

As discussed above, the surface donor states are of fundamental importance to key observable electronic properties of the AlGaN/GaN HEMT such as the 2DEG carrier density and the surface barrier height, and to geometric and material parameters, including the polarization effect. It is therefore highly desirable to be able to describe this relationship quantitatively though a physics-based model. Such a model is of prime importance as a mathematical foundation for the development of optimized structures and new device designs.

Starting with the assumption of a bare AlGaN top surface (no metal gate), the distribution of surface donor states can be characterized by the constant state density n_0 and the donor level E_d, as discussed above and shown in Figure 7. Applying Laplace equation to the AlGaN/GaN structure and requiring overall charge neutrality, it was possible to derive a simple model relating the 2DEG carrier density n_s and the surface barrier height $q\Phi_B$ to n_0 and E_d. These relationships are discussed in more detail in [18] (see Paper A, Part II of this thesis).

The deposition of a metal gate, needed to form a proper Schottky barrier for efficient gate control of the HEMT structure, causes a redistribution of the surface states. In turn, this modifies both $q\Phi_B$ and n_s. Experimentally, it has been shown that the Schottky contacts act to reduce both the 2DEG and the SBH by partially neutralizing the surface states [22]. To address this problem,

the above physics-based model has been extended to describe the surface donor density distribution for metal/AlGaN/GaN structures. This modeling partly relies on experimental observations to describe the reduction that takes place in surface donor density when the metal gate is deposited. We assume that the basic nature of surface states remain unchanged, i.e., that they consist of donor states with a low/intermediate density and a fairly flat distribution in the relevant energy range about the Fermi level, and that only n_0 and E_d changes from those of the bare surface values. Details of this work can be found in the Paper [23], (see Paper C, Part II of this thesis.

Strain relaxation in AlGaN layers and its effects on device properties and behavior

As shown in Figure 9, the top layer in pseudomorphic growth of hetero-structures initially grows with the lattice constant of the substrate. Due to its large thickness, the substrate is always assumed to be in a relaxed state. With a lattice mismatch between the substrate and the barrier, there is always an inherent strain present in the top layer. In the AlGaN/GaN system, a thin layer of AlGaN is grown on a relatively thick GaN substrate. The AlGaN has a lower lattice constant than that of the substrate, and the mismatch gradually increases with increasing Al content. The piezoelectric polarization is an effect of this strain as explained in the previous parts. In addition, spontaneous polarization also increases with increasing Al content. Hence, the total polarization at the AlGaN/GaN interface increases and, consequently, so does the 2DEG charge density.

It has been shown theoretically and experimentally that when the Al content is small, relatively thick AlGaN layers can be grown on GaN since the residual (effective) strain is small [24-27]. When the thickness of AlGaN layer increases, so does the effective total strain energy present in the system. Beyond a certain thickness called critical layer thickness, the strain energy stored in the AlGaN layer can lead to rapid formation of dislocations that relaxes the strain. This can led to plastic deformation by generating surface irregularities. With increasing Al content, needed to produce sufficiently large piezoelectric charges, the critical thickness is reduced and, eventually, the structure may be rendered useless for device applications.

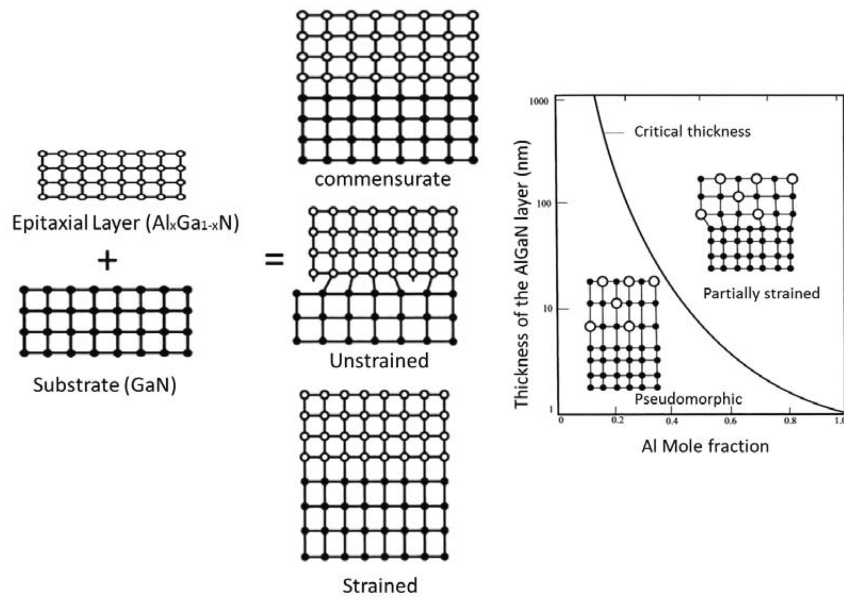

Figure 9. Schematic diagram depicting strained, unstrained and commensurate growth of AlGaN/GaN hetero-structures.

This is partly due to a weakening of the piezoelectric polarization and partly due to a reduction of the channel mobility resulting from interface imperfections. This can reduce the effective polarization significantly. Concomitantly, the piezoelectric polarization gradually weakens. Studies of SBH by Gordon *et al*. [17] and 2DEG by Ibbetson *et al*. [7] showed that beyond the critical thickness, strain relaxation takes place in the barrier layer reducing both SBH and 2DEG. From a practical point of view, it is very important to understand the electrical properties of the heterostructures in terms of the physical attributes of the AlGaN barrier layer. As indicated, its two most important physical parameters are the Al content and the thickness. In order to design highly efficient and reliable HEMT structures, it is important to understand the variation in the SBH and the 2DEG with these physical attributes.

Here, we have proposed a new procedure to extract and to model this critical thickness and to subsequently determine the effective polarization for partially relaxed barrier layers. Details of this analysis are given in [20, 28] (see Papers B and D, Part II of this thesis).

This mathematical model supported with published experimental data enables designers and manufacturers to improve their device characterization focus and their interpretation of characterization results through a better understanding of the physical underpinnings of these devices.

Variation of surface states with Al content in the AlGaN barrier layer and implications on device design

As explained above, donor surface states present at the top interface of AlGaN are the source of electrons in the 2DEG present at the hetero-interface. It was shown using a large number of experiments coupled with numerical simulations [17] and also using ab-intio models [14,15,17], that the density and distribution of these surface states are functions of Al composition in the AlGaN layer. As the Al composition increases, the donor level moves away from the conduction band edge and the surface donor density increases [17]. Our examination of this behavior indicates a nearly linear dependence in the interesting range of Al content of up to 40 %, as shown in Figure 10 (a) and (b). This dependency on the Al composition is very useful for the device designers for specific applications. Hence, for RF applications, thin, un-relaxed AlGaN layers of high Al content can be grown with low source and drain impedances and high transconductance values. On the other hand, for applications requiring devices with high breakdown voltage, thick, unrelaxed AlGaN layers with low Al compositions of up to 12 % can be grown.

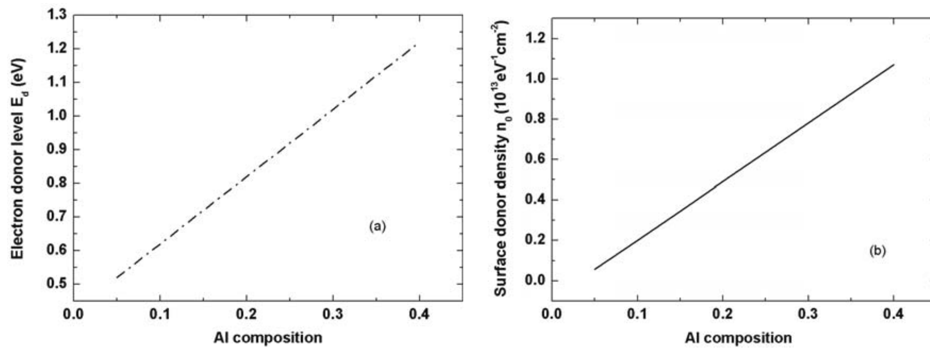

Figure 10. Electron donor level and surface donor density for bare surface AlGaN/GaN heterostructure shown in figure 10 (a) and 10 (b) respectively [19].

LDMOSFET Design with a Zener diode in the drift region (Tunneling LDMOSFET)

As discussed previously, LDMOSFETs are widely used power device for RF applications up to 4 GHz, covering a large range of low to medium operating voltage [1,2,9,10]. It is used extensively in various applications, e.g., base-stations, automobiles, motor speed control and RADAR etc. Due to its compatibility with the standard CMOS process line, SOI (Silicon on Insulator) based LDMOSFETs have opened new possibilities of their implementation in power integrated circuits for applications in very high frequency ranges of mobile applications (see Figure 3), wherein the power drive can be integrated with low power logic circuits [2].

In general, an important design consideration of power MOSFETs is its on-state resistance R_{on} [9,10,29,30], as high values of this parameter increase the power dissipation and also can increase the transient time in the drift region. This, in turn, affects negatively the frequency response. However, due to the presence of a large, lightly doped drift region in LDMOSFETs, needed for obtaining sufficiently high breakdown voltage, a high R_{on} is usually unavoidable.

