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Evaluation of Degradation in GaN High Electron Mobility Transistors Due to the Inverse Piezoelectric Effect

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EVALUATION OF DEGRADATION IN GaN HIGH ELECTRON MOBILITY TRANSISTORS DUE TO THE INVERSE PIEZOELECTRIC EFFECT

by

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ABSTRACT

EVALUATION OF DEGRADATION IN GaN HIGH ELECTRON MOBILITY TRANSISTORS DUE TO THE INVERSE PIEZOELECTRIC EFFECT

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Old Dominion University, 2014
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It has recently been postulated that high voltage stress can result in the degradation of nanoscale structures that are made up of piezoelectric materials. The inverse piezoelectric effect (IPE) is believed to be the likely reason for this degradation mechanism. Basically, the IPE leads to the creation of high internal stresses driven by the presence of an electric field. Consequently, devices based on piezoelectric materials are postulated to undergo defect formation induced by the large mechanical stress arising from the inverse piezoelectric effect in the presence of an applied bias. GaN based devices are mostly observed to show this degradation mechanism, in particular AlGaN/GaN HEMTs. The key feature of this mechanism is the sudden increase in leakage currents due to defect induced energy levels. The leakage currents can contribute to local heating or electromigration, and further enhance defect creation leading to an irreversible device degradation cycle. Given this possibility, and the need to mitigate such deleterious effects, it becomes important to understand and model this degradation mechanism in nanoscale devices.

The aim of this dissertation research is to focus on the particular aspect of the inverse piezoelectric effect, understand its role in potential device degradation of GaN-based High Electron Mobility Transistors (HEMTs), and evaluate the possibilities of minimizing the inverse piezoelectric effect by optimizing the GaN-HEMT geometry and design parameters. The possible modifications of the parameter space include changing device dimensions, varying the Al composition, and employing high-k insulating cap layers. The effect of such changes on various device aspects such as the carrier density, strain, internal electric fields and the related stored energy etc. were carefully and

systematically evaluated in this dissertation research. Details on the salient results, potential summarizing conclusions, and scope for future work are also presented.

I dedicate this dissertation to the God, my advisor and my family for all the blessings, strength, guidance and support.

ACKNOWLEDGMENTS

I would like to express my sincere gratitude to my advisor, Dr. Ravindra Joshi, for his guidance, support and patience during all the years of work. This work wouldn't have been possible without his constant direction and motivation. I would also like to sincerely thank my dissertation committee members for taking time to guide me and assess my work.

I truly appreciate my family for believing in me and for giving me strength to keep working.

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CHAPTER 1

INTRODUCTION

1.1 MOTIVATION

There has been rapid development in Group III nitride material systems. The high breakdown fields that can be sustained in GaN High Electron Mobility Transistor (HEMT) devices, combined with high electron densities of the two-dimensional electron gas (2DEG) in the channel, and the high electron drift velocities, form the important foundation for high power electronic applications of HEMTs with high efficiency. Power consumption of transmission power amplifiers has increased drastically with increasing transmission speeds over 100 Mbps. Thus high power efficiency is required to reduce this increased power consumption for the next generation networks. GaN HEMTs have shown higher efficiencies compared to Si-laterally diffused metal oxide semiconductor (LDMOS) devices [1]. Because of their large band gap, high electron mobility and large piezoelectric coefficients, HEMTs fabricated from GaN can generate four to five times the amount of power that a comparable GaAs HEMT can.

A high output power density of over 40 W/mm was demonstrated for a single HEMT device [2]. Figure 1.1 shows the comparison of On-Resistance as a function of breakdown voltage for Si and GaN materials. For a low value of On-Resistance, which is typically a desirable feature, the breakdown voltage for GaN materials is almost an order of magnitude higher than that for Si-devices. As the feature sizes shrink and hence the internal electric fields scale up, such higher breakdown field limits are very desirable. The high breakdown voltages then mean that the GaN devices are more resistant to breakdown and can sustain much shorter device down-scaling. Furthermore, because of such high power efficiency, smaller devices can be used for the same output power, and high voltage operation is possible. In this regard, the AlGaN/GaN HEMT is the commonly used device structure. This high power efficiency is a result of high concentrations of the two-dimensional electron gas (2DEG) formed at AlGaN/GaN interface due the strong piezoelectric and spontaneous polarization effects[3]. The electric field values can reach several MV/cm during HEMT operation for high power applications.

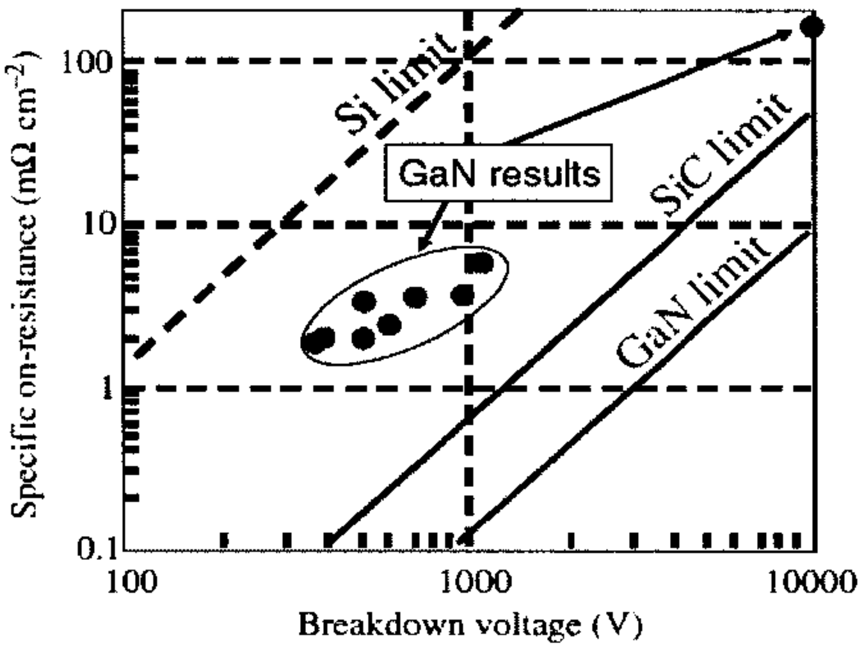


Figure 1.1. Comparison of On-Resistance of materials for power electronics. © 2009 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim. Reprinted, with permission, from [1].

However, it has experimentally been observed that GaN HEMT devices used for high voltage operation can often fail [3]. It was hypothesized that the failure of these AlGaN/GaN devices studied was due to a new defect formation mechanism associated with the inverse piezoelectric effect when biased at high voltages. The inverse piezoelectric effect (IPE) is expected to be more important under high fields [3], since the electric fields drive material stress and ultimate deformation and defect creation. The basic source is the piezoelectric nature of the GaN and AlGaN materials that leads to increased strain and eventual degradation causing crystalline defects at high internal electric fields. Crystalline defects in single crystal semiconductor can degrade the properties of the device such as the background current levels, intrinsic noise, as well as turn-on and turn-off voltage levels. For example, current leakage through dielectric or semiconductor can occur which can degrade the device by affecting charge trapping. This process, in turn, can cause the device properties (such as threshold voltage in Field Effect Transistors and memory devices), or the local electric fields to change dynamically over time. In addition, leakage currents can contribute to internal heating. This presents a potential problem since the temperature at which device operates has profound effects on device operation and its reliability. In the worst scenarios, the deviations in current and operating characteristics may be irreversible, leading to run-away and eventual device failure. Manufacturers and users both desire to minimize or better yet, completely eliminate such device degradation and failures.

GaN microwave power device performance was reported to improve with the MOS HEMT structure. Yue et al. [2] proposed the use of high-*k* layer structure as insulator with thickness of about 10nm grown using Atomic Layer Deposition process. In the process, they were able to achieve reductions in the gate leakage current by six orders of magnitude over HEMT devices without the high-*k* layer, for positive gate biasing [4]. In order to realize the advantages of high breakdown field and high on-off ratio in group III nitride HEMTs, it is required to improve the reliability of the device with reduced leakage currents. The improvement in reliability can result from understanding the physics behind the failure mechanisms and optimizing the device parameters.

1.2 SCOPE AND ORGANIZATION

Several questions and issues must be addressed in order to bring the reliability of these devices to a reasonable point. The first and foremost task is perhaps to understand the mechanisms responsible for the root causes of the failure in GaN-based HEMT devices, especially at the high applied biases. Strain relaxation through the generation of dislocations at the interfaces is observed to be a formidable source of degradation and the inverse piezoelectric effect has been proposed as the mechanism of degradation. However, a complete and quantitative understanding of the mechanisms of device degradation or failure remains. Furthermore, evaluation of the critical magnitudes of the external voltages (or electric fields) and the regions within the device that could potentially trigger failure, needs to be carefully carried out.

This dissertation is organized to basically address the above fundamental issues, and quantitatively access the influence of the inverse piezoelectric effect in driving device failure. In this context then, the dissertation research is organized as given in the following paragraphs.

Chapter 2 reviews the history, advantages, operation and fabrication of AlGaN/GaN High Electron Mobility Transistors (HEMTs). An overview of the different failure mechanisms in HEMTS are discussed for completeness, and to provide a basic background. The basic theory behind the inverse piezoelectric effect (IPE) and its possible role and effect in HEMTs is also presented in Chapter 2. The current solutions to challenges such as addition of cap layers, MOS HFET structures, addition of field plate structure are discussed for completeness. Lastly, this chapter includes possible materials, advantages and challenges in HEMT technology leading to the motivation of this research.

Chapter 3 focuses on the methodology that has been used, adapted and adopted to model the degradation process in an AlGaN/GaN HEMT. This chapter includes details of the HEMT structure used to analyze and study the degradation process. Calculation of different parameters such as stress, strain and elastic energy density that control possible device degradation, the variations in their parameter space, and computations of the optimal values required to reduce device degradation are also investigated. This chapter also provides an introduction to the COMSOL Multi-physics software tool that is used for electrostatics simulations of the HEMT model. Impact of the cap layers on the 2DEG and details of the HEMT structure such as the role of the capping layers for improved device reliability are also discussed.

Chapter 4 presents the results from our simulations using the models presented and discussed in chapter 3. The influence of the variation in parameters such as Al content, the effect of AlGaN thickness on polarization and sheet charge density, quantitative values of the fields and stresses generated within the HEMT structure are also discussed. Finally the effect of capping layers, and the role of possible device heating are presented.

Chapter 5 discusses the summary of the research and the salient points of the results obtained. The optimized parameter space for improving the reliability as observed from the results given in Chapter 4 is also discussed Finally, this chapter presents some scope for possible future work that could be undertaken for further analyses and research evaluations.

CHAPTER 2

LITERATURE REVIEW AND BACKGROUND

2.1 INTRODUCTION

An ideal semiconductor material for power applications should possess excellent transport and thermal properties, a high breakdown voltage, mechanical stability and low parasitics. Traditionally, most of the power devices today are made from silicon or GaAs. However, wide band gap semiconductor materials have attracted a lot of attention as potential candidates for high power applications (3.4eV for GaN versus 1.4 eV for GaAs). In the context of emerging technologies, Group III nitride semiconductor materials have shown great potential in microwave power applications of wireless communication, radar, and automobile electronics. Its mainstream electronic device structure is the AlGaN/GaN high electron mobility transistor (HEMT). During the past few years enormous progress has been made in the development of GaN based HEMTs. GaN based material systems offer important characteristics such as high band gap, high critical field, high thermal stability, high current density, high switching speed and low ON-resistance. Because of their large band gap, high electron mobility and large piezoelectric coefficients, High Electron Mobility Transistors (HEMTs) fabricated from GaN can generate four to five times the amount of power that a comparable GaAs HEMT can. A high carrier density is generated at the AlGaN/GaN hetero-interface due to spontaneous and piezoelectric polarization effects without requiring large doping. The polarization induced contributions to electron density results in low electron scattering since high amounts of dopant impurities (and hence impurity scattering) does not arise. Due to their high breakdown voltages, GaN HEMTs can operate in conditions that are not readily realizable with other device technologies. The GaN technology has been widely accepted as vehicle for high performance and high power applications.

These very high bias conditions, however, induce very high electric field within the device active area that can result in severe device degradation. GaN and AlN have strong piezoelectric properties. The crystal growth direction for these structures is such that these properties directly affect the electric field in the direction perpendicular to the hetero-interface. Several authors have observed that significant degradation effects may take place even when the devices are biased in the "off state". In this cases, the main failures observed are the catastrophic increases in gate leakage current. The existence of a critical voltage beyond which GaN HEMTs start to degrade has led the authors to propose a degradation mechanism based on crystallographic defects. Strain relaxation through the generation of dislocations at the interfaces is observed to be a formidable source of degradation and the inverse piezoelectric effect has been proposed as the mechanism of degradation. Improvements in reliability require a better understanding of failure mechanisms of GaN HEMTs.

2.2 INTRODUCTION TO HEMTs

High electron mobility transistors (HEMT) are presently undergoing intense research due to their usefulness in RF (radio frequency) and microwave power amplifier applications including (but not limited to): microwave vacuum tubes, cellular and personal communications services, and widespread broadband access [5]. One of the main issues being researched in these devices is their reliability.

The frequency of operation and switching speeds are constantly being challenged as advanced semiconductor preparation and processing tools become available. The switching speed of the device is primarily determined by how fast an input pulse can be transmitted to the output. For fast switching time, the capacitances and the transit time through the device must be made smaller. Large amounts of current, if available, can charge and discharge capacitances faster. The transit time can be made smaller by either reducing the current path or by increasing the speed at which the carriers travel. The speed of the carriers, for low electric fields is given by the product of mobility and electric field. Since the current is proportional to the carrier velocity as well as the carrier density, carrier density must be increased for large currents. Increased electron concentration necessary for high currents required for high power devices (and for increased "fan-out") also means increased donor concentration (in n-channel devices) which leads to electron donor interaction called ionized impurity scattering. In general as FETs become smaller, thinner channel layers and higher electron concentrations are required. The requirement for large electron concentrations without deleterious effects of donors (and their associated ionized impurity scattering) can be met by heterojunctions. High Electron Mobility Transistor (HEMT) is the major device application of heterostructures. HEMTs are currently considered as the fastest transistors. Heterostructure Field Effect Transistor (HFET), Modulation Doped Field Effect Transistor (MODFET), Selectively Doped Heterojunction Transistor (SDHT), Two-dimensional Electron Gas FET (TEDFET) are some of the other commonly used names for HEMTs [6, 7, 8].

A heterojuction is defined as a junction formed between two dissimilar lattice matched semiconductors with different energy band gaps (E_G), different dielectric permittivities $\in$, different work functions$(\emptyset)$, and different electron affinities(χ). There are three different types of heterojunctions based on the band alignment as shown in Figure 2.1. In type I, band gap of one semiconductor is completely contained in the band gap of other (e.g. AlGaAs/GaAs) and in type II, the band gaps just overlap (e.g. InP/InSb), while in type III, the band gaps do not overlap (e.g. GaSb/InAs). However, type I is the most commonly used heterojuction due to its applications. Structures formed with same lattice constant but have different band gaps are referred to as lattice mismatched HEMTs and also structures with different lattice constants are called pseudomorphic HEMT (PHEMT).

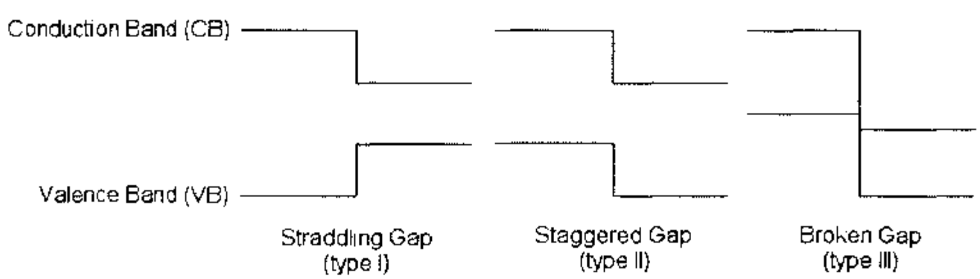


Figure 2.1. Heterojuction types. Reprinted, with permission, from [9].