In the last few years, a large research effort has been directed towards integrating quantum effects into CMOS devices like the tunnel field effect transistors (TFETs), wherein the use of tunneling has been exploited to enhance the performance characteristics [31]. Tunneling is a quantum mechanical phenomenon with only minor dependence on temperature variations. To meet the demand for lowering R_{on} of LDMOSFET, we have proposed a tunneling junction (Zener diode) in series with the LDMOSFET integrated at the drain end of the drift region, as shown in Figure 11. The tunneling junction injects carriers into the drift region during the device turn-on, whereby the overall characteristics of the device are improved. Using 2D numerical simulations, we have shown improvements in the on-state characteristics without having to compromise much on the off-state characteristics. The details of the proposed structure and simulation details can be found in [31] (see Paper E, Part II of this thesis.)

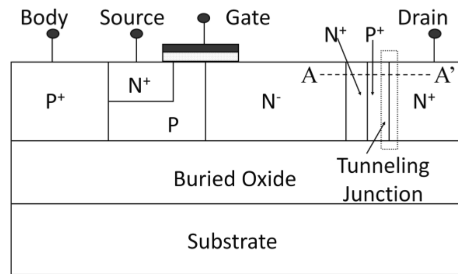

Figure 11. Schematic diagram of the proposed LDMOSFET with tunneling junction for improved on-state performance [31].

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Part II. Papers included in the thesis

Paper-A: Nitin Goyal, Benjamin Iniguez, Tor A. Fjeldly, "Analytical Modeling of Bare Surface Barrier Height and Charge Density in AlGaN/GaN Heterostructures", *Appl. Phys. Lett.* 101, 103505 (2012).

APPLIED PHYSICS LETTERS **101**, 103505 (2012)

Analytical modeling of bare surface barrier height and charge density in AlGaN/GaN heterostructures

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In this paper, a physics based analytical model for the bare surface barrier height and two dimensional electron gas density in AlGaN/GaN heterostructures is presented. The model is based on simple charge neutrality electrostatics across the AlGaN barrier layer and that a low density of surface donor states is the source of the two dimensional electron gas. The model shows good agreement with reported experimental results. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4751859]

GaN based high electron mobility transistors (HEMT) have shown great promise for the future high-power and high-frequency applications due to their wide band gap and high electron mobility. III–V based HEMTs also possess excellent thermal properties, which make them suitable candidates for high-temperature applications. The most interesting feature of these devices is the presence of a high mobility two-dimensional electron gas (2DEG) density of the order of $10^{13}\,\text{cm}^{-2}$ at the AlGaN/GaN interface even in the absence of both doping in the AlGaN barrier layer and gate metal (bare surface). This effect is attributed to the presence of strong piezoelectric as well as spontaneous polarization effects.[1] In the last few years, considerable research has been performed by different groups to explain the mechanism and source of electrons for the formation of this 2DEG. It has been shown, using experiments as well numerical simulations, that the presence of donor states at the AlGaN surface is the main source of the electrons in the 2DEG.[2–7] Till now, this is assumed to be the only valid theory to explain the behavior observed in the experiments. Even in the presence of a gate metal, the effect of surface states is only partially neutralized.[8] Understanding the formation of the 2DEG is very important to explain the mechanism of current collapse and various other effects in ac and dc characteristics[9,10] and is thus very crucial to the device design.

The surface donor model (SDM) by Ibbetson *et al.*[2] was proposed to explain the behavior of 2DEG charge concentration with variation in the barrier layer thickness. They assumed that a high density of surface donor states exists at a particular energy level E_{do} in the forbidden gap measured relative to the conduction band minimum of AlGaN surface (see Fig. 1). With increasing barrier thickness d, this level moves higher due to the constant electric field in the barrier. Once this level reaches the Fermi level, the surface donor states start donating electrons to form the 2DEG at the AlGaN/GaN interface. According to this model, the Fermi level at the surface will remain essentially constant (Fermi level pinning) once the barrier layer reaches the critical thickness d_{cr}, below which the 2DEG vanishes. Therefore, according to SDM, the surface barrier height $q\Phi_B$ remains almost constant (increases only in the range of kT/q) with increasing d once the donor level is reached. This model was justified by certain experimental data as well as by numerical simulations.[2,3]

However, this model could not be reconciled with experimental observations by Koley and Spencer[6] that the $q\Phi_B$ of the bare surface increases with increasing d. But these observations were explained by instead assuming low-density surface donor states distributed over a range of energies below a particular donor energy level E_d in the forbidden gap,[6] as indicated in Fig. 1. Hence, with increasing d, the conduction band can move up and, simultaneously, lift E_d with respect to Fermi level. Thus, when E_d crosses the Fermi level, the surface donor states start donating electrons to form the 2DEG at the hetero-interface. Therefore, in this model, $q\Phi_B$ will be able to increase with increasing d even in the active regime. Experiments and numerical simulations show that both the 2DEG charge concentration qn_s and $q\Phi_B$ first increase linearly and eventually saturate with increasing barrier thickness.[6,7]

Here, we present a physics based analytical model for the variation of the surface barrier height with the variation of the barrier layer thickness. This model is based on the charge neutrality condition across the barrier layer. We assume that the charge contribution due to the unintentional doping in GaN and AlGaN is negligible and that the polarization in combination with the distributed surface donor states is the responsible mechanism for the creation of the 2DEG.

Considering Fig. 1, we observe that to maintain charge neutrality, the electric field across the barrier layer is given by both left and right hand sides of the expression

$$(\sigma_{pz} - qn_s)/\varepsilon_{AlGaN} = (q\Phi_B + E_F - \Delta E_c)/dq, \qquad (1)$$

where ΔE_c is the conduction band offset, E_F is the difference between the Fermi level and the conduction band minimum (CBM) in the GaN at the hetero-interface, σ_{pz} is the positive polarization surface charge at the hetero-interface, and ε_{AlGaN} is the permittivity of the barrier layer. Here, we note that E_F does not change much, at most by a few kT/q, once we enter

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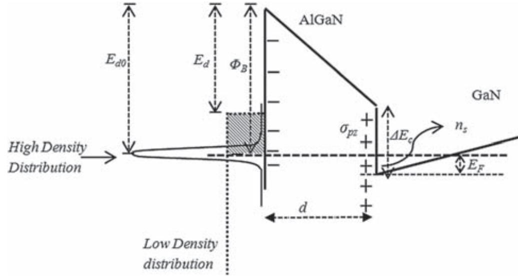

FIG. 1. Band diagrams of a AlGaN/GaN HEMT showing various charges at the different interfaces and illustrating the formation of a 2DEG with electrons supplied by surface donor states. Two cases with different distributions of the surface donor states in the energy gap are shown: (a) single surface donor level with high density; (b) distributed surface donor states with low density.The shaded box shows the number of electrons per unit area donated by low density surface donor states.

the active regime. As a reasonable approximation, we therefore assume $E_F \approx 0$ (see further comments below). Next, we assume a constant surface donor density below the donor level E_d with the population n_o states per unit area and energy, as proposed by Gordon *et al.*[7] The number of empty surface donor states above the Fermi level can then be written as $n_o(q\Phi_B - E_d)$ per unit area, which corresponds to the 2DEG electron density n_s at the hetero-interface. Applying this to Eq. (1) and solving for the surface barrier, we find

$$q\Phi_B \approx \frac{K_1 d + K_2}{n_0(d + K_3)}, \tag{2}$$

where $K_1 = \sigma_{pz}/q + n_o E_d$, $K_2 = \varepsilon_{AlGaN}\Delta E_c/q^2$, and $K_3 = \varepsilon_{AlGaN}/q^2 n_o$. From Eq. (2), we see that for sufficiently thick barriers, the barrier height saturates at the value $q\Phi_B \approx E_d + \sigma_{pz}/qn_o$. Moreover, when the surface state density is high, $q\Phi_B$ approaches the value E_d.

Figure 2 shows a comparison of the modeled barrier height versus barrier thickness against experimental data from Gordon *et al.*[7] for two different Al compositions in the barrier layer. The experimentally determined values for n_o and E_d were used in the model. The model is found to reproduce quite well the experimental results, especially for small barrier thicknesses. At higher thicknesses, there is a slight deviation between model and experimental data, which can be attributed to the strain relaxation in the barrier layer[7] as well as the finite value of the difference between Fermi level and the CBM in GaN at the AlGaN/GaN interface[10] that we have neglected in order to simplify the mathematical analysis. As can be seen from Fig. 2 and from additional experimental results in Ref. 7, the model is fairly accurate up to a barrier layer thickness of close 25 nm at the Al composition of 19%. For higher Al compositions, the range of accuracy decreases to about 15 nm at 24% Al. For this practical range of barrier compositions, the present model explains the effect of barrier thickness in a simple manner, which can be used to understand and develop new concepts of GaN HEMTs. Figure 3 illustrates graphically how E_F and $q\Phi_B$ behave with increasing d, and why the approximation for E_F is justified for thin barriers.