A good example of heterojunction devices with different band gaps and similar lattice constant is made of $Al_xGa_{(1-x)}As$ and GaAs. Here when x=0, GaAs is obtained with band gap of 1.42 eV and lattice constant of 5.6533 A°, x=1 gives AlAs with band gap of 2.17 eV and lattice constant of 5.6605 A°. Therefore, even for extreme cases, the lattice mismatch is 0.1% [9]. In most of the device applications AlAs mole fraction (x) lies between 0.2 and 0.3. The band diagram for two isolated semiconductors is shown in Figure 2.2(a) and the band diagram of heterojuction formed at thermal equilibrium is shown in Figure 2.2(b). Here the difference in the energy of conduction band edges in the two semiconductors is denoted by ΔE_c and the difference in energy of the valence band edges is denoted by ΔE_v. According to the electron affinity rule, the conduction band offset at a heterojunction interface is equal to the difference in the electron affinities between two semiconductors which is $\Delta E_c = \chi_1 - \chi_2$ as shown in band diagram. The valence band offset is then $\Delta E_v = \Delta E_G - \Delta\chi$ with $\Delta E_G = E_{G1} - E_{G2}$. Depending upon the difference between χ_2 and χ_1 different heterojuction interfaces are formed as shown in Figure 2.1. Also, as can be seen from the band diagram, there is a band bending across the junction and therefore potential difference exists across junction. This is the built in potential which is the difference in the Fermi levels on the two sides of the junction given as $qV_{bi} = E_{f1} - E_{f2}$.

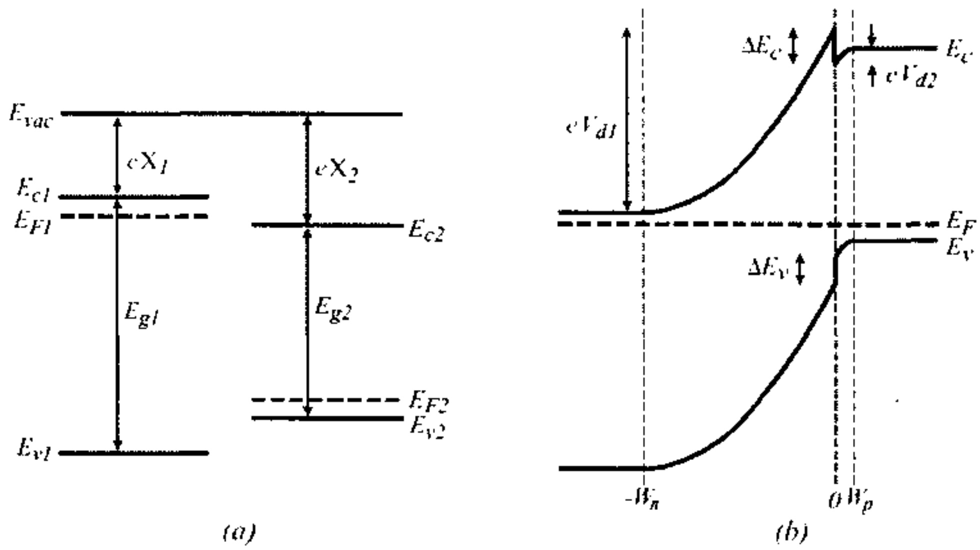


Figure 2.2. (a) Band diagrams for isolated semiconductors, (b) at thermal equilibrium.© 2008 Springer. Reprinted, with permission, from [6].

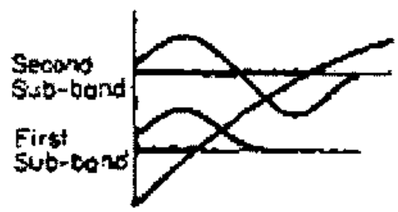


Figure 2.3. Discrete energy levels of the electrons trapped in conduction band notch of the AlGaAs/GaAs heterostructure. © 1984 IEEE. Reprinted, with permission, from [7].

Fermi level must be same on both sides of the interface at thermal equilibrium. Therefore, from Figure 2.2, it can be observed that due to difference in electron affinity there is discontinuity formed in the conduction band at the interface creating a notch. Therefore at the interface, the electrons coming from AlGaAs, confine in the conduction band notch due to large barrier height. This notch can also be called as quantum well and Figure 2.3 shows the energy levels permitted for this particles trapped are obtained by solving Schrodinger's equation as discrete energy levels. Here, since the thickness of the potential well is very thin of the order of nanometers, the tunneling of electrons occurs due to wave like nature of the electrons [7, 11]. Since these electrons are confined in one direction in potential well and can only move in two directions which are parallel to the interface, it is called as two dimensional electron gas (2DEG).

This confinement of electrons becomes the basic principle of most widely used heterostructures in high frequency applications, also called High Electron Mobility transistors (HEMTs) [7] as mentioned previously.

2.2.1 HETEROSTRUCTURE FABRICATION AND OPERATION

The AlGaAs/GaAs heterojunction structures needed for HEMTs are grown by molecular beam epitaxy (MBE) on semi-insulating substrates. The buffer layer, typically GaAs, is epitaxially grown on the substrate. This is to create a smooth surface and isolate defects so that active layers of transistor can be grown. An AlGaAs spacer layer, a donor layer n+ AlGaAs layer and a Schottky contact layer are then grown above the buffer layer which results in a two dimensional electron gas (2DEG) due to band gap difference between AlGaAs and GaAs. In a conventional HEMT fabrication process, first a nominally 1 μm thick undoped GaAs layer is grown at a substrate temperature of about 580°C. Gallium flux which determines the growth rate is adjusted to yield a growth rate of about 1 μm/h. This is followed by the growth of the AlGaAs layer, about 20 – 60 A° of which is not doped near the interface. Its purpose is to ensure the separation of the hetero-junction interface from the doped aluminum gallium arsenide region. This is critical if the high electron mobility is to be achieved. The doped AlGaAs layer, about 600 A° thick, may be capped with a doped GaAs layer. The source and drain areas are then defied in positive photoresist, and typically AuGe/Ni/Au metallization is evaporated. Following the lift-off, the source drain metallization is alloyed at or above 400°C for a short time to obtain ohmic contacts and a gate is then defined [7].

The basic operation of HEMT is based on the electrons that diffused from the doped AlGaAs to the GaAs and are confined by the energy barrier forming a two dimensional electron gas. The n+ AlGaAs layer acts as source of electrons and spacer layer serves to separate donor ions from the 2DEG. However, increased spacer layer thickness will decrease the sheet carrier concentration. The region of AlGaAs depleted of electrons forms a positive space charge region which is balanced by the electrons confined at the interface. The electric field set up by the charge separation causes a severe band bending in the GaAs layer with a resultant triangular potential barrier where the allowed energy states are no longer continuous in energy, but discrete as shown in Figure 2.5. Since the 2DEG is located in undoped GaAs layer, the columbic scattering by donors is avoided resulting in very high mobility. Thus high electron mobility is achieved in these heterostructures with mobility of about 2x10^{6} cm^{2}/V [7].

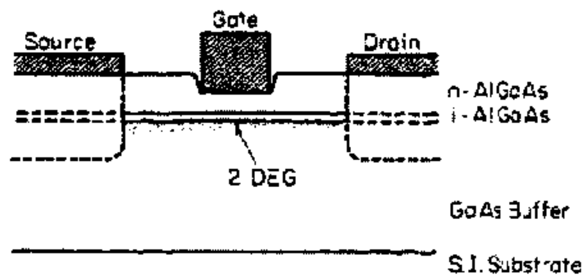


Figure 2.4. AlGaAs/GaAs heterostructure. © 1984 IEEE. Reprinted, with permission, from [7].

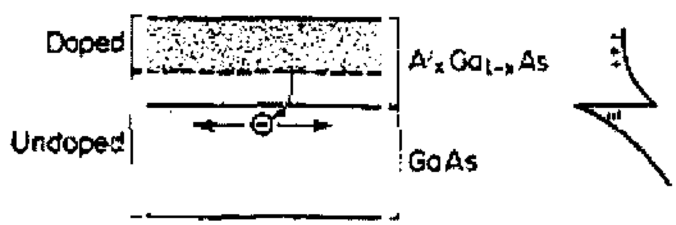


Figure 2.5. AlGaAs/GaAs heterostructure and energy band diagram. © 1984 IEEE. Reprinted, with permission, from [7].

Similar to the Junction Field Effect Transistor (JFET) and Metal Semiconductor Field Effect Transitor (MESFET), electric field applied in HEMT devices controls the flow of current through the device. The gate forms a schottky contact with AlGaAs layer. When a negative bias is applied to gate, the Schottky barrier becomes depleted. As gate is biased further, the 2DEG becomes depleted. Therefore, modulation of 2DEG is obtained by negatively applied gate biasing wherein gain and amplification are achieved until the channel is fully depleted or pinched off. Since the conduction of electrons takes place in the well confined undoped channel resulting in high saturation velocity, the transconductance given by $g_m = \in V_{sat}W/d$ remains very high where V_{sat} is saturation velocity, is permittivity, W is gate width and d is the distance from gate to 2DEG. Also, the higher mobility achieved in HEMT results in lower parasitic drain and source resistance. As a result, the figure of merits of a device like cut off frequency given as $f_T = \frac{g_m}{2\pi C_{gs}}$ where C_{gs} is the gate to source capacitance and maximum frequency of oscillation are increased leading to higher gain and lower noise figure.

2.3 III-V NITRIDE BASED HEMTs

In the past 40 years, the focus of GaAs-based device technologies shifted from Metal Semiconductor Field Effect Transistors (MESFETs) to various types of High Electron Mobility Transistors (HEMTs) and then to Heterojunction Bipolar Transistors (HBTs). More recently, GaN-based HEMTs have received much attention for their use in high power and high frequency applications due to large energy band-gaps, great electron mobility, high breakdown voltages, and considerable 2-D electron gas densities as compared to their GaAs counterparts. Two of the most important requirements for switching devices are large breakdown voltage and low "ON" resistance. Silicon has long been the dominant semiconductor for high voltage power switching devices but silicon power devices are rapidly approaching the theoretical limits for performance. GaN material system attracted much attention due its number of potential advantages over silicon. GaN has projected saturation velocities of 2.5×10^7 cm/s and 3.4 eV band gap that leads to a critical breakdown field of 3.3 MV/cm [12]. Also, the ability to form a high density 2DEG by polarization doping allows for very high electron mobility while maintaining high carrier density. A high mobility and carrier density product in devices results in low on resistance. Table 2.1 compares some of the fundamental physical properties of GaN to those of other major semiconductors.

Employment of GaN HEMTs for high power radar systems will require devices to be subjected to large-signal RF while being driven into saturation, resulting in devices experiencing high electric fields and high current densities. Impressive mean-time-to-failure values of greater than 10^7 hours have been reported at operating temperatures below 200 °C, with activation energies ranging from 0.18 eV to 2 eV [13]. Wide bandgap semiconductor technology for high-power microwave devices has matured rapidly over the last several years as evidenced by the fact that AlGaN/GaN High Electron Mobility Transistors (HEMTs) have been available as commercial-off-the-shelf (COTS) devices since 2005. AlGaN/GaN HEMTs possess high breakdown voltage, which allows large drain voltages to be used, leading to high output impedance per Watt of RF power, resulting in easier matching and lower loss matching circuits. The high sheet charge leads to large current densities and transistor area can be reduced resulting in high Watts per millimeter of gate periphery. The high saturated drift velocity leads to high saturation current densities and Watts per unit gate periphery. In turn, this leads to lower capacitances per Watt of output power. Low output capacitance and drain-to-source resistance per Watt also make GaN HEMTs suitable for switch-mode amplifiers. Research and development of GaN HEMTs gained considerable momentum in the late 1990s and early 2000s when it became possible to reproducibly grow high-quality 4H-SiC substrates. High total RF powers from GaN HEMT transistors over a wide frequency range have been reported for single die up to several hundred Watts [14]. However, these high power densities, in terms of Watts per millimeter, also present extreme power dissipation demands on both the transistor layouts, as well as the semiconductor substrates. Fortunately, the high thermal conductivity of SiC substrates (~330 W/m K) allows these high power densities to be efficiently dissipated for realistic drain efficiencies, preventing the extreme channel temperatures that would result due to self-heating with other substrate technologies [12-15]. Figure 2.6 shows the merits of GaN based material systems compared to Si and GaAs for different applications. The room temperature mobility of 2DEG which is typically between 1200 $cm^2 V^{-1} S^{-1}$ and 2000 $cm^2 V^{-1} S^{-1}$ and saturation velocity of 2DEG at AlGaN/GaN interface is very suitable for high power and high frequency applications. The 2DEG carrier density of AlGaN/GaN structure is around 10^{13} cm^{-2} due to piezoelectric and spontaneous polarization induced effects [16].

Table 2.1. Physical properties of various semiconductors relevant to high voltage applications [1-16].

Si	1.12	11.9	1.5	3×10^5
GaAs	1.43	12.5	0.45	4×10^5
GaN	~3.4	9.5	1.3	3×10^6

GaN based and other group III Nitride based semiconductors exist in different crystal structures like Wurtzite, Zinkblende and Rocksalt. Most of AlGaN/GaN HEMTs crystal structures exist in the Wurtzite phase. Wurtzite GaN based semiconductors have a polar axis resulting from a lack of inversion symmetry in the <001> direction. Due to this electronic charge redistribution inherent to the crystal structure, the group III-N semiconductors exhibit exceptionally strong polarization called spontaneous polarization (P_{sp}). Because of their wurtzite structure, GaN based semiconductors can have different polarities, resulting from uneven charge distribution between neighboring atoms in the lattice. The polarity of the crystal is related to the direction of the group III-N dipole along the <0001> direction. Figure 2.7 shows the two possible polarities, in cation-face i.e., Ga face where polarization field points away from surface to substrate and in anion face i.e., N-face where direction of polarization is inverted [17].

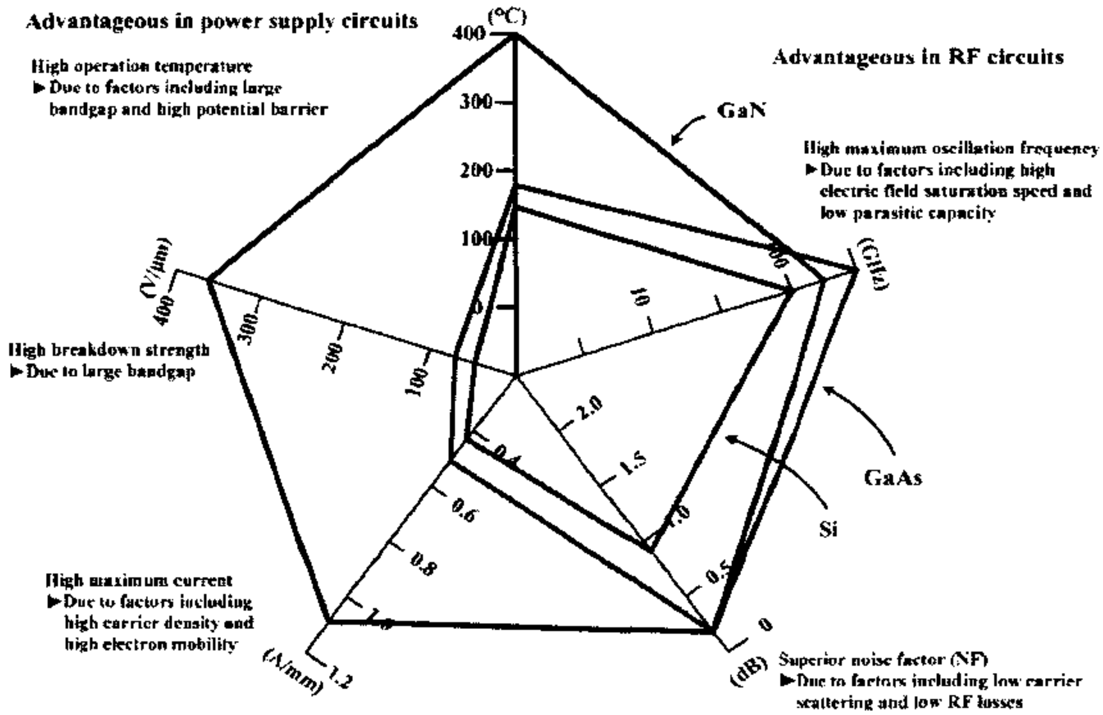


Figure 2.6. GaN material merits compared to Si and GaAs. © 2013 GaN Systems. Reprinted with permission from [16].

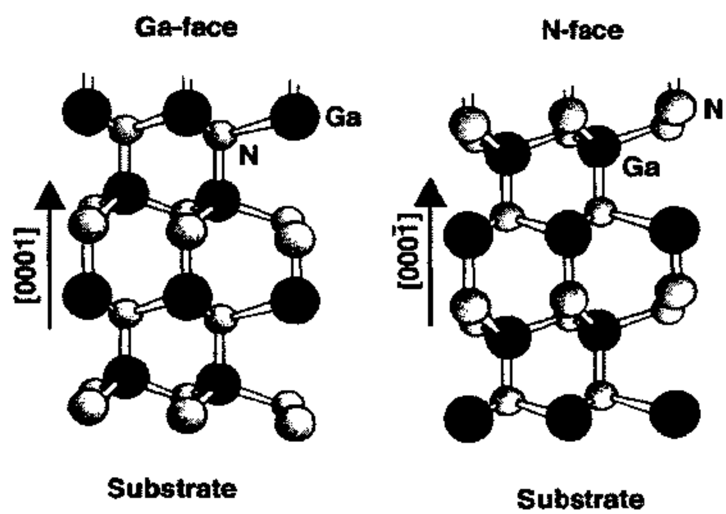


Figure 2.7. Illustration of a) Gallium face, and (b) Nitrogen face ideal Wurtzite GaN lattice structure. © 2000, AIP Publishing LLC. Reprinted, with permission, from [17].

Due to this lack of inversion symmetry, when stress is applied along the <0001>direction to the group III-N semiconductors lattice, the lattice parameters of the crystal structure will change to accommodate the stress. This additional polarization is called piezoelectric polarization (P_{pe}). For example, if nitride crystal is under biaxial compressive stress the in-plane lattice constant will decrease and the vertical lattice constant will increase. Hence the total polarization strength of the crystal will decrease because piezoelectric and spontaneous polarizations will act in opposite direction. If tensile stress is applied to the crystal, the total polarization will increase because the piezoelectric and spontaneous polarizations in that case act in the same direction. The values of piezoelectric polarization is in Group III Nitrides is always negative due to negative piezoelectric coefficient (e_{31}) value and for layers under tensile stress spontaneous and piezoelectric polarizations are parallel. For layers under compressive stress both are anti-parallel. In AlGaN/GaN HEMTs this polarization induced doping is the source of two dimensional electron gas (2DEG). Unlike GaAs based HEMTs, GaN based HEMTs show high values 2DEG density without intentional doping, as previously mentioned.

2.3.1 GaN versus GaAs

The combination of GaAs and AlGaAs has long been used in fabricating HEMT devices. In recent years another material combination, AlGaN/GaN, has been the subject of intense research. This is because GaN has attractive electrical properties such as a large bandgap (3.2 eV comparing with 1.4 eV of GaAs), high electrical breakdown field ($2x10^6$ Vcm^{-1} comparing with 4x105 Vcm^{-1} of GaAs), high peak and saturation carrier velocity (3x107 cm/s and $2x10^7$ cm/s comparing with $2x10^7$ cm/s and 10^7 cm/s of GaAs) and good thermal conductivity (1.3 $Wcm^{-1}K^{-1}$ comparing with 0.55 $Wcm^{-1}K^{-1}$ of GaAs). Furthermore, nitride-based devices are chemically inert and have high temperature stability which makes them more reliable.

These superior properties of GaN are adequate for high power amplifiers, since for power applications the three most important device characteristics are breakdown voltage, current carrying capability, and speed (including operation at higher frequencies) [17]. A typical AlGaN/GaN HFET device is shown in Figure 2.8.

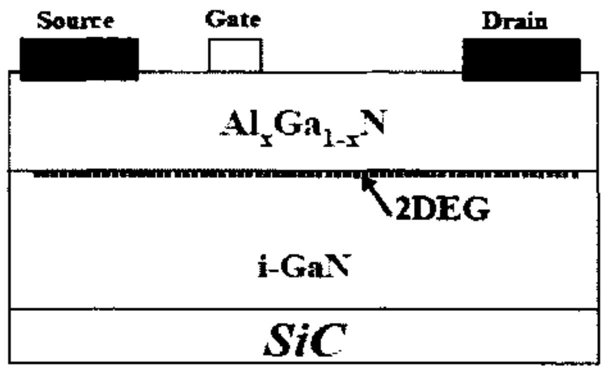


Figure 2.8. Typical AlGaN/GaN HFET – with source, gate, and drain metallization contacts, and SiC substrate. The approximate location of the two-dimensional electron gas (2DEG) is depicted, just below the heterojunction of AlGaN. © 2005 IEEE. Reprinted, with permission from, [18].

Due to lattice mismatch between the GaN and substrate layer, sometimes a buffer layer such as AlN is used between these layers to mediate. Mismatch between GaN and the substrate generates defects such as dislocations. In the case of SiC substrate, this dislocation density may reach 10^8-10^9/cm2 [19]. Because AlGaN has a wider band gap than that of GaN, the electrons diffuse from the AlGaN layer into the GaN and form the 2DEG on the GaN side of the AlGaN/GaN heterojunction.

AlGaN/GaN HEMTs are generally considered to have better high-power application performance than the better studied AlGaAs/GaAs HEMT due to the favorable larger 2DEG density [20]. In an AlGaN/GaN HEMT of (common) wurtzite lattice structure, both the AlGaN and GaN have high polarization present, with that of AlGaN is much stronger [21]. In this type of HEMT, the AlGaN possesses 5 times the piezoelectric polarization than that of an AlGaAs/GaAs HEMT. This large polarization results in greater 2DEG density and confinement at the heterointerface than what is experienced in GaAs devices [22]. This occurs because the change (i.e., difference) in polarization at the AlGaN/GaN junction is greater than for AlGaAs/GaAs.

The device is put into active mode with applied electric bias. From there, the band gap difference between GaN and AlGaN, caused mainly by their high conduction band offset, stimulates the transfer of electrons from AlGaN to the adjacent GaN. The transferred electrons are there confined to a very narrow "potential well," or steep canyon, in the heterostructure's conduction band of electrons. There, they can move freely only in the two spatial directions parallel to the heterojunction but not back into the AlGaN. This drastic transfer of electrons leaves the AlGaN layer "depleted," which produces the isolation required between the device gate and body in order for the device to function. Once part of the 2DEG, the electrons move unimpeded by any dopants in the GaN since these dopants are spatially separated from the 2DEG region; thus the mobility of these electrons is enhanced [21].

Although both doping conditions and band offsets in the materials help create 2DEG in a general HEMT device, one key characteristic unique to the AlGaN/GaN type is that the electron concentration in the 2DEG is enhanced by the presence of high polarization. This polarization induces a large positive charge at the AlGaN/GaN heterointerface, which consequently leads the electrons on the AlGaN side to compensate by contributing an additional 2DEG component on the GaN side. The polarization consists of two kinds: spontaneous (i.e., "instant") and piezoelectric [21]. Spontaneous polarization is the polarization that exists in each material when in its individual bulk (i.e., "free") state [23], or at zero strain [5]. Both AlGaN and GaN exhibit spontaneous polarization individually, but that of AlGaN is higher. Piezoelectric polarization is added in as a result of the tensile strain induced in the pseudomorphic (i.e., epitaxial) AlGaN layer from being grown on the relaxed GaN layer. An important quantity for pseudomorphic AlGaN/GaN heterostructures is the critical layer thickness of the AlGaN. If it is not too thick, the result is that its atoms adjust themselves according to the lattice structure of the GaN, creating more densely packed atoms in the AlGaN. After the AlGaN growth is complete, the GaN is relaxed back to its original bulk lattice structure state, but not without a large number of resultant dislocations forming near the heterointerface [21]. At that point in time, the spontaneous and piezoelectric polarizations present are parallel and all act in the same direction [5]. The overall polarization effect is what allows the 2DEG to have such a high electron density even when the AlGaN does not contain dopants [22].

2.3.2 OHMIC CONTACTS

The ohmic contacts (source and drain) and Schottky contact (gate) are made of metallic materials (i.e. non-semiconductors), and most commonly consist of layers. In literature, the specific layering configuration is written in order of deposition (e.g. "x/y/z" means x is the bottom layer and z is the top layer of the overall contact) and the layers are nano-scale (e.g., Ti/Al/Ni/Au (15 nm/50 nm/15 nm/50 nm) [24]). Common ohmic contacts used in research are Ti/Al/Ni/Au [25] and Ti/Al [16]. Gong et al. [26] recently developed a novel Ti/Al-based ohmic contact structure Ti/Al/Ti/Al/Ti/Al/Ti/Al/Ni/Au capable of obtaining both much lower contact resistance and specific contact resistivity than the conventional Ti/Al/Ni/Au structure. Low-resistance ohmic contacts are important for HEMTs, particularly because they carry high power and thus demand both high power conversion efficiency and heat dissipation [27]. Common Schottky contacts used in research are Ni/Au [25], Ni [16], and Pd/Ni/Au [24]. This contact is commonly referred to as a Schottky "barrier" and causes a space-charge region to develop directly beneath it in the AlGaN layer [28]. Additionally, the surface potential of the AlGaN is nearly fixed to the Schottky barrier value, which allows the AlGaN/GaN heterojunction polarization charge to induce a 2DEG in the GaN. Research continues in optimizing both ohmic and Schottky contacts.

2.3.3 GATE LEAKAGE CURRENT

Factors that limit GaN transistor performance are primarily dispersion and gate leakage. The main obstacle to progress has been in controlling the trap densities in the bulk and surface of the material. Since material quality is essential to obtaining a high power device, research is being done in improving the quality of GaN and AlGaN layers. However, surface states are thought to be unavoidable in the material system. Spontaneous and piezoelectric polarization effects lead to charge sheets of opposite polarity at the top and bottom surfaces of AlGaN layer in an AlGaN/GaN heterostructure. Experimentally, it is observed that the output power measured at frequencies of interest

(4-18 GHz) is well below the actual calculated power. This reduction in power is caused by a decrease of maximum drain current which is referred to as current collapse or dispersion. The process of current collapse becomes is dependent upon the supply of electrons to fill up the empty surface states which are observed to come from gate metal. Electric field lines which concentrate at drain side edge of the gate cause charge injection into the surface traps. This reduces field concentration at the drain side of the gate leading to high frequency current dispersion. Dispersion is eliminated with effective surface passivation. Surface passivation prevents the formation of virtual gate on the surface of the device in the gate drain access region. The passivation buries the surface donors and make them inaccessible to electrons leaking from the gate metal.

Figure 2.9 shows a sketch of an AlGaN/GaN HEMT. Both GaN and AlGaN are intrinsically piezoelectric materials. In the context of GaN, its polarizability coupled with mechanical strain can cause degradation of the device. The very high fields which AlGaN/GaN is supposed to withstand, can be produced upon device biasing at the gate edge on the drain side, causing local strain and parametric changes. When high reverse bias voltages are applied to the gate, degradation of electrical characteristics has been observed with increases in gate leakage, worsening of current collapse, increases in drain and source parasitic resistance and decreases in saturated drain current [29]. It involves the presence or generation of defects at gate edges where electric field is high. These defects and strains can couple with local defects to create more distortions at the macroscopic level, ultimately leading to failure.

The built-in lattice mismatch between the AlGaN and GaN results in in-plane tensile stress and stored elastic energy in AlGaN barrier layer at rest. This stress increases with an applied bias during device operation. When this elastic energy exceeds a critical value, defects can be produced, which can behave as electron traps introducing a leakage path between gate and channel through AlGaN barrier layer. Also, due to the filling of electrons in these traps, the electrostatics of the channel is affected reducing the maximum current that flows through the device. This mechanism has been reportedly observed by several researchers. The defects promote the injection of electrons from gate into AlGaN barrier layer through a trap assisted tunneling mechanism as shown in Figure

2.10 [29]. This device failure is attributed to new failure mechanism called the Inverse Piezoelectric Effect in which the dominant feature is a significant increase in gate leakage current [29].

Strain relaxation in AlGaN/GaN HFETs leading to increased gate leakage current due to converse piezoelectric effect was identified using micro Raman spectrum at a wavelength of 532nm [30]. Figure 2.11 shows the increase in gate leakage current with increase in drain bias where most significant shift occurred in the first 5 hours.

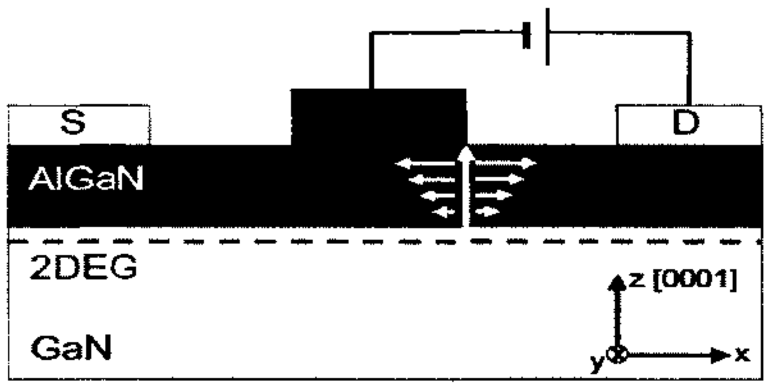


Figure 2.9. Sketch of GaN HEMT under electrical stress. © 2009 Elsevier. Reprinted, with permission, from [29].

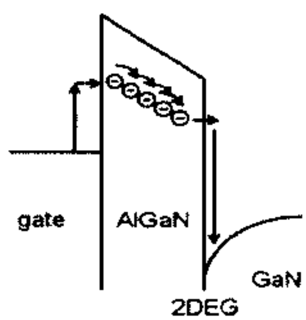


Figure 2.10. Trap assisted tunneling mechanism through AlGaN layer. © 2009 Elsevier. Reprinted, with permission, from [29].

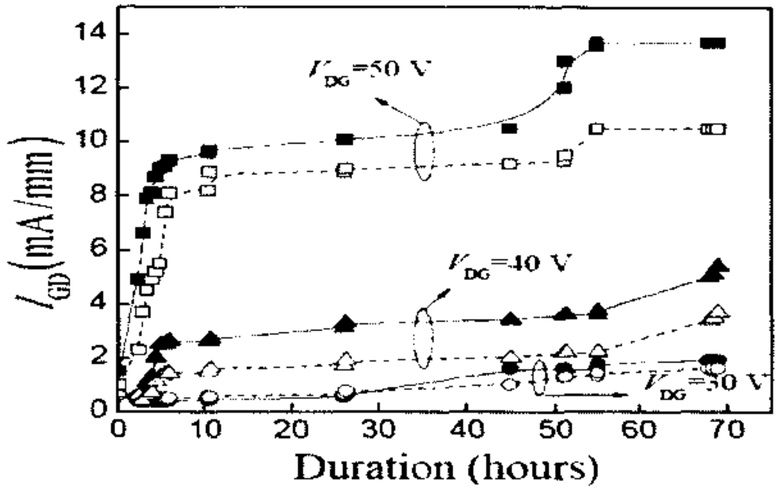


Figure 2.11. Time dependent characteristics of gate leakage current under different gate bias configurations. © 2012 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim. Reprinted, with permission, from [30].