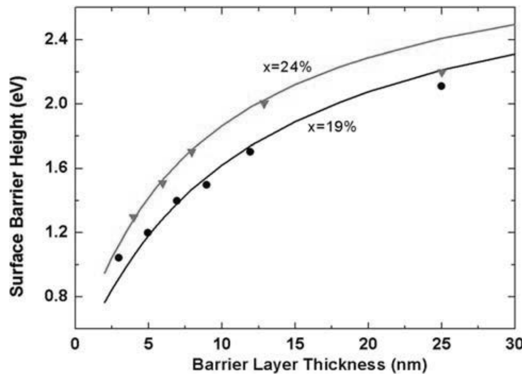

FIG. 2. Comparison between the model (curves) and experimental data (symbols) obtained from Ref. 7, for two different Al compositions in the barrier. The density of surface donor states used were $n_o(x = 0.19) = 4.6 \times 10^{12}\,\mathrm{cm^{-2}V^{-1}}$ and $n_o(x = 0.24) = 6.1 \times 10^{12}\,\mathrm{cm^{-2}V^{-1}}$.[7]

The critical thickness $d = d_{cr}$ is the barrier layer thickness below which n_s can be approximated to be very small. It can easily be calculated from Eq. (1) by setting $n_s = 0$, $q\Phi_B = E_d$, and $E_F = 0$, resulting in

$$d_{cr} = \left(\frac{\varepsilon_{AlGaN}}{\sigma_{pz}q}\right)(E_D - \Delta E_c). \tag{3}$$

Finally, we may also develop an explicit expression for n_s versus d for a given d_{cr} by combining Eq. (1) to (3). This results in the following expression:

$$n_s = \frac{\sigma_{pz}}{K_4 q}\left(1 - \frac{d_{cr}}{d}\right), \tag{4}$$

where $K_4 = 1 + \varepsilon_{AlGaN}/dqn_o$ can be regarded as a correction factor relative to SDM by accounting for the variation in the surface barrier height with increasing barrier layer thickness. For large n_o, K_4 approaches unity, which corresponds to SDM. This correction is illustrated in Fig. 4, where we choose $E_d = E_{d0}$ to emphasize the magnitude of the correction.

The importance of this work lays in the fact that this model predicts the experimental observations in AlGaN/GaN HEMTs in a simple analytical manner. For any given HEMT structure, only the donor level of the surface states and the surface state density are required for this model to calculate barrier height as well as the 2DEG for any value of the barrier

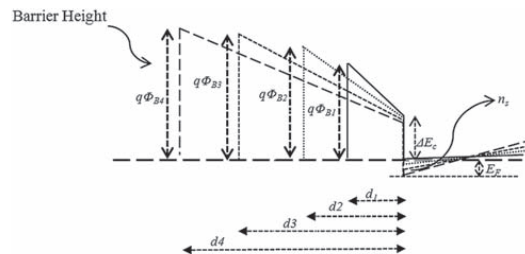

FIG. 3. Schematic view of band diagrams of a AlGaN/GaN HEMT showing surface barrier heights versus barrier layer thicknesses (not to the scale). Here, E_F is indicated for a relatively thick barrier.

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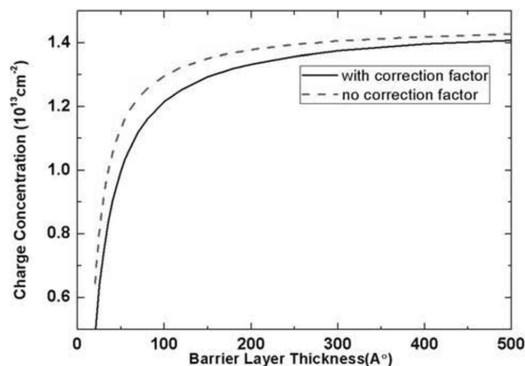

FIG. 4. Comparison between the proposed model according to Eq. (4) (low density surface states) and the model given by Ibbetson *et al.*[2] (high density of surface states where $K_4 = 1$) for dependence of n_s versus barrier layer thickness.

thickness. We have also verified that using the corresponding values in Ref. 6, the saturating value of barrier height has been observed as approximately 1.7 eV, which demonstrates the validity of the model for different sets of samples. From our analysis, we can observe that d_{crit} is dependent on σ_{pz} and ΔE_c. Therefore, to design HEMTs with better gate control, there is a need for new materials for barrier layers that can provide strong polarization as well as large conduction band off-set values. AlN/GaN and lattice matched InAlN/AlN/GaN are such material combinations and have been demonstrated to possess superior gate control as well as high n_s at small barrier layer thicknesses due to strong spontaneous polarization and large effective ΔE_c. These materials can be used for high aspect ratio designs.

In conclusion, we have presented a physics based model for the sheet carrier density (2DEG) at the AlGaN/GaN interface, including the effect of piezoelectric and spontaneous polarization charges. We have shown that the sheet carrier density as well as barrier layer height are functions of the density, location in the band gap, and distribution of surface donor states. By assuming a uniform distribution, a completely analytical model has been presented, which can be used to further understand the physics of AlGaN/GaN based HEMTs. The present model is in good agreement with the reported experimental data.

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Paper-B: Nitin Goyal and T. A. Fjeldly, “Effects of Strain Relaxation on Bare Surface Barrier Height and Two-Dimensional Electron Gas in AlxGa1−xN/GaN Heterostructures”, *J. Appl. Phys.*, vol. 113, 014505 (2013).

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Effects of strain relaxation on bare surface barrier height and two-dimensional electron gas in $Al_xGa_{1-x}N$/GaN heterostructures

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A physics based analytical model is presented to describe the bare surface barrier height and the two-dimensional electron gas density in AlGaN/GaN heterostructures versus barrier layer thickness and Al content. Details of the model rely on the extraction of the critical thickness for strain relaxation based on the identification of a signature cusp in experimentally obtained bare surface barrier heights. This information is used to obtain the residual strain and total effective polarization when strain relaxation takes place. The model, which covers both unrelaxed and relaxed barriers, shows good agreement with reported experimental results and promises to become a useful tool in advanced design and characterization of GaN based heterostructures. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4773334]

I. INTRODUCTION

III-V based AlGaN/GaN heterostructures have been a topic of intensive research over the last decade because of their excellent properties such as high saturation velocity, high band gap, excellent thermal stability, and superior sheet carrier concentration on the order of $10^{13}\,cm^{-2}$, even in the absence of any doping and gate metal (bare surface). The high sheet carrier concentration arises due to the strong polarization fields present at the AlGaN/GaN interface, which is the result of the strong piezoelectric and spontaneous polarization present in these materials.[1] These properties make the AlGaN/GaN structure, where AlGaN acts as a barrier layer, an excellent basis for high electron mobility transistors (HEMTs) for use in future high-power and high-frequency applications. It is accepted that the surface donor states residing at the top AlGaN surface are the primary source of electrons present at the AlGaN/GaN interface,[2] where the donated electrons form a two-dimensional electron gas (2DEG). The presence of a gate metal on top of AlGaN affects the density and distribution of these surface states, but the effect of the surface states is only partially neutralized and they remain the source of the 2DEG. Understanding the formation of the 2DEG is very important to explain the mechanism of current collapse, inverse piezoelectric effect, and various other effects in ac and dc characteristics, and is thus very crucial to the device design.

The surface barrier height (SBH) is the topic of continuing research related the nature and distribution of the surface states in the band gap of AlGaN. Ibbetson *et al.*[2] initially proposed a fixed SBH based on the assumption of a high density of surface donor states (Fermi level pinning). Later, Koley and Spencer[3] and Gordon *et al.*[4] showed that the SBH changes with the barrier layer thickness, which implies a relatively low donor state density. It was subsequently shown experimentally as well as by numerical simulations that the Al mole fraction in AlGaN has a significant impact on both the SBH and the 2DEG density owing to its effect on the piezoelectric and spontaneous polarizations.

In pseudomorphic growth of heterostructures, the top layer initially grows with the lattice constant of the substrate. Due to its large thickness, the substrate is always assumed to be in a relaxed state. With a lattice mismatch between the substrate and the barrier, there is always an inherent strain present in the top layer. In the AlGaN/GaN system, a thin layer of AlGaN is grown on a relatively thick GaN substrate. The AlGaN has a lower lattice constant than that of the substrate, and the mismatch gradually increases with increasing Al content. The piezoelectric polarization is an effect of this strain. In addition, spontaneous polarization also increases with increasing Al content. Hence, the total polarization at the AlGaN/GaN interface increases and, consequently, so does the 2DEG charge density.

It has been shown theoretically that when the Al content is small, relatively thick AlGaN layers can be grown on GaN since the residual (effective) strain is small.[5–7] When the thickness of AlGaN layer increases, so does the effective total strain energy present in the system. Beyond a certain thickness called critical layer thickness, the strain energy stored in the AlGaN layer can lead to rapid formation of dislocations that relaxes the strain. This can lead to plastic deformation by generating surface irregularities. With increasing Al content, needed to produce sufficiently large piezoelectric charges, the critical thickness is reduced and, eventually, the structure is rendered useless for device applications. This is partly due to a weakening of the piezoelectric polarization and partly due to a reduction of the channel mobility resulting from interface imperfections. From a practical point of view, it is very important to understand the electrical properties of the heterostructures in terms of the physical attributes of the AlGaN barrier layer. As indicated, its two most important physical parameters are the Al content and the thickness. In order to design highly efficient and reliable HEMT structures, it is important to understand the variation in the SBH and the 2DEG with these physical attributes.