In other studies [31-33], cap layers are commonly used to realize various goals in GaN based devices. It has been proposed that InGaN cap on GaN, or a GaN cap on AlGaN could reduce the resistance of Ohmic contacts. It was also shown that a GaN cap layer can be used to increase the Schottky barrier height of AlGaN/GaN heterostructures by which gate leakage current was significantly reduced. Also, AlN cap layer could act as a good gate insulator and a passivation layer.

2.4 PIEZOELECTRICITY & INVERSE PIEZOELECTRIC EFFECTS

In 1880, Pierre and Jacques Curie discovered that positive and negative charges can be observed on some portions of crystal surface when these crystals were compressed in particular directions. These charges were proportional to the pressure applied. Later, this effect was termed as the Piezoelectric effect, with the prefix "Piezo" meaning "to press". This effect is closely related to Pyroelectric effect in which electric polarity is produced on certain crystals by a change of temperature [34].

The term piezoelectricity can precisely be defined as electric polarization produced in certain crystals that lack inversion symmetry, due to mechanical strain and is directly proportional to the strain. This polarization reverses its sign if the stress is changed from tensile to compressive. This is also called as the direct piezoelectric effect. This effect was observed to be reversible and termed as the converse effect or Inverse Piezoelectric effect, wherein a piezoelectric crystal becomes strained when electrically polarized. Here the amount of strain is proportional to the polarizing field as shown in Figure 2.12. These effects were found in zinc blende, sodium chlorate, boracite, tourmaline, quartz, tartaric acid, and Rochelle salt [34].

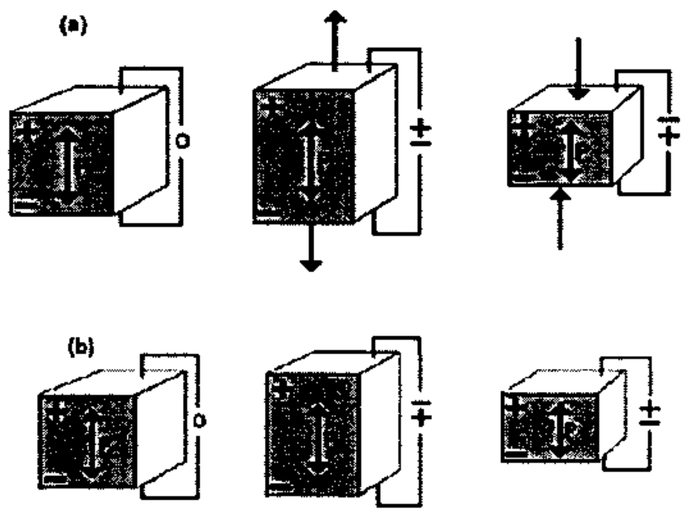


Figure 2.12. Schematic representation of the (a) direct, and (b) Inverse Piezoelectric effects. © 2008 Springer. Reprinted, with permission, from [35].

These effects are observed in crystals belonging to certain classes of materials that lack a center of symmetry. Such materials are called anisotropic. The classification of crystals based on their periodic molecular arrangement, is restricted by geometrical laws to a known finite number. This restriction to a finite number of classifications arises from the variety of atomic arrangements capable of forming crystals having a repetitive arrangement. Based on atomic configuration, different crystals are classified into finite number of space groups which have certain geometrical characteristics in common. Overall, thirty-two (32) crystal classes were formed from these space groups which possess certain symmetry characteristics. If symmetry is with respect to a point, the body is centro-symmetrical and possesses no polar properties. Therefore no piezoelectric crystals are found in centro-symmetrical classes. With one exception (Class 29), all classes devoid of a center of symmetry are piezoelectric. The piezoelectric effect was first used by Curie to measure the charge emitted by radium. Later Langevin used it for exciting quartz plates electrically to serve as high frequency sound wave emitters and receivers under water, thus becoming the originator of the modern science (and art) of ultrasonics [34].

In piezoelectric effect, field E causes a piezoelectric stress X. This stress is linearly related to the driving electric field, i.e., $X = \varepsilon E$, where ε is the piezoelectric stress coefficient. Similarly, strain x causes electric polarization with $P = \varepsilon x$. Stress for a homogeneous solid in equilibrium is defined as force per unit area exerted by the portion of the body on one side of surface element upon the portion on the other side. Its state of deformation is then called the strain. This definition involves tensors. The symmetrical stress tensor that represents a stress system may be resolved into 6 components. Compressions along the 3 coordinate axes, and shearing stresses with respect to 3 planes normal to these axes. The axis nomenclature is as shown in Figure 2.13 below. The six components are designated as X_x, Y_y, Z_z, Y_z, Z_x, and X_y. The first letter indicates the direction of force and the second (subscript) indicates the direction of the normal to the surface on which force acts. Similarly the components of strain are denoted as x_x, y_y, z_z, y_z, z_x and x_y.

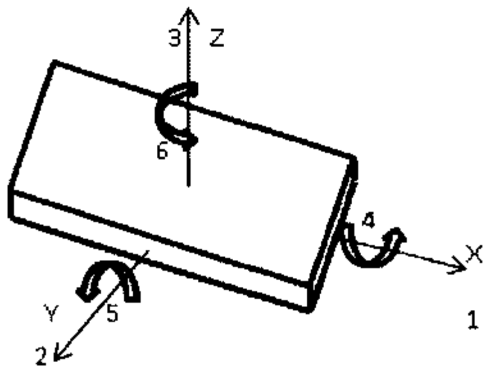


Figure 2. 13. Crystallographic axes.

Since there are six possible components of stress and three of electric polarization, it is evident that there are 18 possible relations between mechanical and electrical states of crystal. These relations are expressed by 18 piezoelectric constants whose values are independent and differ from zero except when the symmetry of the class is such that some of the constants have identical values including zero.

According to Lippmann's reasoning given in [34], when a piezoelectric crystal is placed in an electric field of strength E and at the same time subjected to mechanical stress X, electric polarization P and strain x are induced in the crystal. Assuming the process to be reversible, it can be expressed as:

$$\left(\frac{\partial P}{\partial X}\right)_E = \left(\frac{\partial x}{\partial E}\right)_X \quad . \tag{2.1}$$

This represents a situation where in both the direct and converse effects have the same piezoelectric constants. The fundamental equations for the direct and inverse piezoelectric effects are as given below:

$$P_m = \sum_k^3 \eta''_{km} E_k + \sum_h^6 e_{mh} x_h \quad , \tag{2.2a}$$

and, $$X_h = \sum_i^6 c_{hi}^E x_i - \sum_m^6 e_{mh} E_m \quad . \tag{2.2b}$$

These equations states that the externally applied stress consists of two parts. First which would produce prescribed strain if E=0 and second part which is necessary to hold strain constant when E is applied. From the above equations, the principal equation for direct and inverse effect is given below as:

$$P_x = d_{11}X_x + d_{12}Y_y + d_{13}Z_z + d_{14}Y_z + d_{15}Z_x + d_{16}X_y \quad , \tag{2.3a}$$

$$P_y = d_{21}X_x + d_{22}Y_y + d_{23}Z_z + d_{24}Y_z + d_{25}Z_x + d_{26}X_y \quad , \tag{2.3b}$$

$$P_z = d_{31}X_x + d_{32}Y_y + d_{33}Z_z + d_{34}Y_z + d_{35}Z_x + d_{36}X_y \quad , \tag{2.3c}$$

$$X_x = e_{11}E_x + e_{21}E_y + e_{31}E_z \quad , \tag{2.3d}$$

$$Y_y = e_{12}E_x + e_{22}E_y + e_{32}E_z \quad , \tag{2.3e}$$

$$Z_z = e_{13}E_x + e_{23}E_y + e_{33}E_z \quad , \tag{2.3f}$$

$$Y_z = e_{14}E_x + e_{24}E_y + e_{34}E_z \quad , \tag{2.3g}$$

$$Z_x = e_{15}E_x + e_{25}E_y + e_{35}E_z \quad , \tag{2.3h}$$

and $$X_y = e_{16}E_x + e_{26}E_y + e_{36}E_z \quad , \tag{2.3i}$$

where the *d's* and *e's* are piezoelectric strain coefficients and stress coefficients relating the mechanical stress to electric polarization and electrical stress to strain, respectively, and η'' is the susceptibility. These *d* and *e* coefficients are related by elastic constants as given below:

$$e_{mh} = \sum_i^6 d_{mi} c_{ih}^E \quad . \tag{2.4}$$

In the above equations for the *d* and *e* coefficients, the first letter in the subscript indicates the direction of the field or polarization, and the second letter expresses the type of stress or strain. For a given strain, the associated direction of polarization is always the same, regardless of whether polarization and strain are due to an impressed electrical filed or to mechanical stress. According to piezoelectric effect, all components of piezoelectric tensor should vanish in crystals possessing a center of symmetry [36].

Majority of AlGaN HFETs are grown with the Wurtzite structure. The inverse Piezoelectric effect in HFET can be written using equations described above as [28]:

$$X = c_E S - eE \quad , \tag{2.5}$$

$$\begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & (C_{11}-C_{12})/2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} - \begin{bmatrix} 0 & 0 & e_{31} \\ 0 & 0 & e_{31} \\ 0 & 0 & e_{33} \\ 0 & e_{15} & 0 \\ e_{15} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix}$$

where *X* and *x* are stress and strain tensors, respectively, *E* is electric field vector, c_E is stiffness coefficient tensor at constant field and *e* is piezoelectric coefficient tensor.

Considering the HFET devices made of AlGaN, this material typically has the symmetry of the Wurtzite crystal, and the equations can be written in matrix form as shown above [28].

2.5 RELIABILITY ISSUES – A BRIEF OVERVIEW

Reliability issues such as gate contact degradation through metal diffusion, thermal instability of semiconductors, poor electrical reliability under high-electric-field operation and strain relaxation of material have all been identified, and limit the use of these devices for long term applications [37,38]. Stresses that are developed in materials due to multiple physical phenomena including lattice mismatch, piezoelectric effect, self-heat generation due to electric current, and coefficient of thermal expansion (CTE) mismatch may cause local stress concentration at the interfaces and result in cracks and failures. Local defects such as pit-shaped defects and cracks in the AlGaN layer beside the drain-side edge of the gate may form [19] due to high stress concentration.

Understanding contribution of these physical phenomena in activating the failure mechanisms is the key to diminishing these mechanisms. In particular, understanding the response of the structure to thermo-mechanical stresses that develop in the material due to high temperatures can provide insights in understanding temperature-dependent degradation of the device [39].

Studies conducted by Kisielowski et al. [40] showed that cracks may occur in thin layers of material due to biaxial and hydrostatic residual stresses resulting from both fabrication and the presence of defects. Self-heating has been shown to have a strong effect on the development of mechanical stresses in these devices, as shown in an experimental study by Bykhovski et al. [41]. Over time, relaxation of the strains caused by high temperatures in the device channel (i.e. region of the two-dimensional electron gas) results in degradation in electrical performance of the device and early failure. Use of near-perfect material with low dislocation density helps reduce this effect, but fabrication of such material is still under investigation.

In Sarua et al. [42], two-dimensional (2D) finite element (FE) simulation in conjunction with Raman optical spectroscopy were used to show that a source-drain voltage (Vds) of 40 V applied to AlGaN/GaN HEMTs was found to cause piezoelectric strain, resulting in high compressive stress levels (< -300 MPa) located between the gate and drain, and also underneath the drain contact. The observed strain was found to be directly related to the electric field component normal to the GaN layer.

2.6 FIELD INDUCED DEGRADATION MECHANISMS

Although much progress has been made, GaN HEMTs are not yet reliable as they degrade over time. The understanding of the physics behind failure mechanisms of AlGaN/GaN devices such as HEMTs is increasingly important due to their widespread use. Several questions and issues must be addressed in order to bring the reliability of these devices to a reasonable point. The first and foremost task is perhaps to understand the mechanisms responsible for the root causes of the failure.

The failure mechanisms for AlGaN/GaN HEMTs can be grouped together into three main categories that affect device lifetime: Contact degradation, hot electron effects, and the IPE. Both Schottky and Ohmic contacts have shown excellent stability below 300 °C [43]. Piazza *et al.* [44] have reported an increase in contact resistance and passivation cracking due to Ga out-diffusion and Au inter-diffusion after a 100-hour thermal storage test stress at 340 °C [44]. Nickel based Schottky contacts have been shown to form nickel nitrides on GaN at annealing temperatures as low as 200 °C, resulting in a significant decrease in Schottky barrier height [19]. The observed current collapse and gate lag in AlGaN/GaN HEMTs under high voltage and high current operation have been attributed to hot electrons. These are electrons that have been accelerated in a large electric field, resulting in very high kinetic energy, which can result in trap formation. Creation of traps can occur in both the AlGaN layer and the buffer, leading to reversible degradation of transconductance and saturated drain current [24]. GaN is a piezoelectric material and under high bias conditions, the electric field induces additional tensile stress to the already strained AlGaN layer [25, 26]. Several authors have shown that upon reaching a "critical voltage", irreversible damage to the device occurs resulting in defect formation through which electron leakage can occur [27, 28].

(A) <u>Hot Carrier and Trap Generation</u>: Permanent device degradation after high voltage (drain-to-gate) stress under on-state conditions has been attributed to the presence of hot electrons. In GaAs-based devices, hot electrons generate holes which are accumulated by the gate and result in a negative shift in the threshold voltage V_T [26, 45]. Typically, the gate current is used to derive the field-acceleration laws for failure. Impact ionization, however, is negligible in GaN HEMTs. This is due to the fact that tunneling injection dominates gate current, preventing gate current from being used as an indicator for hot electron degradation [22, 46]. However, these hot electrons likely lead to trap generation at the AlGaN/GaN interface and/or at the passivation GaN cap interface. As in GaAs and InP based HEMTs, traps lead to an increase in the depletion region between the gate and the drain, ultimately resulting in an increase in drain resistance and subsequently a decrease in saturated drain-source current. Comparatively, under reverse bias or so-called "OFF-state" conditions the degradation is greatly reduced due to the reduction of electrons present in the channel. There have been reports that GaN/AlGaN/GaN HEMTs that underwent a 3000-hour "ON-state" stress resulted in an increase in surface traps with an activation energy of about 0.55 eV [12]. On the other hand, devices stressed under "OFF-state" conditions saw a very small increase in traps.

Meneghesso *et al.* employed the use of electroluminescence (EL) to study the effect of hot-carriers and its dependence on stress conditions [46]. Uniform EL emission was observed along the channel for devices stressed at $V_{GS} = 0$ V and $V_{DS} = 20$ V, which is due to hot electrons. However, there is no presence of hot spots or current crowding. On the other hand, under OFF state conditions with $V_{GS} = -6$ V and $V_{DS} = 20$ V (resulting in a $V_{GD} = -26$ V), the EL emission from the channel is not uniform. These hot spots may be due to injection of electrons from the gate into the channel. Due to the high bias conditions, the electrons acquire enough energy to give rise to photon emission.

(B) Contact Degradation: Contact degradation and gate sinks for currents are significant degradation mechanisms at elevated temperatures in GaAs and InP based HEMTs. Contact degradation has not yet proven to be a significant issue with AlGaN/GaN HEMTs at temperatures below 400 °C for Pt/Au Schottky contacts and Ti/Al/Pt/Au annealed Ohmic contacts [47-49]. An increase in Schottky barrier height was observed for Ni/Au Schottky contacts after dc stress at elevated junction temperatures of 200 °C [50, 51]. This was due to a consumption of an interfacial layer between the Schottky contact and the AlGaN layer. Though the resulting positive shift in the Schottky barrier height, and thus the pinch-off voltage, is ideal, the subsequent change in IDSS is not favorable. Unstressed devices were subjected to an anneal after the Schottky contact was deposited in order to decrease the interfacial layer between the gate and semiconductor. Devices that underwent the gate anneal showed 50% less degradation during a 24 hour stress test as opposed to devices that did not receive a gate anneal [22]. Thermal storage tests up to 2000-hour on Ti/Al/Ni/Au ohmic contacts at and above 290 °C showed an increase in contact resistance as well as surface roughness due to growth of Au-rich grains that ultimately led to cracks in passivation [51, 52]. The two primary degradation mechanisms were determined to be Au inter-diffusion within the metal layers and Ga out-diffusion from the semiconductor into the metallic compounds. Similar degradation was observed after dc stress tests that resulted in junction temperatures equivalent to the thermal storage tests. Due to the high power capability of AlGaN/GaN HEMTs, proper temperature management is crucial in order to optimize device performance under high current and high voltage operation [53, 54]. Self-heating of devices can ultimately result in poor device performance through contact degradation. Reliability of contacts is highly dependent upon both metal schemes as well as processing during fabrication.

(C) Inverse Piezoelectric Effects: Several research groups have shown that high reverse bias on the gate results in the generation of defects that provide a path for gate current leakage [55]. This defect formation mechanism is a result of the inverse piezoelectric effect. Due to the fact that GaN and AlGaN are intrinsically piezoelectric materials, the presence of high electric fields will result in an increase in stress within the GaN and AlGaN layers. AlGaN is lattice mismatched to GaN, resulting in significant tensile strain, even in the absence of an electric field. If under electric stress the elastic energy within the AlGaN/GaN layers surpasses a critical value, then the strained layer can relax only through crystallographic defect formation. It is possible that the defects could be electrically active and result in device degradation [55].

J. Joh et al. [56] have established that drain current (ID) and gate current (IG) degradation under high reverse gate bias occurs at a critical voltage, typically above VDG = 20 V [57]. This is also correlated with a sharp rise in both source and drain resistance as well as a positive shift in threshold voltage VT. However, the critical voltage for devices can deviate substantially within one wafer, though adjoining devices appear to exhibit similar performance. The critical voltage corresponds to a threshold field that leads to immediate device degradation if it is exceeded. The degradation exhibits a time dependence at lower fields, being slower the further below critical voltage that the device is biased. The broad distribution of critical voltage observed, ranging from VDG of ~15 V to ~30 V, has been attributed to slow changes within the substrate or epi-layer growth over the wafer [51, 52]. To verify the inverse piezoelectric effect, transmission electron microscopy (TEM) cross sections were studied by Chowdhury et al. [19] after stressing with VDS = 40 V and ID0 = 250 mA/mm at various base-plate temperatures, which corresponded to junction temperatures of 250 °C, 285 °C, and 320 °C based on device modeling [46]. Unstressed devices showed no evidence of pits or cracks near the edge of the Schottky contact. However, all stressed devices showed evidence of pit-like defects on the drain side of the gate. The depth of the pit was about 10 nm, and remained within the AlGaN layer. Crack-like defects were observed in a few of the stressed devices, and appeared to originate at the bottom of the pit defect, extending to the heterointerface of the AlGaN/GaN layer and occasionally into the GaN buffer. As the junction temperature increased, the time after which the crack appeared decreased, developing within 6 hours at a temperature of 320 °C. Gate metal was also observed to diffuse ~2 nm into the defect crack. The formation of the crack was hypothesized to originate in the deepest points in the defect pit and spread along the gate width, thus explaining the presence of cracks in very shallow defect pits [46].

Figures 2.14 and 2.15 show the cross section of AlGaN/GaN layer before and after stress as investigated in [19]. The unstressed device shows no sign of defects with a sharply defined interface between gate metal and semiconductor, but the evidence of various defects can be seen in the stressed devices.

Figure 2.14. Cross sectional HREM image of an unstressed device-source-side edge, middle part and drain side edge of the gate. © 2008 IEEE. Reprinted, with permission, from [19].

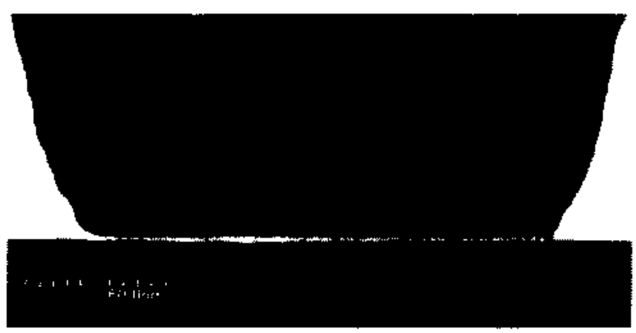


Figure 2.15. Formation of crack and degradation on drain side gate edge of stressed device. © 2008 IEEE. Reprinted, with permission, from [19].

The inverse piezoelectric effect is solely an electric field driven degradation mechanism due to the fact that it is the induced mechanical stress that results in the relaxation of the AlGaN layer. It has also been hypothesized by the del Alamo group [56] that current should not drive this mechanism, except for indirect self-heating that would accelerate degradation of the device. Device design that affects the profile of the electric field on the drain side of the gate will also, in turn, impact the critical voltage.

A pictorial view of the degradation mechanism in GaN based HEMTs is shown in Figure 2.16. Traps are created in the AlGaN layer near to gate edge to the drain side when the device is stressed beyond the critical voltage. Electrons flow from gate to the channel through these traps. In this process, these traps are filled with electrons depleting the sheet charge in the channel degrading the output current and drain resistance [56].

Other issues can lead to additional compressive and tensile strains on the underlying epitaxial layers, including SiN passivation, which is used extensively to minimize surface traps on the AlGaN surface. Typically, SiN has a relatively small magnitude of stress as compared to the tensile strain present in the AlGaN layer due to lattice mismatch. The strain in SiN is highly dependent on processing conditions, *i.e.*, thickness, frequency of the plasma during Plasma Enhanced Chemical Vapor Deposition (PECVD), pressure, and temperature. When deposited on the device, variations and discontinuities can increase the stress fields. For instance, the opening at the edge of the gate metal will result in a force on the AlGaN which will be perpendicular to the gate edge and parallel to the surface of the AlGaN. It was predicted [58] that as the gate length decreases, the magnitude of the strain fields increases. This effect on gate length is of great importance due to the desire to continuously scale down the dimensions of the devices.

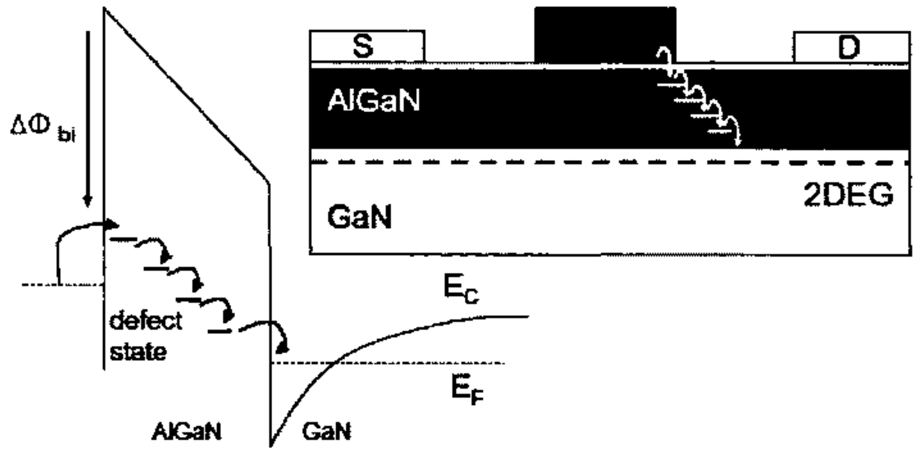


Figure 2.16. A mechanism for IG degradation. © 2010 Elsevier. Reprinted, with permission, from [56].

The physics of GaN devices introduces the possibility for several new failure mechanisms. AlGaN/GaN HEMTs operate at higher drain bias, electric fields, and temperatures with respect to conventional GaAs transistors. Their quality and reliability may be affected by the defectiveness of the AlGaN/GaN epitaxial layers grown on SiC substrate. The piezoelectric nature of GaN introduces potential risks related to the additional strain induced by high electric fields. Figure 2.17 shows a cross section of schematic AlGaN/GaN HEMT showing failure mechanisms.

A.F.M. Anwar *et al.* [59] investigated gate bias dependence of piezoelectric polarization and its implications on GaN based device performance and Figure 2.18 (a) shows variation of the piezoelectric polarization charge density with applied bias. The application of bias greater than threshold induces 2DEG and with increasing 2DEG corresponding the applied gate bias the strain along the c-axis in the AlGaN layer increases as shown in Figure 2.18 (b).

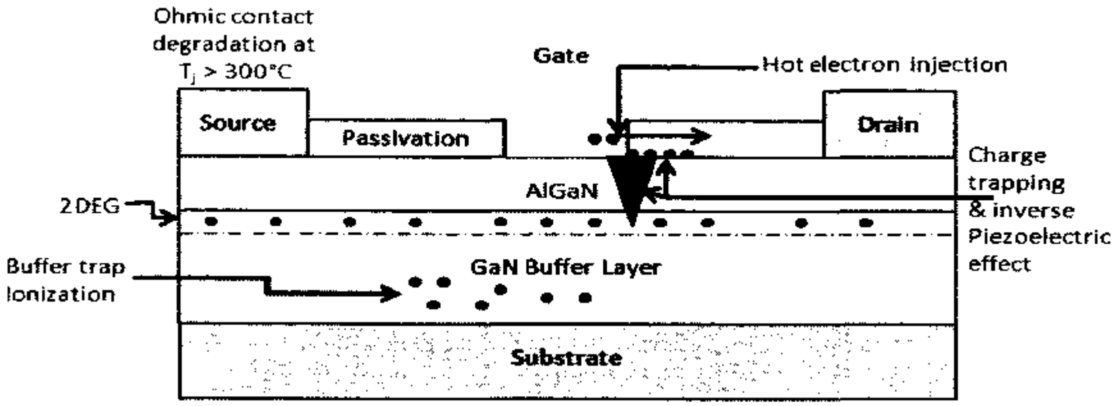


Figure 2.17. Schematic of degradation mechanisms in AlGaN/GaN HEMTs.© 2012 Creative Commons Licence. Reprinted, with, permission, from [58].

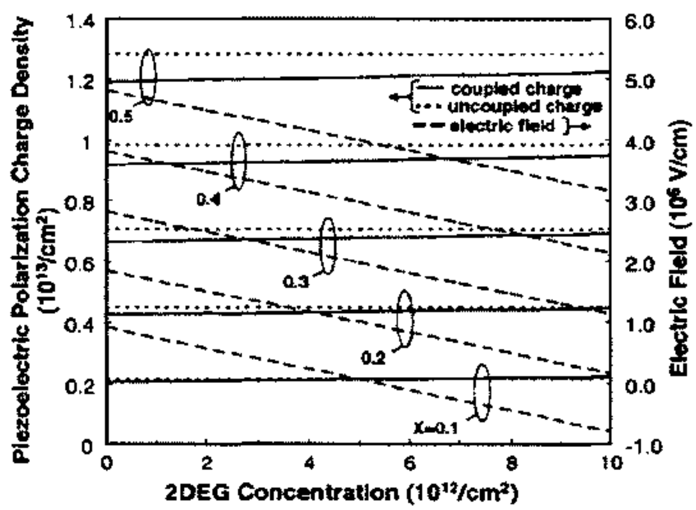


Figure 2.18. (a) Piezoelectric charge component as a function of 2DEG concentration. © 2006 AIP Publishing LLC. Reprinted, with permission, from [59].

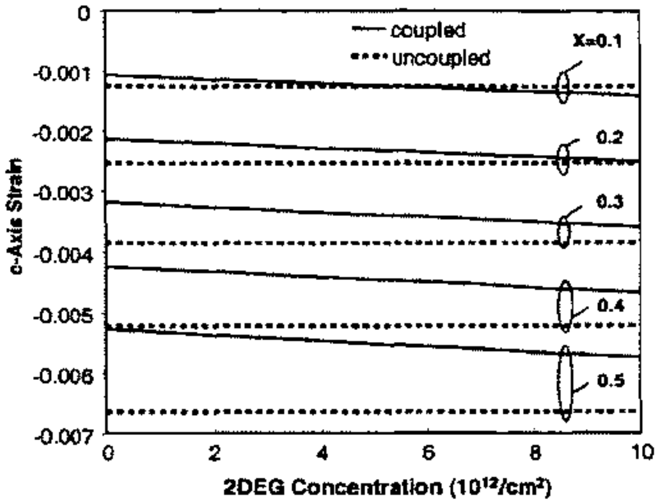


Figure 2.18 (b) Strain in the direction of c-axis as a function of 2DEG concentration. © 2006 AIP Publishing LLC. Reprinted, with permission, from [59].

C. H. Lin *et al.* [60] reported evolution of electronic defects inside AlGaN/GaN HEMT's operating under electric field induced stress measured using depth resolved catholuminescence spectroscopy and Kelvin probe force microscopy. Figure 2.19(a) shows dc-IV and $I_{G\text{-}off}$ before and after an off state stress where $I_{G\text{-}off}$ increases by 2.6 times with V_{DG} above a critical voltage of 28V. Figure 2.19(b) shows increase in near band edge energy upto 7 meV corresponding to a 0.27GPa compressive stress at the edge of the gate on the drain side. These measurements reveal that above a characteristic V_{DG}, field induced stress induces electrically active defects supporting inverse piezoelectric effect model degradation in AlGaN/GaN HEMTs [60].

Attempts to mitigate the field induced stress in the AlGaN has been done by using a thinner barrier layer [59, 61], or AlGaN layer with low Al composition [62, 63], or thorough GaN cap layer [62], or by SiN passivation [64, 65].

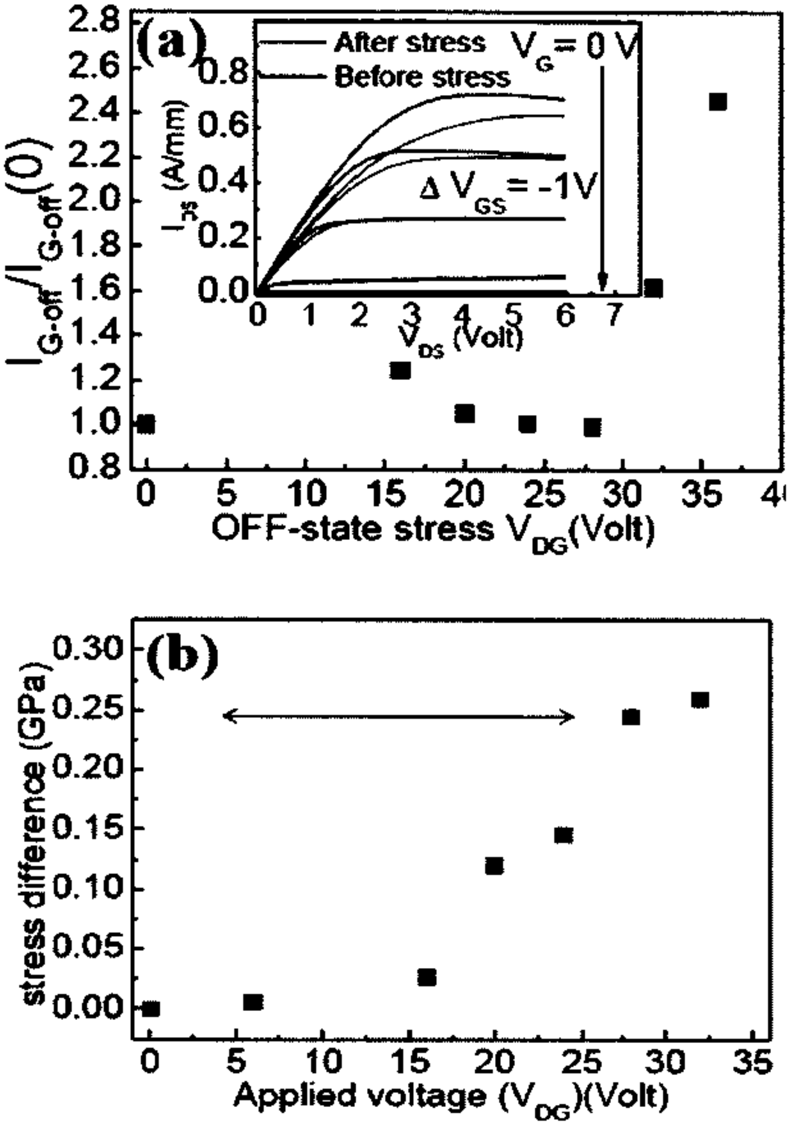


Figure 2.19. (a) DC characteristics and IG-off as a function of off-state stress, (b) External stress caused by applied voltage under off state stress. © 2010 AIP Publishing LLC. Reprinted, with permission, from [60].