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In the past, theoretical work on deformation energy by Bykhovski *et al*.[5,6] and experiments by Bourret *et al*.[8] were performed on relaxation effects. This included the critical thickness d_{crr} for onset of relaxation in various configurations of GaN-AlN-GaN superlattices. The work also considered semiconductor-insulator-semiconductor (SIS) systems where a thin layer of AlN or AlGaN is sandwiched between two thick layers of GaN, which may be considered an extreme case of a superlattice. But, to our knowledge, no analytical model has been published on studies of d_{crr} for practical AlGaN/GaN or related structures.

II. PRESENT MODEL

The present analytical model describes the variation of SBH and 2DEG charge density with barrier layer thickness and includes the effects of strain relaxation. The model is divided into two parts. First part is based on our previous work on the bare surface barrier height for unrelaxed barrier layers for thin AlGaN layers.[9] The second part is based on the extraction and incorporation of the critical thickness and the resultant effective polarization in partially relaxed thick AlGaN layers.

A. Model for unrelaxed AlGaN thin barriers

In the Fig. 1, we show the low-density surface donor states distributed over a range of energies below a particular donor energy level E_d in the forbidden gap. E_d is measured relative to the conduction band minimum (CBM) of the AlGaN surface. With increasing barrier thickness d, this level moves higher due to the constant electric field in the barrier. Once it reaches the Fermi level, the surface donor states start donating electrons to form the 2DEG at the AlGaN/GaN interface. Because of the low surface donor density, the surface barrier height $q\Phi_B$ will be able to increase with increasing d in the active regime. Experiments and numerical simulations in the past have shown that both the 2DEG charge concentration qn_s and $q\Phi_B$ first increase linearly and eventually tend to saturate with increasing barrier thickness.[3,4]

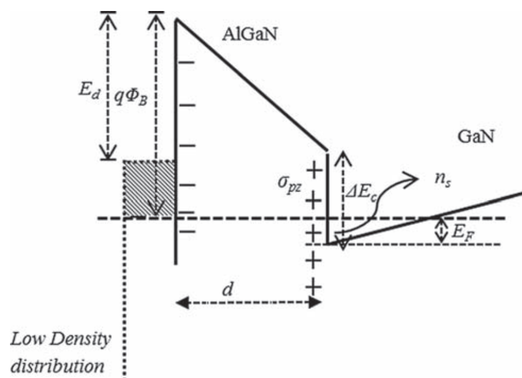

FIG. 1. Band diagram of a AlGaN/GaN heterostructure showing various charges at the different interfaces illustrating the formation of a 2DEG with electrons supplied by surface donor states. Distributed surface donor states with low density are shown. The shaded box shows the number of electrons per unit area donated by low density surface donor states.

If we assume charge neutrality condition across the barrier layer and solve Poisson equation using proper boundary conditions, we obtain the following expression for the SBH:

$$q\Phi_b = \frac{(n_o E_d + \sigma_{pz}/q)d + \varepsilon_{AlGaN}\Delta E_c/q^2}{n_o(d + \varepsilon_{AlGaN}/q^2 n_o)}, \tag{1}$$

where ΔE_c is the conduction band offset, E_F is the difference between the Fermi level and the CBM in the GaN at the hetero-interface, σ_{pz} is the positive density surface charge at the hetero-interface, n_o is density of surface states per unit area and energy, and ε_{AlGaN} is the permittivity of the barrier layer. From this expression, we find that for sufficiently thick barriers, the barrier height saturates at the value $q\Phi_B \approx E_d + \sigma_{pz}/qn_o$. This variation is shown schematically in Fig. 2 in the form of conduction band profiles for different AlGaN thicknesses.

We can also solve Poisson's equation for the 2DEG sheet density, which leads to the following relationship:

$$n_s = \frac{\sigma_{pz}/q}{1 + \varepsilon_{AlGaN}/dq^2 n_o}\left(1 - \frac{d}{d_{cr}}\right), \tag{2}$$

where $d_{cr} = \varepsilon_{AlGaN}(E_d - \Delta E_c)/\sigma_{pz}q$ is the critical thickness for onset of significant charge at the interface.

B. Model for partially relaxed AlGaN thick barriers

Studies of SBH by Gordon *et al*.[4] and 2DEG by Ibbetson *et al*.[2] for different barrier layer thicknesses, showed that beyond a certain critical thickness, strain relaxation takes place in the barrier layer, as discussed in Sec. I. This can reduce the effective polarization significantly. Concomitantly, the piezoelectric polarization gradually weakens. Here, we propose a new procedure to extract and to model this critical thickness d_{crr}, and to subsequently determine the effective polarization for partially relaxed barrier layers. A useful indication of how d_{crr} depends on the Al content in AlGaAs/GaN heterostructures is found in the above mentioned work on superlattices and SIS structures.[5] However, d_{crr} can also be extracted by comparing experimental data on SBH versus barrier thickness with our earlier model for unrelaxed barriers,[9] allowing us to observe where the experimental data start deviating from this model. This was done for barrier layers with Al mole fractions of $x = 0.19$, 0.24, and 0.29, for which experimental data have been reported.[4] The extracted values for d_{crr} were 22.5 nm, 18.4 nm, and 15.5 nm, respectively. Inspired by the corresponding behavior in d_{crr} for superlattices and SIS structures,[5,6] we fitted our extracted values by the empirical expression

$$d_{crr} = d_o x^k, \tag{3}$$

where $d_o \approx 4.17$ nm and $k \approx -1.04$. This relationship, together with the extracted values for d_{crr}, is shown graphically in Fig. 3 and compared with the corresponding relationships reported for the superlattices and SIS structures.

From a consideration of the strains involved, the present heterostructures are expected to have critical thicknesses somewhere between those of GaN-AlN-GaN superlattices

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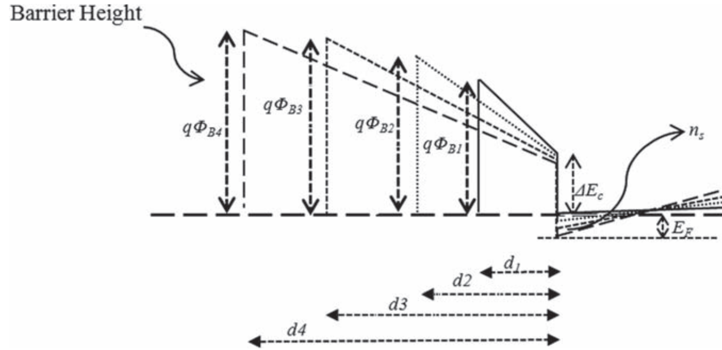

FIG. 2. Schematic view of band diagrams of a AlGaN/GaN HEMT showing surface barrier heights versus barrier layer thicknesses (not to the scale). Here, E_F is indicated for a relatively thick barrier.

and GaN-AlGaN-GaN SIS structures, in good qualitative agreement with the results in Fig. 3. The superlattice has the highest values of d_{crr} since, in this case, the unrelaxed strain is more equally distributed between the GaN and AlN layers. In the SIS structure, which consists of a thin AlGaN layer between two thick GaN layers, the strain is more fully located within the thin layer. The above comparison, therefore, serves to verify the extraction procedure discussed above.

The piezoelectric and spontaneous polarizations of non-relaxed AlGaN are calculated from the following expressions, respectively,[1]

$$P_{PE} = 2\left(\frac{a_{AlGaN}}{a_{GaN}} - 1\right)\left(e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right), \quad (4)$$

$$P_{SP} = -0.052x - 0.029, \quad (5)$$

where a_{AlGaN} and a_{GaN} are lattice constants, e_{13} and e_{33} are the piezoelectric coefficients, and C_{13} and C_{33} are elastic constants. The lattice constants and the elastic constants for the AlGaN have been extrapolated from the corresponding values of AlN and GaN for the given Al mole fraction x using linear and quadratic relations.[1] While the spontaneous polarization is known to be independent of the AlGaN layer thickness and therefore is not affected by strain relaxation, Bykhovski *et al.*[5] showed that the total strain induced polarization is reduced in an exponential manner with increasing barrier layer thickness d once the critical thickness is exceeded. Bourret *et al.*[8] indicated that the strain behaves in a similar manner. Based on this and data available in the literature,[5–8] we estimate that for $d > d_{crr}$ the residual strain can be expressed as

$$s_r = s_{crr}\exp\left(1 - \frac{d}{d_{crr}}\right), \quad (6)$$

where s_{crr} is the critical strain at onset of relaxation. This behavior is shown in Fig. 4 for the three Al fractions used above.