The converse piezoelectric effect in AlGaN/GaN HFETs was studied using micro Raman scattering spectroscopy by Balaz *et al.* [66]. Large strains related to the vertical electric field induced by source drain bias were observed. Also, it was analyzed that electric field and piezoelectric strain are more concentrated near the AlGaN/GaN interface for Fe-doped devices whereas in undoped devices, electric field and piezoelectric strain extended into the buffer layer [66].

D. Marcon et al. [64] reported on common failure modes in AlGaN/GaN HEMTs using stress step experiments and showed that critical voltage for increases in gate leakage current depends on step time and formation of crystallographic defects in AlGaN layer. This was in agreement with inverse piezoelectric theory and is the main cause of the permanent output current drop as illustrated in Figure 20 [64].

Increased stability for devices with reduced Al content in AlGaN layer is also shown highlighting the fundamental role of strain on reliability of AlGaN/GaN-based devices. Figure 2.21 shows the relative variation of output current during high power stress on devices with 26% and 30% Al content in the barrier.

Y. Ando et al. [28] investigated inverse piezoelectric effect in AlGaN/GaN HFETs with field plate (FP) electrodes and suggested that FP structure drastically reduces the elastic energy due to inverse piezoelectric effect and minimizes the degradation associated with this effect. Figure 2.22 shows elastic energy density profiles calculated for 3 different device configurations: a rectangular gate device, a single FP device and a dual FP device indicating a significant reduction in elastic energy peak for dual FP device [28].

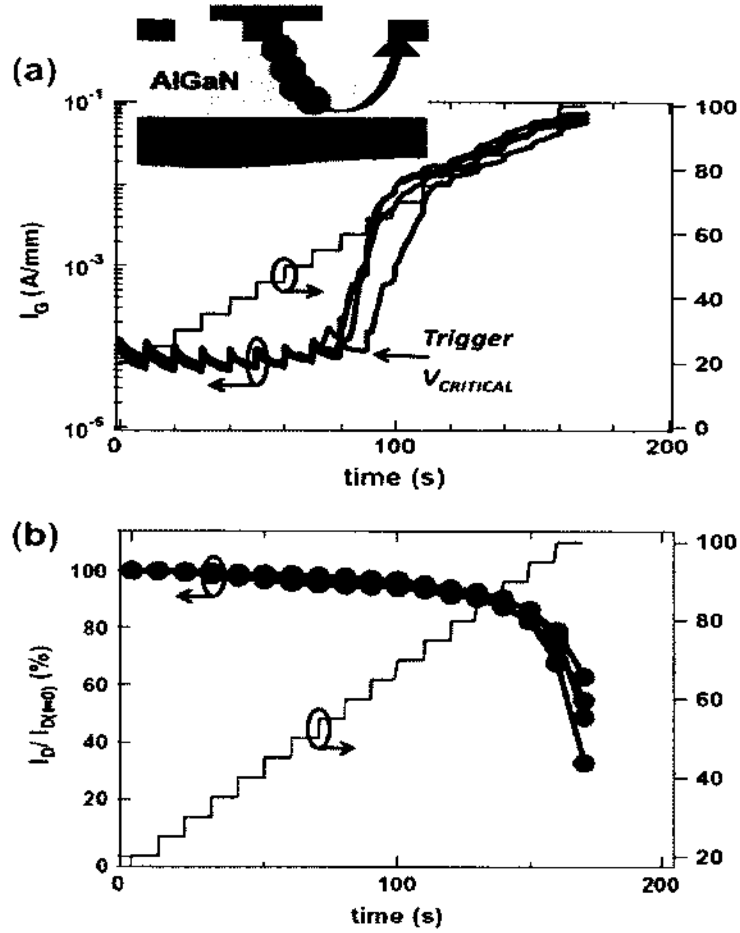


Figure 2.20 (a) Gate leakage current monitored during reverse gate bias step-stress, (b) relative drop of output current after each step. © 2012 Elsevier. Reprinted, with permission, from [64].

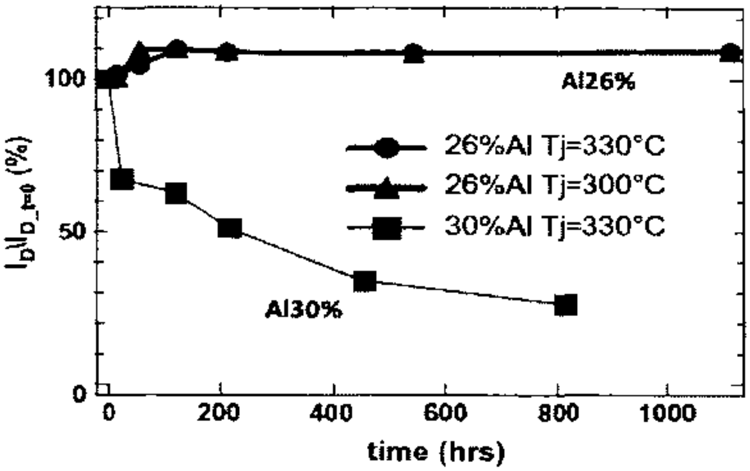


Figure 2.21. Relative variation of output current during high power DC stress © 2012 Elsevier. Reprinted, with permission, from [64].

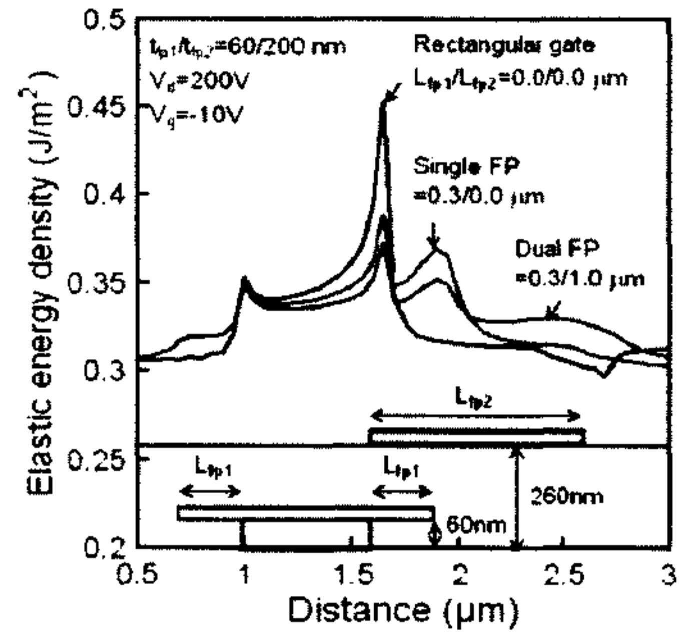


Figure 2.22. Comparison of elastic energy density profiles.© 2012 IEEE. Reprinted, with permission, from [28].

(D) GaN based HEMTs with High k Gate Insulators

GaN has emerged as promising material for high speed, high power device applications. However, AlGaN/GaN HEMTs suffer from high gate leakage current which reduces the reliability and efficiency of the devices. Considerable interest in this issue has initiated the exploration of dielectrics to reduce the gate leakage in the GaN material system. In other works [67-69] high k dielectrics are used as gate insulators to prevent tunneling in AlN/GaN HEMT structures which exceeded 100GHz small signal frequency performance. The commonly used dielectrics are HfO2 and Ta2O5. Next generation networks will need higher power efficiency requiring AlGaN/GaN HEMT to be used at saturation region which will lead to increased forward gate leakage current under large input signal condition creating problems in terms of reliability and amplification characteristics. Improvements for this problem have been suggested in by Kanamura et al. [68] to develop MIS HEMT as shown in Figure 2.23. GaN based MIS HEMTs with high-k materials and very low leakage currents have been reported in [68].

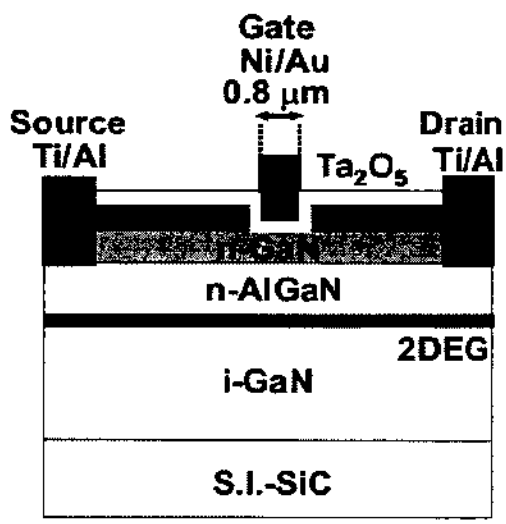


Figure 2.23. Cross section of AlGaN/GaN MIS HEMT. © 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim. Reprinted, with permission, from [68].

2.7 CURRENT COLLAPSE

Current collapse in AlGaN/GaN HEMT has been one of the most exciting topics in recent years. This is basically an observation in which the output power achieved from a device at microwave frequency of interest is considerably smaller than the expected one based on d.c. characterization. This is shown schematically in Figure 2.24. The presence of surface and epitaxy related defects, traps or deep levels in the device structure are responsible for this observation.

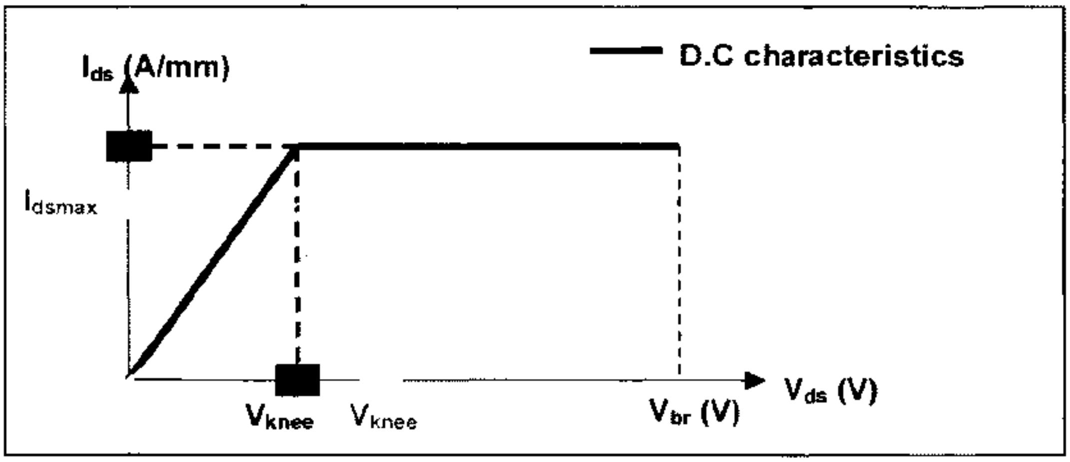


Figure 2.24. Schematic showing the current collapse phenomena. © 2001, IEEE. Reprinted, with permission, from [70].

The charge transfer process in these levels is too slow to follow high frequency signal therefore the electrons get trapped in them [70]. This disturbs the balanced charges in 2DEG and reduces the number of electrons available for current conduction. As a result of which the drain current reduces with an increase in knee voltage, thereby limiting the device power output. Hence this current collapse problem is a major obstacle in boosting up the overall device performance.

Intensive research works and studies have been performed worldwide to analyze and to solve this problem. Wu [71] was the first one to detect the problem of current collapse. Vetury [70] proposed the possible locations of traps, which were responsible for current collapse. He first directly measured the negative surface potential between gate and drain. This suggested the presence of net negative charge on the surface. This negatively charged region therefore acts as a second gate or a virtual gate and limits the drain current conduction in the channel. In the context of current collapse, Ibbeston [72] proposed the theory of surface states as the origin of 2DEG, while Binari [73] presented the current collapse effect attributed to surface and buffer layer trapping. Figure 2.25 shows charge distribution and virtual gate formation due to electrons that leak from the gate at large negative gate voltages.

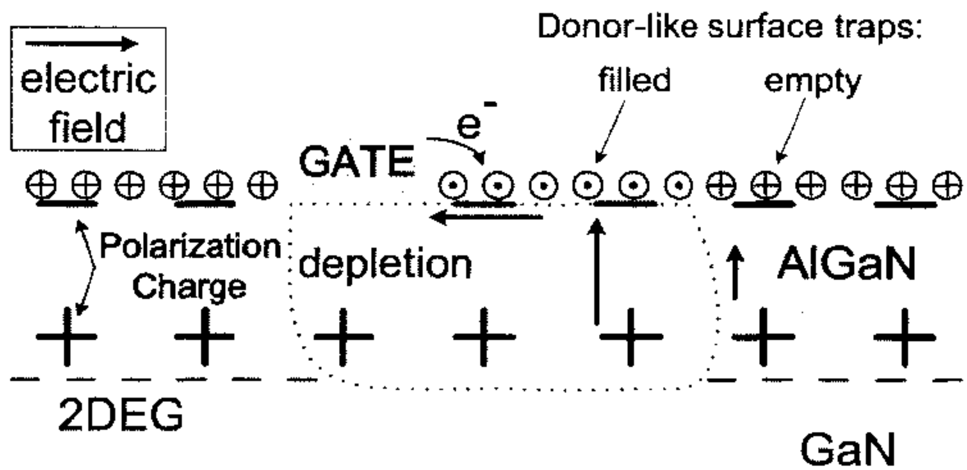


Figure 2.25. Virtual gate formation at large negative Vg. © 2001, IEEE. Reprinted, with permission, from [70].

Gate lag is a significant reduction in the drain current when the gate voltage is changed abruptly. When the gate voltage is suddenly changed (say made negative from a zero value), the electrons beneath the gate are pushed out and these electrons get trapped in surface interface states. Once trapped at the interface sites, they are unable to follow the fast (RF) changes in the gate voltage.

As a result, the surface becomes rich in negative charge and behaves like a virtual gate, which modulates the 2DEG. Hence, the drain current gets reduced as a result of expanded depletion region, and such a gate lag effect can be attributed to surface states.

Drain lag is a combined effect of change in gate bias and drain bias voltages on current response. It is believed that increase in device gate widths probably increase the defect density and hence current collapse percentage. Large area devices are, therefore, needed in order to achieve high power levels.

The difference between current collapse and device degradation due to inverse piezoelectric effect is that current collapse is caused by electrons trapping in existing traps while due to IPE, new traps are created at energy levels that can retain the trapped charges. Passivation has been largely used to suppress current collapse. But, device degradation due to inverse piezoelectric effect is still a challenge in GaN technology and requires careful analyses and the understanding of failure mechanisms [74].

CHAPTER 3

METHODOLOGY

3.1 INTRODUCTION

This chapter covers methodology and steps undertaken to investigate the inverse piezoelectric effect in High Electron Mobility Transistors (HEMT). Inverse piezoelectric effect causes irreversible degradation in HEMTs due to the formation of defects induced by excessive mechanical stress. To improve the electrical reliability of these HEMTs, this degradation process has been modeled in this chapter.

Section 3.2 details the HEMT structure used to understand the degradation process and includes the calculation of different parameters such as stress, strain and elastic energy density that lead to computation of optimal parameters to reduce device degradation. Section 3.3 introduces COMSOL Multi physics software used for electrostatics simulation of the HEMT model. Impact of high-k layers on 2DEG and on the improvement of device reliability are studied in section 3.4.