The corresponding effective piezoelectric polarization for $d > d_{crr}$ then becomes

$$P_{PE} = 2s_r\left(\frac{a_{AlGaN}}{a_{GaN}} - 1\right)\left(e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right) \quad (7)$$

and the total polarization charge will be

$$P_{Total} = P_{PE} + P_{SP}. \quad (8)$$

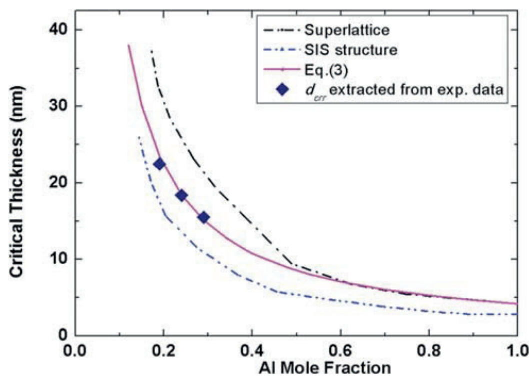

FIG. 3. Critical thickness for relaxation versus Al mole fraction for (a) AlGaN on GaN substrate (solid curve and symbols) from present work, (b) dashed-dotted curves for superlattices (top) and SIS structures (bottom) from Ref. 5.

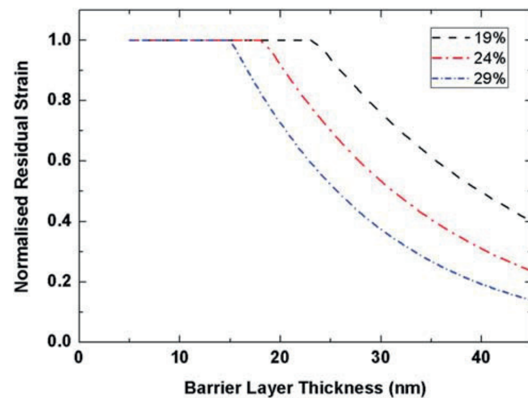

FIG. 4. Modeled variation in normalized residual strain due to piezoelectric effect as function of AlGaN layer thickness for three Al mole fractions in the barrier: 0.29 (lower), 0.24 (middle), and 0.19 (upper).

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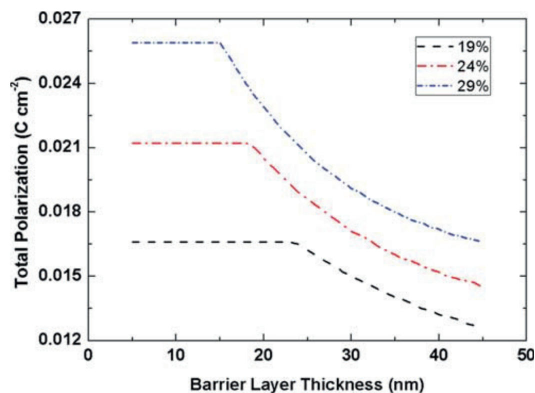

FIG. 5. Modeled total polarization as function of AlGaN layer thickness for three Al mole fractions in the barrier: 0.29 (upper), 0.24 (middle), and 0.19 (lower).

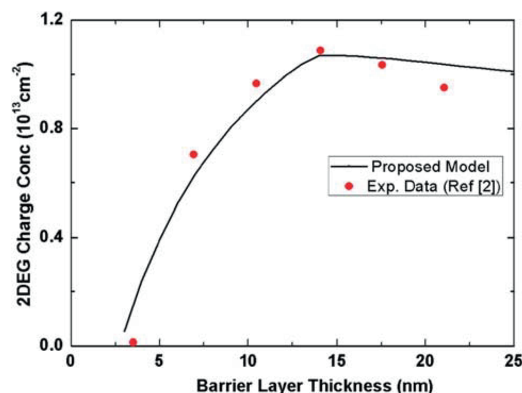

FIG. 7. Comparison of modeled (solid curve) and experimental (symbols) 2DEG sheet density versus barrier layer thickness for Al mole fraction in the barrier of 0.35. Experimental data from Ref. 2.

The total polarization versus the barrier layer thickness according to this is shown in Fig. 5. We note that at lower thicknesses, the piezoelectric polarization component is dominant. However, when d is substantially larger than d_{crr}, only the spontaneous polarization remains.

By combining these results with Eq. (1), the dependence of the bare surface SBH on the barrier Al fraction and thickness can now be generalized to cover both the unrelaxed and the relaxed states of the barrier. This is done by incorporating the information about the residual strain according to Eqs. (6)–(8) in the total polarization sheet charge density at the interface, $\sigma_{pz} = P_{Total}/q$. Figure 6 shows a comparison between the prediction by this updated model and experimental data[4] for the bare SBH versus the barrier layer thickness for the three Al fractions used above. Apart from some scatter in the experimental data, we observe a quite satisfactory agreement with the model predictions.

Similarly, for the 2DEG sheet charge density, the model (2) is compared with experimental data[2] in Fig. 7 for a device with an Al mole fraction of 0.35. Again, a good agreement is found.

Since the inception of inverse piezoelectric effect,[12] new design approaches are being proposed for devices that can withstand high electric field at high stress off-state bias conditions. Therefore, it is important to know the magnitude of the initial electric field present in the barrier. SBH is also a direct measure of this electric field. Figure 8 shows the modeled effective electric field present in the AlGaN barrier layer for fully strained and partially relaxed AlGaN layers for different thicknesses. We observe that the effective field is reduced at higher thicknesses due to reduction in the effective polarization. We note that the electric field in the AlGaN layer can be measured by means of the electro-reflectance method, as recently shown for doped GaN.[10] The reported trend is very similar to that of Fig. 8, except for a difference in magnitude owing to the difference in material systems considered. The electric field may serve as a measure of the initial structural reliability of the barrier since it gives an indication of how much relaxation has taken place in the layer.

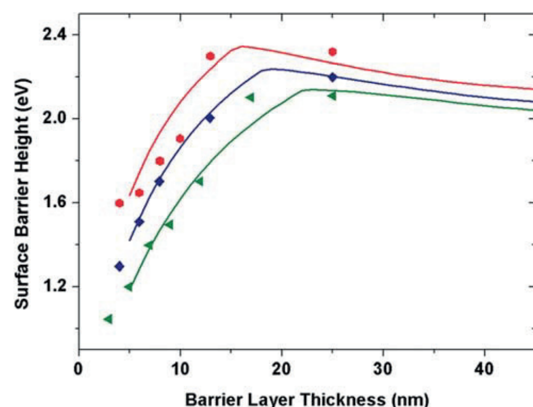

FIG. 6. Comparison of model (curves) with experimental data[4] of surface barrier height versus barrier layer thickness for three Al mole fractions in the barrier: 0.29 (upper), 0.24 (middle), and 0.19 (lower).

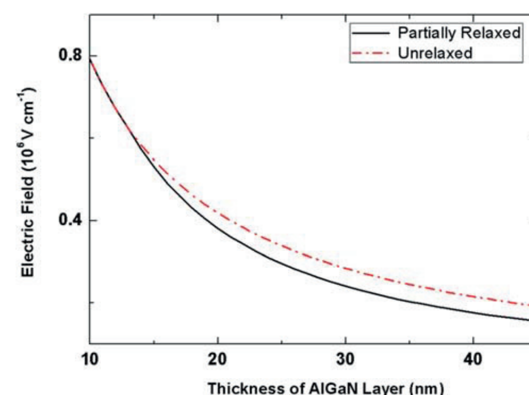

FIG. 8. Comparison of electric field in partially relaxed (solid curve) and unrelaxed (dotted-dashed) versus barrier layer thickness for an Al mole fraction of 0.35 in the AlGaN layer.

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III. DISCUSSION

In studies of degradation in AlGaN/GaN HEMTs related to the inverse piezoelectric effect, Jimenez and Chowdhury[11] and del Alamo *et al.*[12] reported that the composition and thickness of the AlGaN layer should affect device reliability owing to changes the initial level of elastic energy in the AlGaN. They reported that a high electric field in the AlGaN layer at bias conditions of negative gate and positive drain can generate very strong mechanical stress in addition to the piezoelectric stress. If the total stress exceeds a certain limit, it can do irreversible damage to the AlGaN layer structure by producing dislocations from the top to the interface of the AlGaN layer. It was also reported that high electric field enhances the formation of pits.[12] The solutions suggested for counteracting this degradation mechanism rely on advanced device designs that serve to mitigate the electric field in AlGaN barrier layer. To achieve device performance optimization, thick dislocation-free AlGaN layers are needed, for which a reduction of the barrier Al content is one of the proposed and favored solutions. Layers of low Al content are also beneficial due to reduced amounts of oxygen at the AlGaN top surface. Therefore, there is a strong need of physics based models for insight in and design of suitable barrier layers of low Al content. But, to our knowledge, there are no analytical models, prior to the one presented here, for predicting 2DEG and SBH including strain relaxation effects for thick AlGaN layers with practical Al fraction in the full range between $0 < x < 0.4$.