3.2 HIGH ELECTRON MOBILITY TRANSISTOR (HEMT) STRUCTURE

Figure 3.1 shows the AlGaN/GaN HEMT model used for the calculations [29]. The device operation has been discussed in chapter 2. The objective of this section is to outline the calculations for sheet carrier concentration, stress, strain and elastic energy density in AlGaN/GaN HFET structures. Appropriate equations and formulas are provided.

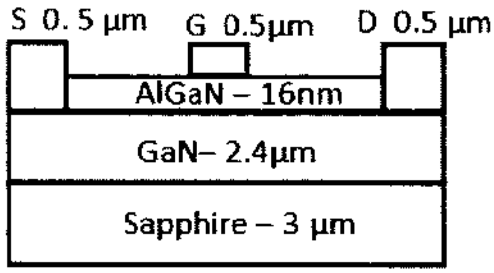


Figure 3.1. HEMT structure.

3.2.1 CALCULATION OF SHEET CARRIER CONCENTRATION

The sheet carrier concentration (n_s) at AlGaN/GaN interface can be calculated using the following equation outlined by Ambacher [75], and is given as:

$$n_s(x) = \frac{\sigma(x)}{q} - \left(\frac{\epsilon_0\epsilon(x)}{dq^2}\right)[q\varphi_b(x) + E_F(x) - \Delta E_c(x)], \quad (3.1a)$$

$$\text{where } \sigma(x) = \left|\frac{2(a(0)-a(x))}{a(x)}\left\{e_{31}(x) - \frac{e33(x)C13(x)}{C33(x)}\right\} + P_{sp}(x) - P_{sp}(0)\right|, \quad (3.1b)$$

$$E_F(x) = E_o(x) + (\pi\hbar^2/m^*(x)) * n_s(x), \quad (3.1c)$$

$$E_0(x) = \left\{\frac{9\pi\hbar^2 q^2}{8\epsilon_0\epsilon\sqrt{8m^*(x)}} n_s(x)\right\}^{\frac{2}{3}}. \quad (3.1d)$$

Also, in the above, x denotes Al content, $q\varphi_b$ denotes the Schottky barrier height, d is the AlGaN layer thickness, a(0) and a(x) are lattice constants, σ represents polarization induced sheet charge density, e_{31} and e_{33} are piezoelectric constants, C_{13} and C_{33} are elastic constants, E_F is the fermi level with respect to GaN conduction band edge energy, ΔE_c is the conduction band offset at AlGaN/GaN interface, P_{sp} denotes spontaneous polarization, q is electron charge and $\mathcal{E}$ denotes dielectric constant. In the above, the sheet charge is determined by the polarization consisting of both the piezoelectric (PZ) and spontaneous polarization (SP) components.

Ambacher [75] found that the dominant factor for the sheet carrier concentration was the total polarization induced sheet charge which can be controlled by the alloy composition (i.e., the Al mole fraction) of the barrier. The sheet carrier concentration is directly related to the thickness of the Schottky barrier and inversely proportional to the height of the barrier.

Also, a number of useful physical properties such as the dielectric constant $\varepsilon(x)$, the Schottky barrier height $q\varphi_b(x)$, the conduction band offset $\Delta E_c(x)$ and band gap $E_g(x)$, the lattice constant $a(x)$, and the piezoelectric coefficients $C_{13}(x)$, $C_{33}(x)$, $e_{ij}(x)$, can be calculated as a function of the mole fraction (x) of Al in the AlGaN layer (i.e., in $Al_xGa_{1-x}N$). The specific equations connecting the mole fraction x are:

$$\varepsilon(x) = -0.3\,x + 10.4, \tag{3.2a}$$

$$\varphi_b(x) = (1.3\,x + 0.84)\ eV, \tag{3.2b}$$

$$\Delta E_c(x) = 0.7\,|\,E_g(x) - E_g(0)|, \tag{3.2c}$$

$$E_g(x) = [6.13\,x + 3.42\,(1-x) - x\,(1-x)]\ eV, \tag{3.2d}$$

$$\varepsilon(x) = -0.3\,x + 10.4, \tag{3.2e}$$

$$C_{13}(x) = (5x + 103)\ GPa, \tag{3.2f}$$

$$C_{33}(x) = (-32x + 405)\ GPa\ , \tag{3.2g}$$

$$e_{ij}(x) = [e_{ij}(AlN) - e_{ij}(GaN)]\,x + e_{ij}(GaN), \tag{3.2h}$$

$$P_{SP}(x) = (-0.052x - 0.029)\ C/m^2, \tag{3.2i}$$

$$a(x) = (-0.077\,x + 3.189)\,Å, \tag{3.2j}$$

where the unstrained value of the lattice constant for GaN is 3.189 Angstroms. Also, the piezoelectric coefficients for AlN and GaN were taken from [75] and were set to: e_{31} = -0.6 and e_{33} = 1.46 for AlN, and e_{31} = -0.49 and e_{33} = 0.73 for GaN.

Given these formulas for PZ and SP, the induced charge density ρ_P can be calculated as: $\rho_P = -\nabla P$. Ambacher [75] showed the Fermi level (E_F) to be dependent on the Al mole fraction of the AlGaN layer. Based on their data for the sheet carrier concentration versus Al mole fraction, the following relation can be obtained: $E_F(x)$ = -0.102967 + 2.1917x - 7x^6.

The above set of equations (3.1a-3.1d) is solved self consistently to obtain an n_s value. The procedure stars by assuming a small E_F (0.005eV) to obtain n_s based on equation 3.1(a). Using this n_s value, equations 3.1 (c) and (d) are solved for E_f and E_0. These values are then substituted back into equation 3.1(a) to obtain n_s values. These steps are repeated until there is negligible change in n_s value. Parameters used for these calculations are given in Table 3.1. For these parameters, the value of n_s was obtained as 1.5x10^{17} m^{-2} at zero bias. This n_s value can be used as the initial value of 2D charge density uniformly distributed along AlGaN/GaN interface and the self-consistent algorithm is implemented to calculate the n_s value after applying bias. Here, electric field values midway between discrete grid points are calculated across the channel layer using the COMSOL Multiphysics software. Corresponding drift velocity at these midway points can then be calculated for the corresponding electric fields using the equation given below:

$$v(x) = \frac{\left\{\mu_0 E(x) + v_s * \left[\frac{E(x)}{E_1}\right]^5\right\}}{\left\{1 + \left[\frac{E(x)}{E_0}\right]^5\right\}} \quad , \qquad (3.3a)$$

where $v(x)$ represents drift velocity values at grid points and v_s is the saturation velocity (2.1x10^7 cm/s). The other constant values used are μ_0= 260 cm^2/V s, E_0 = 15.9x10^4 V/cm, E_1= 17.2x10^4 V/cm [76]. Using these drift velocity values, flux at right ($F_{i+1/2}$) and left side($F_{i-\frac{1}{2}}$) of grid points is calculated as:

$$F_{i-\frac{1}{2}} = -\left[\frac{n_{i-1}+n_i}{2}\right] * v_{i-\frac{1}{2}} + D_n * \left[\frac{n_{i-1}-n_i}{\Delta x}\right] \quad , \qquad (3.3b)$$

$$F_{i+1/2} = -[(n_{i+1} + n_i)/2] * v_{i+1/2} + D_n * [(n_i - n_{i+1})/\Delta x], \tag{3.3c}$$

$$\frac{\left[F_{i-\frac{1}{2}} - F_{i+\frac{1}{2}}\right]\Delta t}{\Delta x} = \Delta n_i , \tag{3.3d}$$

where Δn_i is the calculated change in n_s value at i^{th} grid point and Δt is a fixed time step equal to $(\Delta x/10^6)\ s$ and D_n is diffusion constant equal to $5\text{x}10^{-3}$ m^2/s for GaN. The n_s values can be updated along the grid points as:

$$n_i(t + \Delta t) = n_i(t) + \Delta n_i, \quad i=2...N-1. , \tag{3.3e}$$

where N represents total number of grid points. The n_s values at the first and last grid points are calculated using the average flux ($\bar{F}$) value as:

$$\bar{F} = \frac{\sum_{i=2}^{N} F_{i=\frac{1}{2}}}{N} - 1 , \tag{3.4a}$$

$$n_1(t + \Delta t) = n_1(t) + \Delta n_1 , \tag{3.4b}$$

$$n_N(t + \Delta t) = n_N(t) + \Delta n_N , \tag{3.4c}$$

$$\Delta n_1 = \frac{(\bar{F} - F_{1.5})\Delta t}{\Delta x} , \tag{3.4d}$$

$$\text{and, } \Delta n_N = \frac{\left(F_{N-\frac{1}{2}} - \bar{F}\right)\Delta t}{\Delta x} , \tag{3.4e}$$

Table 3.1: Parameters used for the AlGaN-GaN HEMT simulations [29, 77].

Parameter	**Value**
x (Al fraction)	0.26, 0.28, 0.3
a (lattice constant)	$3.189e^{-10}$(GaN), $3.112e^{-10}$(GaN),
ε_0 (permittivity of free space)	$8.85\text{x}10^{-12}$ F/m
ε (dielectric constant)	9.5 (GaN), 9.0 (AlN)
$\hbar$ (Planck's constant)	$6.5\text{x}10^{-16}$ eVs
m^* (Effective mass)	$0.22\text{x}10^{-31}$ Kg
e_{31} (piezoelectric constant)	-0.49C/m^2 (GaN), -0.6C/m^2(AlN)
e_{33} (piezoelectric constant)	0.73 C/m^2 (GaN), 1.46 C/m^2 (AlN)
C_{33} (elastic constant)	405 Gpa (GaN), 373 Gpa (AlN)
C_{11} (elastic constant)	350 Gpa
C_{12} (elastic constant)	110 GPa
C_{13} (elastic constant)	103Gpa (GaN), 108 Gpa (AlN)
ρ (Density)	6095 (GaN), 3965 (Substrate) kg/m^3
K (Thermal Conductivity)	160 (GaN), 49 (substrate) W/ m K
C_p (Heat capacity at constant pressure)	410 (GaN), 730 (Substrate) J/ kg K
α_a(In-Plane thermal expansion coefficient)	48 x 10^{-7} (GaN) K^{-1}
α_c(Out of Plane thermal expansion coefficient)	43 x 10^{-7} (GaN) K^{-1}

This process is repeated until the changes in n_s values are negligible. The following convergence condition is used here in this research:

$$|n_i(t+\Delta t) - n_i(t)| / (|n_i(t+\Delta t) + n_i(t)|/2) < 10^{-4} \ . \qquad (3.4f)$$

3.2.2 STRESS, STRAIN AND ELASTIC ENERGY DENSITY

First order calculations of stress, strain and elastic energy density along the channel in AlGaN barrier layer are modeled to understand the electrical degradation of the device due to inverse piezoelectric effect. Here, the vertical direction is direction normal to the interface and is called z direction. The channel direction is along x axis. The planar strain in AlGaN barrier is set by thick GaN buffer layer. The equations for stress, strain and elastic energy density are given as:

Planar Strain: $S_{10} = (a_{GaN} - a_{AlGaN}) / a_{AlGaN}$, (3.5a)

Vertical Strain: $S_3 = -\frac{2C_{13}}{C_{33}} S_{10} + \left(\frac{e_{33}}{C_{33}}\right) E_z$, (3.5b)

Vertical (Normal) Stress:

$$T_1 = \left(C_{11} + C_{12} - \frac{2C_{13}^2}{C_{33}}\right) S_{10} + \left(\frac{C_{13}e_{33}}{C_{33}} - e_{31}\right) E_z \ , \qquad (3.5c)$$

Elastic Energy Density : $W = \frac{C_{33}}{C_{11}C_{33} - 2C_{13}^2 + C_{12}C_{33}} * T_1^2$, (3.5d)

where E_z is the electric field in vertical (normal to interface) direction. Parameters used for the GaN layer in the present calculations are given in Table 3.1.

3.3 THE COMSOL SOFTWARE TOOL – FEATURES AND IMPLEMENTATION

3.3.1 ELECTRICAL MODELING

The two-dimensional (2D) electrostatics of the HEMT model were computed using software called COMSOL Multiphysics. This is a general purpose Finite Element application software tool. It contains a graphical user interface which has full CAD, meshing and post processing capabilities. This software includes different application modes. Electrostatics application mode was used for this model. This mode gives electric field and electric potential distribution across the device. The governing equation is:

$$-\nabla.\epsilon(\nabla V) = \rho \ , \tag{3.6}$$

where ρ is the space charge density. COMSOL is useful for various physics and engineering applications, especially coupled multi-physics phenomena. COMSOL Multiphysics also offers an extensive interface to the MATLAB application, and its toolboxes for a large variety of programming, preprocessing and post-processing capabilities. The packages are supported across a variety of platforms such as Windows, Mac, and Linux. In addition to conventional physics-based user interfaces, COMSOL Multiphysics also allows for entering coupled systems of partial differential equations (PDEs). The PDEs can be entered directly into the COMSOL software tool. In two-dimensional (2D), finite element (FE) modeling, it is required for the user to define whether a state of planar strain or planar stress is being assumed to represent true 3D geometry. It is very common in literature to see 2D illustrations of HEMT devices, because their geometry as well as the profiles of electron flow, do not change as it extends into the third dimension (i.e., into the page). Add to that the fact that this third dimension of the HEMT device is commonly a factor or two larger than the other two modeled dimensions, a plane strain assumption for a 2D model then is often quite logical.

The simulated AlGaN/GaN HEMT model is shown in Figure 3.1 and is based on the device defined by Joh *et al.* [29]. Geometry as well as material properties were taken from literature as relevant and appropriate. The material properties required to run this model are given in Table 3.1.

The boundary conditions used for calculations are as given below:

- Zero charge ($n.D = 0$ where D is electric displacement, and n the unit normal) condition is used for all the exterior boundaries.
- Charge conservation ($n.(D_1 - D_2) = 0$) used for interior boundaries with zero surface charge.
- Interface charge density ($n.(D_1 - D_2) = \rho$) set at the AlGaN/GaN interface with $\rho = \sigma - ns * q$ where σ represents the spontaneous and piezoelectric polarization charge density and n_s represents sheet carrier concentration and q is the electron charge.
- Ground (i.e., $V=0$ Volts) applied for the Source contact.
- Electric potentials V_G and V_D (Volts) for Gate and Drain contacts, respectively.

This finite element COMSOL Multiphysics model has also been used to determine the stress/strain behavior of select HEMT device structures, in keeping with the experimental reports in the literature. The focus of the overall approach to this research will be to emphasize the electro-mechanical issues in the HEMT device, while making some simplifying assumptions, in order to understand the device stress/strain mechanics. In reality, the 2DEG region of an HEMT device has a highly complex quantum nature [78]. However, due to this thesis's mechanical approach of identifying stress/strain present in an active HEMT device, it is important to specify that the 2DEG will be represented at the AlGaN/GaN heterointerface using a surface charge density resulting from polarization present in the GaN and AlGaN materials as a boundary condition. In addition, for any thermal calculations, a heat source value (i.e. power dissipation) needs to be included. Other crucial boundary conditions applied in the 2D model will be voltage levels applied to source, drain, and gate terminals, as well as the surface charge density resulting from polarization at the 2DEG location. The 2D model could also be coupled to a thermal model to include effects of heating and thermal expansion.

It is important to mention that the external source, drain, and gate voltages were not applied at the top of the contacts, but rather at their base (i.e., at their interface with the underlying AlGaN layer). This effectively assumes that the voltage drop across the contact regions is negligible due to the high doping levels. Additionally, a gradual transition of voltage within the source-gate and gate-drain regions along the top AlGaN edge was introduced. This was done by applying a boundary condition in those two regions which resulted in a linear transition of potential. The above numerical step was implemented to overcome the possible issue of adverse voltage spikes in the device at the boundary edges.