The importance of the present model lays in the fact that optimized AlGaN layers can be designed for desired barrier heights and 2DEG concentrations. Large 2DEG density and barrier height are always among the most important design priorities. SBH and 2DEG also reflect the effective internal polarization field. Therefore, the present model in combination with transport models can be used to design optimized AlGaN/GaN structures for reliable low-resistivity and high-performance HEMT devices. High aspect ratio design involves a suitable ratio of AlGaN thickness and gate length. The model can also be useful in the characterization of top surface properties of AlGaN. Different surface properties like the energy donor level and the surface donor density can be obtained from Hall measurements and Kelvin probe spectroscopy measurements on different samples. Top surface properties are also very important in the study of passivation of AlGaN surfaces to avoid effects like current collapse and RF-dispersion. Selection of passivation materials also depends on these surface properties. It is also important to know the accurate bare surface barrier height for the selection of suitable gate metals for Schottky gate contacts. Large Schottky barrier heights are very desirable for device design to reduce gate leakage in power devices. Reliability of high-power and optoelectronic devices also depends on the dislocation density at the AlGaN/GaN interface. Strain relaxation practically depends on the amount of generated dislocations at the interface. Therefore, the model can also be used to assess the reliability of given structures for a particular application during the design phase. Another important design aspect of GaN based heterostructures is accurate surface potential and transport modeling. In heterostructures with a thin AlGaN or AlN layer, the Coulomb scattering due to surface positive charges can be one of the dominant mechanisms of the mobility degradation. The present model can be used to determine the density of donor states that donate electrons to form the 2DEG and become positively charged. Also, a reliable prediction of the critical barrier thickness for onset of relaxation is very important for reliable designs, as thicker layers can lead to increased dislocation density, which degrades the device transport characteristics.

IV. CONCLUSION

In conclusion, an analytical model is presented for the bare surface barrier height and the 2DEG sheet charge density in AlGaN/GaN heterostructures for unrelaxed thin and partially relaxed thick AlGaN layers. Based on this model, we propose an extraction procedure to determine critical thickness for strain relaxation from experimental measurement of the bare surface barrier height. This model enables designers and manufacturers to improve their device characterization focus and their interpretation of characterization results through a better understanding of the physical underpinnings of these devices.

ACKNOWLEDGMENTS

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Paper-C: Nitin Goyal and Tor A. Fjeldly, "Impact of gate metal on surface states distribution and effective surface barrier height in AlGaN/GaN heterostructures", *Material Research Society, Spring Meeting*, San Francisco, Vol. 1538, USA, April 2013.

Impact of Gate Metal on Surface States Distribution and Effective Surface Barrier Height in AlGaN/GaN Heterostructures

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ABSTRACT

A physics based model is presented to describe the surface donor density distribution for metal/AlGaN/GaN structures. This model partly relies on experimental observations to describe the reduction that takes place in surface donor density when the metal gate is deposited. This new model is based on our previous work on the bare surface barrier height for both unrelaxed and partially relaxed barrier layers. The model predictions are consistent with reported experimental data.

INTRODUCTION

GaN based High Electron Mobility Transistors (HEMTs) have shown great promise for future high-power and high frequency applications due to their wide band gap and high electron mobility. Wide bandgap III-V based HEMTs also possess excellent thermal properties, which make them suitable candidates for high-temperature applications. The most interesting feature of these devices is the presence of a high mobility, two-dimensional electron gas (2DEG) with a sheet density of the order of 10^{13} cm^{-2} at the AlGaN/GaN interface, even in the absence of both AlGaN barrier layer doping and a gate metal (bare surface). This phenomenon is attributed to the strong piezoelectric as well as spontaneous polarization effects in the structure[1].

In the last few years, considerable efforts have been made to explain the mechanism and source of electrons for the formation of this 2DEG. It has been shown that the presence of distributed donor states in the forbidden gap of the barrier AlGaN surface is the main source of the 2DEG [2-6]. We have previously shown how the bare surface (Schottky) barrier height (SBH) relates to polarization, thickness, and Al content of the barrier, as well as to the surface donor state distribution. This model applies well to bare surface AlGaN/GaN [7,8], but the understanding of what happens when a gate metal is deposited on top AlGaN layer is still lacking. Understanding of metal contacts on AlGaN/GaN heterostructures is important, since these contacts are required for an efficient gate control in practical HEMTs. A large SBH implies low leakage current as well as high breakdown voltage.

THEORY

The SBH of a metal-semiconductor contact is defined as the energy difference between the conduction band minimum (CBM) and the Fermi level E_F at the interface. The SBH has been a constant topic of research for several decades. In their basic model, Schottky and Mott assumed ideal interfaces with no surface states, where SBH is given by $q\Phi_b = q\Phi_m - \chi$, where Φ_m is the

metal work function and χ is the electron affinity of semiconductor [9] . Bardeen later introduced a model based on the assumption of a very high density of surface states in order to explain an observed pinning of the Fermi level. A part of this problem is that the metal can give rise to so-called metal induced gap states (MIGS) in the forbidden gap of semiconductor, and that defects present at the interface can introduce defect induced gap states (DIGS) [9]. These surface states can be of acceptor or donor type depending on the position in bandgap. Cowley and Sze explained the variation observed in the barrier height for non-polar materials with different metal contacts in terms of a corresponding change in the surface state properties post metal deposition [10]. But this theory is not applicable to AlGaN/GaN heterostructures. The underlying reason is that the inherent polarization present in a thin AlGaN layer fully depletes this layer and that the thickness of the AlGaN layer also strongly affects the barrier height. In reality, for the AlGaN/GaN heterostructures, the surface state density will be somewhere in between, where the Mott model does not quite apply and where the Fermi level is not fully pinned.

Experimentally, it has been shown that deposition of metals to form Schottky contacts reduces both the 2DEG and the SBH by partially neutralizing the surface states, but it also causes a redistribution of the surface states [11]. In turn, this modifies both the SBH and the charge carrier density n_s in the 2DEG. The density and distribution of the surface states are strongly dependent on the surface treatment technique used and the Al content in the AlGaN layer [12]. However, to date no satisfactory theoretical model has been proposed to explain the change in the 2DEG and the SBH in the presence of the metal gate. This requires a careful consideration of surface donor density and its distribution post metal deposition. Other experiments show a large unexplained difference between SBH measured on bare $Al_{0.29}Ga_{0.71}N$ surfaces (about 2.4 eV) and on surfaces with deposited metal (1.4-1.6 eV found using internal photoemission spectroscopy) [13-15]. An interfacial oxide is usually etched away prior to the metal deposition to improve reliability and reproducibility. The effect of the metal on this post-deposition distribution is found to depend on the metal work-function, which, in effect, rules out the existence of high-density surface states that would otherwise have pinned the Fermi level. On the other hand, the Mott theory applies to semiconductor surfaces with no surface states and therefore gives inaccurate results for practical semiconductors [9].

To simplify the development of an analytical model for the modifications resulting from the metal gate deposition on the AlGaN/GaN heterostructures, we assume that basic nature of surface states remain unchanged, i.e., that they consist of donor states with an intermediate density and a fairly flat distribution in the relevant energy range about the Fermi level. We base the present modeling on our recent work on the SBH and 2DEG sheet density in the bare surface AlGaN/GaN structure for strained thin and partially relaxed thick AlGaN layers [7,8]. As indicated above, the deposition of a metal gate has been observed to diminish both the SBH and the 2DEG density which, in turn, corresponds to a reduction in both the surface donor density n_o and in the surface donor level E_d . These changes are schematically illustrated in Figure 1, where E_{db} and E_{dm} are the donor level for the bare and the metalized surface, respectively, ΔE_c is the conduction band offset at the hetero-interface, and d is the AlGaN layer thickness.

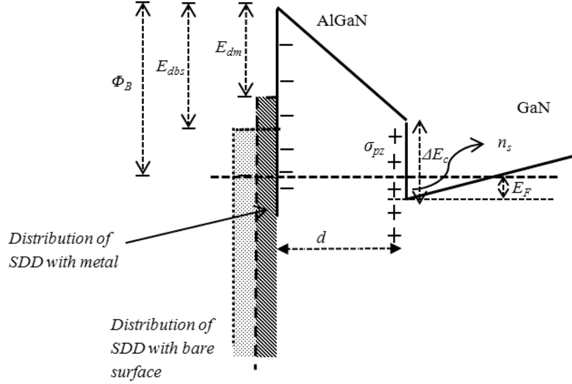

Figure 1. Schematic illustration of the band diagram in the AlGaN/GaN hetero-structure, with indication of surface density and energy distribution with a bare and a metallized surface.

The bare surface model for the unrelaxed AlGaN/GaN hetero-structure gives the following expression for the SBH and the 2DEG charge density

$$q\Phi_b = \frac{\left(n_o E_d + \sigma_{pz}/q\right)d + \varepsilon_{AlGaN}\,\Delta E_c/q^2}{n_o(d + \varepsilon_{AlGaN}/q^2 n_o)} \tag{1}$$

$$qn_s = n_o d\,\frac{\sigma_{pz} - \varepsilon_{AlGaN}(E_d - \Delta E_c)/q}{n_o d + \varepsilon_{AlGaN}/q^2} \tag{2}$$

where σ_{pz} is the polarization charge density, ε_{AlGaN} is the permittivity of the barrier layer, and ΔE_c is the conduction band offset at the heterointerface.
Based on the assumptions above, (1) and (2) also apply after deposition of the metal gate, but with modified values of the parameters n_o and E_d. Since n_o and E_d depend on the metal work function, so do $q\Phi_b$ and qn_s.

DISCUSSION

As indicated, the reduction in the surface barrier height and the 2DEG density, observed after deposition of the metal gate, occurs because of a reduction in both the surface donor level and surface donor density. We show in the Figure 2 the experimentally observed values of the SBH for a 25nm thick AlGaN barrier layer versus the Al mole fraction. These values are considerably lower than those reported for the similar bare surfaces [4-7]. Similar trends for the 2DEG density for bare and metallized surfaces are also shown in Figures 3 and 4,

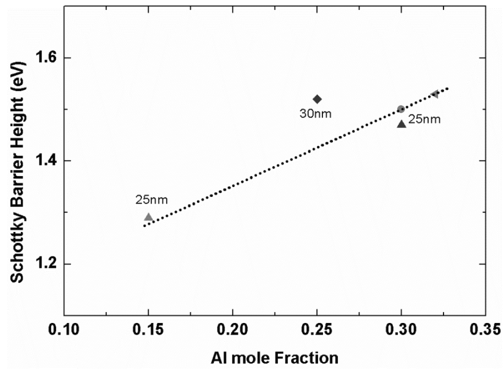

Figure 2. Experimental values of SBH versus the Al mole fraction in the barrier of an AlGaN/GaN heterostructure with deposited metal gate (Ni). AlGaN thickness: 25 nm.

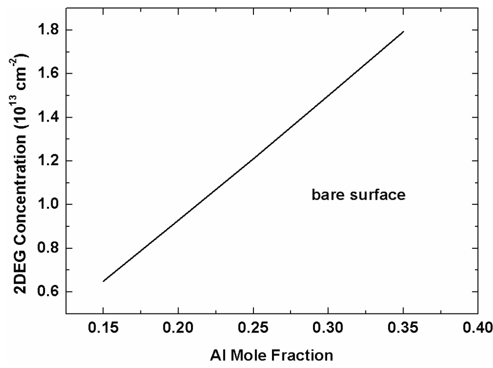

Figure 3. 2DEG density at the AlGaN/GaN heterointerface versus Al mole fraction in the barrier with a bare surface (no metal), calculated from the bare surface model formulation [7,8]. AlGaN thickness: 25 nm.

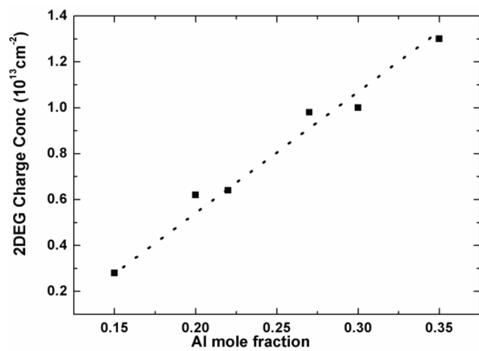

Figure 4. Experimental data for the 2DEG density at the AlGaN/GaN heterointerface post metal gate (Ni) deposition. AlGaN thickness: 25 nm.

To determine the surface donor density n_o, we extract from Figure 4, $n_s = (5.14x - 0.49)\mathrm{x}10^{13}$ cm^{-2} and $q\Phi_b = (1.41x + 1.07)$ eV for the 25nm thick AlGaN barrier layer. By substituting these

values in equation (1) and (2) and solving, we obtain n_o for post metal gate deposition for any Al mole fraction. The result is shown in Figure 5 and compared with n_o of the bare surface case.

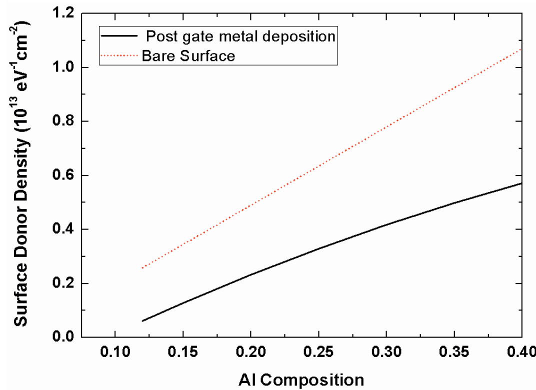

Figure 5. Modeled surface donor density versus Al mole fraction for bare surface and after deposition of metal (Ni) on top AlGaN barrier layer.

As shown in the Figure 5, the surface donor density reduces considerably when the metal gate is deposited. These calculations are consistent with the experimental observations and the proposal by Shin *et al.* that the gate metal causes a reduction in 2DEG by partial neutralization of the surface donor states [11]. This also shows the necessity for understanding the surface physics of metal AlGaN interface, which determines the 2DEG at the AlGaN/GaN interface. A theoretical understanding of this surface is also important for design of efficient gate control and design of Schottky contacts with different metals. To the best of our knowledge, this is first such theoretical attempt in this direction and more theoretical and experimental efforts are needed. This result can be used to derive a threshold voltage model and to develop advanced concepts related to these surface properties of the GaN HEMTs.

CONCLUSIONS

In this paper, we have developed a model framework for the effect of the metal gate deposition on the top surface of an AlGaN/GaN heterostructure. The model predicts how this leads to a reduction in the donor density and distribution at the top surface. This model can be useful in understanding how various physical phenomena in AlGaN/GaN HEMT devices are related to the surface donor states and can also be used for the calculation of threshold voltage. The model agrees well with experimental observations.

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Application of bare surface barrier height to assess structural reliability in AlGaN/GaN heterostructures

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Keywords Surface barrier height, reliability, strain, polarization, critical thickness, dislocations.

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A new characterization procedure for assessing structural reliability in AlGaN/GaN heterostructures is presented, relying on measurements of the bare surface barrier height. This procedure is based on a proposed new model for calculating the critical thickness for dislocation formation in thick AlGaN layers for different Al mole fractions, and for deriving the effective polarization, the effective electric field, and the residual strain in unrelaxed and partially relaxed structures. This procedure can be used to characterize the post stress effects (both electrical and high temperature) for harsh environment conditions.

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1 Introduction GaN based heterostructures devices show great promise in the field of optoelectronics and high-power and high-frequency semiconductor devices applications. This is largely attributed to their superior electrical properties, such as high breakdown field, high saturation velocity, and high two-dimensional electron gas (2DEG) densities even in undoped heterostructures. The underlying reason of the high 2DEG density is the strong spontaneous and piezoelectric polarization present in these heterostructures (see Fig. 1). The lattice mismatch between AlGaN and GaN is the key effect producing strong piezoelectric charges [1]. This mismatch creates a strain energy energy that increases with increasing Al content as well as the thickness of the AlGaN barrier.

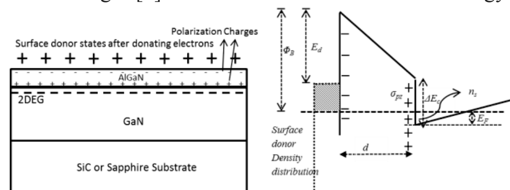

Figure 1 Typical structure of a AlGaN/GaN HEMT showing various charges at the different interfaces and illustrating the formation of 2DEG with electrons supplied by surface donor states.On the left is shown the band diagram.

Over the last few years, the bare surface barrier height (SBH), i.e., the energy difference between the Fermi level and the conduction band minimum, has been an active area of research. The reason for this interest is its coupling to the low density distributed surface donor states that reside in the forbidden gap of the top AlGaN surface. These surface states are considered to be the source of the electrons that form the 2DEG at the AlGaN/GaN interface. Different groups in the last decade have used Kelvin probe microscopy and Kelvin force microscopy to measure the surface barrier height in the AlGaN/GaN heterostructures [2, 3]. Recently, results from capacitance voltage characteristics were applied for the calculation of the surface barrier height in different GaN based heterostructures [4]. To our knowledge, the application of surface barrier height has till now only been used for calculation of surface potential for studies related to current collapse [2]. However, since the surface barrier height is a function of the density and distribution of the surface donor states, it can be used as signature for the characterization of GaN based devices. Due to a lack of a viable model, this feature has previously not been exploited to the full extent. In this paper, based on our previous work, we propose a procedure to model the struc-

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tural reliability of these devices prior to and at post stress conditions.

2 Theory The bare SBH of the AlGaN layer depends on the effective total polarization charge as shown in our earlier work [5]. The polarization depends on the strain energy and the total effective residual strain in the AlGaN layer. However, with increasing AlGaN layer thickness, dislocations start to form once the thickness reaches a certain critical value, whereby some of the strain energy is released. The critical thickness is shown to decrease with increasing Al content in the barrier [6]. At large thicknesses, even plastic deformation can occur, relaxing the whole structure. In the strain relaxation regime, the effective polarization decreases. This, in turn, tends to lower the SBH. Hence, measurements of the SBH will contain information about the internal structural state of the barrier layer, which relates closely to its structural reliability. To design high-performance devices, one objective is to increase the barrier thickness while avoiding strain relaxation. An apparent solution is to use barriers with a low Al content [6].

Understanding the physical mechanisms related to device degradation is essential for reliable device design. SBH provides an accurate estimate of the residual strain, the total effective polarization, and the total internal field in the barrier [5, 6]. Therefore SBH can be used as an initial performance metric for the reliability of AlGaN/GaN HEMTs. During the off-state of AlGaN/GaN HEMTs, the gate is negatively biased and a very high electric field is applied across the AlGaN layer. This field can lead to device degradation by producing additional strain through the so-called inverse piezoelectric effect [7]. Hence, SBH is potentially an important tool for characterization and assessment of device reliability following various stress conditions, such as after application of high electric fields and, in fresh devices, just after the growth of the barrier layer. The effective polarization and 2DEG at high temperatures is also important for applications at extreme conditions, where SBH measurements can be used to search for signatures related to changes in these properties.

3 Results and discussion Based on our model for bare SBH in the AlGaN layers [5], we can divide the effects of barrier thickness into two regions – the unrelaxed region and partially relaxed region for each given Al content as shown in Fig. 2. Using this model, the effective residual strain present in the AlGaN layer can be calculated, as indicated in Fig. 3. This is a direct measure of the degradation of piezoelectric effect and the number of dislocations forming. We observe that the trend indicated is very similar to that of experimental data reported by Bykhovski *et al.* [8], where the reported data was extracted from C-V measurements on a metallized AlGaN/GaN surface. The resultant total polarization versus the barrier thickness can also be calculated as shown in Fig.4.

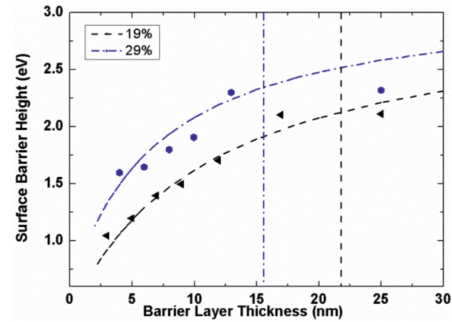

Figure 2 Comparison between SBH experimental data from Ref. [5] (symbols) and the modeled SBH assuming unstrained layers (lines). The vertical lines indicate the critical thicknesses for the different Al content (shown as percentages).

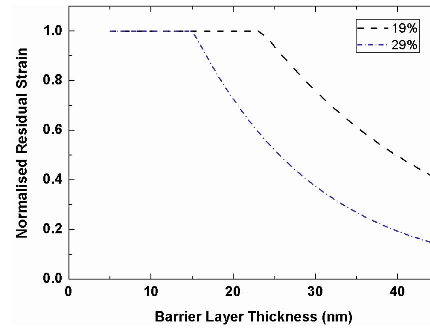

Figure 3 Modeled normalised residual strain for two Al contents in the AlGaN barrier layer. At large Al content, strain relaxation occurs at lower thickness and dislocations form to reduce strain energy.

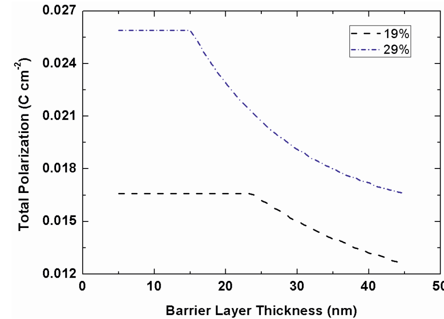

Figure 4 Modeled effective total polarization in AlGaN layer versus thickness for two different Al contents. Beyond the critical thickness, the piezolectric polarization weakens owing to strain relaxation and the total polarization tends towards the spontaneous polarization value.

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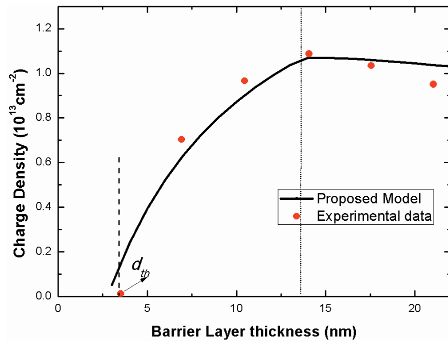

Figure 5 Calculated 2DEG density versus AlGaN barrier layer thickness for a barrier Al content of 35 %, compared with experimental data given in Ref. [9]. The vertical line atthe cusp separates the unrelaxed and partially relaxed regions.

Based on these results, our model allows us to calculate 2DEG at AlGaN/GaN interface, an example of which is shown in Fig. 5.

As demonstrated above, measurements of the SBH will contain information about the internal structural state of the barrier layer, which relates closely to its structural reliability. SBH can be used as a performance metric for the reliability of AlGaN/GaN heterostructures resulting from different stress conditions, providing a quantitative measure of the structure degradation in the barrier layer. Hence, SBH measurements can potentially become an important tool for the characterization and assessment of the AlGaN barrier layer. This also includes assessment of the effective polarization, which, for example, is important for high temperature applications, where SBH measurements can be used to search for signatures related to changes in the polarization. Likewise, the dependence of the surface donor level and surface donor density on temperature can be characterized this way to enable an enhanced power of predictability in our model.

In conclusion, we have presented a modeling and characterization framework for AlGaN/GaN hetero-structures, which relates important surface donor state properties to measurable quantities such as the surface barrier height and the 2DEG density at the heterojunction. Specifically, we have demonstrated how this framework can be utilized, together with experimental data, as a diagnostic and predictive tool for reliability assessment of these structures when used in electronic devices such as AlGaN/GaN HEMTs.

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Part III. Future work and Conclusions

As mentioned previously, AlGaN/GaN based HEMTs are projected to become widely used in harsh environments and at high power and voltage conditions. For this reason, the longtime reliability of these devices, both in on-state and off-state operation, is of major concern and has been a topic of study over the last decade. Current collapse and inverse piezoelectric effect have been suggested as two major reliability problems for these AlGaN/GaN based devices [1-10]. Both of these effects occur due to the high electric field in the AlGaN layer produced under external bias conditions. Recently, Rivera et al [6], Alamo *et al.* [1][7][8], Jimenez *et al.* [5], Sarua *et al.* [9] and Ando [10] identified the inverse piezoelectric effect as one of the major reliability issue for off-state bias conditions in AlGaN/GaN heterostructures. Since then, different groups have reported many experimental observations showing degradation due to this effect. This may occur, for example, when a large negative gate bias is applied during off-state (with source and drain connected to ground), which leads to a strong electric field inside the AlGaN barrier layer. This electric field can generate an electrically induced mechanical strain (inverse piezoelectric effect), which, when combined with built-in strain, may cause structural deformation and can lead to permanent degradation of the AlGaN/GaN hetero-structure. This is typically initiated at source and drain side corners of the metal/AlGaN interface, where the electrical field peaks. The off-state gate voltage at which the onset of this degradation happens is called the critical voltage for inverse piezoelectric effect. This problem is closely associated with device design. A suitable choice of thickness and Al composition of the AlGaN layer can increase the critical voltage to allow a wider operational range. Such device design guidelines depend of the initial estimate of the critical voltage for a given structure and need to be modeled in the future. We have initiated a modeling of this effect starting with an analysis of the precise electrostatic field distribution adjacent to the gate corners using conformal mapping techniques. We expect that this, in combination with experimental data, can lead to a suitable model of the critical voltage for onset of degradation.

Some of the still unsolved on-state reliability effects in AlGaN/GaN HEMTS's are the DC current collapse, RF dispersion, gate- and drain-lag, and a reduction in RF output power. Vetury *et al.* explained some of these phenomenon by the virtual gate model based on surface states [11]. They assumed that due to negative gate bias, some of the electrons get trapped in the region near the gate edge and make the surface potential negative. These trapped electrons in the vicinity of gate act as a negatively biased electrode, thus depleting the 2DEG in the channel region beneath.

But the theory by Vetury *et al.* didn't explained the kink observed in drain current when drain voltage increases for the gate bias close to threshold voltages. Also the theory was based on the assumption of a pinned Fermi level at 1.65 eV in the bare AlGaN surface while it has been established that AlGaN surface has low density surface states and that the Fermi level moves up and down with the occupancy of surface states and the thickness of AlGaN layer [12][13]. Recently, some research groups have used scanning probe microscopy to study the surface potential near the gate edge after application of gate and drain voltages [14] and calculation of surface potential using electrochemical capacitance-voltage measurements [15]. But still a complete understanding is lagging in terms of distributed surface donor states and observed negative surface potential at the gate drain edge as well as the complete profiling of the defect states. This needs to be explained with the relevant device physics backed by experimental data in the future so as to develop efficient GaN HEMTs for future applications.

In conclusion, this PhD thesis is focused on issues ranging from the fundamental understanding of the 2DEG formation in AlGaN/GaN heterostructures to the development of mathematical modeling explaining the physical behavior. We then modeled strain relaxation related calculations in the basic model. Impact of gate metal was also presented with the developed understanding and is consistent with the reported experimental data. We also proposed a new procedure to access reliability of GaN heterostructures quantitatively. Two major reliability issues inverse piezoelectric effect and current collapse have been recommended for future work for guidelines of efficient GaN based HEMT design. The proposed formulation can be used for the development of design guidelines for optimum design of AlGaN/GaN HEMTs for different applications. Proposed modeling framework is consistent with the reported experimental data published by different groups.

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Part IV. Errata

Paper A:

In equation 4, $K_4 = 1 + \varepsilon_{AlGaN} / dq^2 n_0$

Paper B:

In section B: Model for partially relaxed AlGaN thick barriers, there is AlGaN/GaN instead of AlGaAs/GaN.