For completeness, a discussion on the COMSOL implementation of meshes and numerical grids is briefly given next. The numerical meshing available in COMSOL include the Lagrange 1st-order through the 5th-order techniques, where each progressively higher order requires greater memory storage but smoother derivatives. The discretization includes free triangular/quadrilateral/mapped meshing on two-dimensional (2D) boundaries, and free tetrahedral meshing in three-dimensional (3D) domains. The most important factor in the choice for mesh generation depends on the accuracy of the solution in critical areas (e.g., areas of high gradients, or large temperature or voltage variations. In the COMSOL FE modeling, once these critical areas are identified, the mesh can be refined in these areas until convergence is achieved. While one can attempt to manually refine the mesh in the critical areas, COMSOL offers a feature called "Adaptive Mesh Refinement." Using this feature, an initial solution is found for the quantities of interest (e.g., voltage, carrier density, temperature etc) based on the initial mesh defined by the user. The software then identifies the areas of greatest gradient (i.e., critical areas), refines the mesh in those regions, and then proceeds to solve the model once again. This process undergoes a user-defined number of iterations until proper convergence of the quantities of interest in the critical areas is achieved. One drawback to this feature, however, is that it does not support 2D quadrilateral meshes, nor does it support 3D hexahedral (i.e., "brick") or prism meshes[77]. In this thesis, a 2D triangular mesh with manual refinement is used here as shown in Figure 3.2.

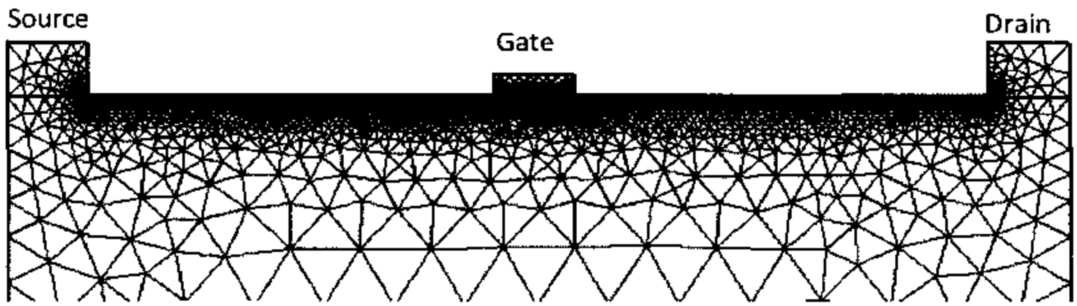


Figure 3.2. AlGaN/GaN HEMT Structure showing mesh elements. The maximum mesh element size was set to 0.2μm and minimum element size in AlGaN region was set to 0.002 μm.

3.3.2 THERMAL MODELING

Current carried by the HEMT in 2DEG layer at the GaN-AlGaN interface gives rise to dissipation and Joule heating, that provides a distributed source term for temperature increases and thermal effects. Such temperature increases result in thermal expansion which can create strain and thus thermo-mechanical stress, within the device. Such temperature changes due to device operation can be analyzed by the COMSOL tool, using its Heat Transfer module. This application mode gives the user the option to incorporate conduction, convection, and/or radiation under steady-state (i.e. stationary) or transient (i.e. time-dependent) conditions. The governing equation is, upon neglecting viscous heating and pressure-work terms:

$$\rho\, C_p \frac{\delta T}{\delta t} - \nabla.(\mathrm{k}\nabla T) = Q - \rho\, C_p\, \boldsymbol{u}.\nabla T \quad , \tag{3.7a}$$

where k is the thermal conductivity (W $m^{-1}\cdot K^{-1}$), ρ is the mass density (kg m^{-1}), C_p is the specific heat capacity at constant pressure (J Kg^{-1} K^{-1}), T is the absolute temperature (K), Q the heat source term (W m^{-3}), and $\boldsymbol{u}$ the velocity vector. If both radiation and convection effects are excluded, equation (7a) simplifies to:

$$\rho\, C_p \frac{\delta T}{\delta t} - \nabla.(\mathrm{k}\nabla T) = Q \ , \tag{3.7b}$$

The main task in this thermal modeling aspect is to obtain an FE solution of the temperature distribution in the device and quantify the 2DEG channel temperature.

All thermal boundary conditions were assigned similar to the boundary conditions discussed in an FE model by Menozzi et al. [79]. The bottom substrate surface has been maintained here at a constant 300 K (i.e., isothermal room-temperature condition). The top GaN surface and the remaining exterior model boundaries were considered adiabatic (i.e., insulated). The most crucial boundary condition applied in the thermal model is that of the power dissipation value applied to the active device area (i.e., the AlGaN/GaN interface). This is taken to be E*J (W/m^2), with E being the Electric field values across the interface, and J the channel current density calculated as ns*q*υ where ns is sheet carrier concentration, q is electron charge and υ is the drift velocity. These values are calculated as described in sections 3.2. Electric field values are obtained from COMSOL. This E*J value represents the power dissipation value across the AlGaN/GaN interface. This value is applied as the heat source on the 2D GaN surface of a 3D thermal model as shown in Figure 3.3. Parameters used for thermal modeling are given in Table 3.1.

3.4 IMPACT OF HIGH-*K* LAYER

A thin insulating layer above AlGaN barrier layer (used as a capping layer) can possibly influence the transport properties of 2DEG in AlGaN/GaN heterostructures. With increasing degree of relaxation of the AlGaN barrier layer, electron mobility is observed to decrease [80, 81]. AlN or GaN have been used as cap layers which lead to decrease in 2DEG density due to the additional negative polarization charges formed at the interface. Variation of strain state of AlGaN barrier layer is studied with different kinds of thin cap layers. Since, HEMTs are used for high power applications, under large input signal condition gate leakage current increases. To improve reliability, high-k dielectric layers were used as insulator between gate and semiconductor. Very low leakage currents were reported for GaN MIS HEMT with high-k layer [82]. Figure 3.4 shows the AlGaN/GaN model used to study the impact of high-k layer [80-82].

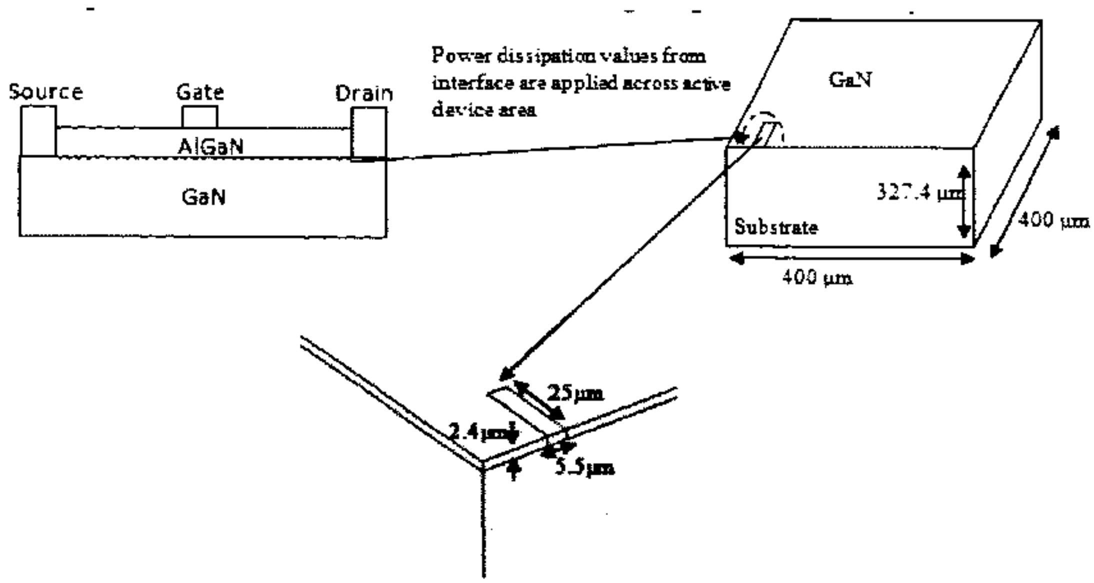


Figure 3.3. Schematic of thermal model.

The calculation of 2DEG density (n_s) at the interface for AlGaN/GaN model with the inclusion of a high-*k* cap layer is given as [81]:

$$n_s(x) = \left\{\frac{\sigma(x)}{q} - \left(\frac{\epsilon_0 \epsilon_{AlGaN}(x) \epsilon_{high-k}}{(\epsilon_{high-k} d_{AlGaN} + \epsilon_{AlGaN}(x) d_{high-k}) q^2}\right) [q\varphi_b(x) + E_F(x) - \Delta E_c(x)]\right\}, \quad (3.8)$$

where σ is the spontaneous and piezoelectric polarization charge density, ϵ_0 is vacuum permittivity, ϵ_{AlGaN} is relative permittivity of AlGaN, $q\varphi_b$ is the metal/GaN schottky barrier height, E_F is the Fermi level, ΔE_c is conduction band offset at AlGaN/GaN interface and d_{GaN}, and d_{high-k} are insulating layer and AlGaN barrier layer thickness, respectively. The equation for n_s is solved self consistently similar to the case as AlGaN/GaN without cap layer described in section 3.2. The value of n_s was observed to increase with the addition of a high-*k* layer.

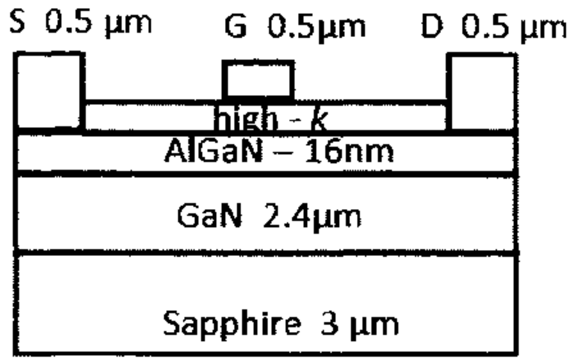


Figure 3.4. HEMT structure with cap or high k layer.

3.5 THERMAL STRAIN MODELING

Heating within the HEMT device can lead to internal stresses as the various materials (e.g., GaN and AlGaN) have different coefficients of expansion. Calculation of such stresses is then a coupled linear elastic thermal-mechanical problem which can be solved using COMSOL. The total strain ε will in general be comprised of three components, namely the elastic strain (ε_{el}), the thermal strain (ε_{th}), and the residual strain (ε_0). Thus: $\varepsilon_e = \varepsilon_{el} + \varepsilon_{th} + \varepsilon_0$. Of these, the thermal strain is determined by the thermal expansion coefficient α, and given by [83]:

$$\varepsilon_{th} = \alpha \, \Delta T \ , \tag{3.9}$$

where ΔT is the change in temperature from the equilibrium ambient value. The paramaters used are given in Table 3.1. In the present research work, temperature dependent dynamic changes to the material parameters (such as the mobility) were ignored. Hence, the calculations were not self-consistent, and could be improved by incorporating an iterative scheme that first computes temperature changes, which are then fed into updating material parameters, and these in turn used to re-evaluate the temperature changes in a self-consistent manner.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 INTRODUCTION

Modeling and quantitative evaluations of the inverse piezoelectric effect in AlGaN/GaN HEMT structures described in section 3.2 were carried out using COMSOL and MATLAB software tools. For the purpose of demonstration, polarization charge densities and sheet carrier concentrations for various Al contents and AlGaN thickness as described in Chapter 3 were determined. The goal was to evaluate the role and significance of both the Al content and AlGaN thickness of the internal electric fields that influence the degradation process due to the inverse piezoelectric effect. Later in this chapter, the effects of a high-*k* layer on the AlGaN layer are discussed. For completeness, the influence of 2DEG channel temperature on strain in AlGaN layer has also been probed and studied through numerical simulations. In general, our model simulations were implemented with an aim to obtain quantitative analysis and to investigate the optimal parameter set that might reduce the degradation and failures due to the inverse piezoelectric effect in AlGaN/GaN HEMTs.

4.1.1 MODEL VALIDATION

The model used in our simulation was taken from the report by Joh et al. [29], and the validation of our simulation and its implementation for the HEMT model was carried out by comparing our results with the values reported by Joh et al. [29].

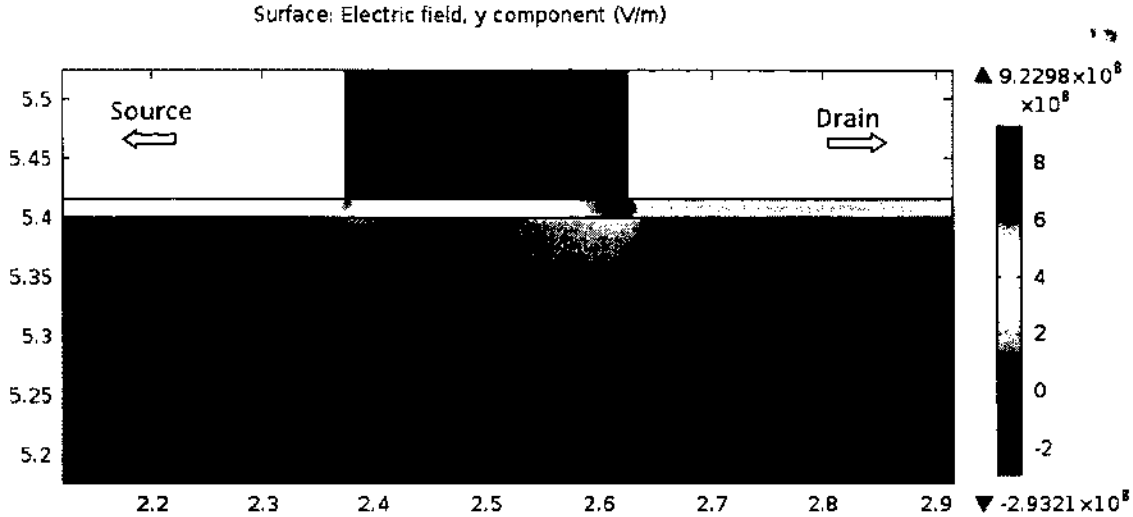


Figure 4.1 (a). Vertical electric field profile in AlGaN/GaN HEMT with Vd=33V and Vg=-5V.

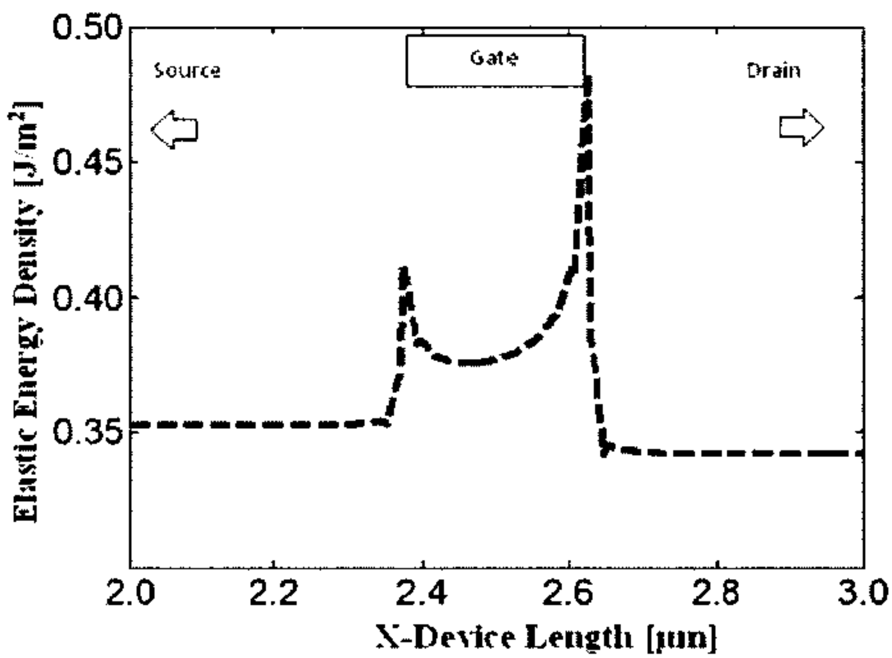


Figure 4.1 (b). Elastic energy density in AlGaN layers.

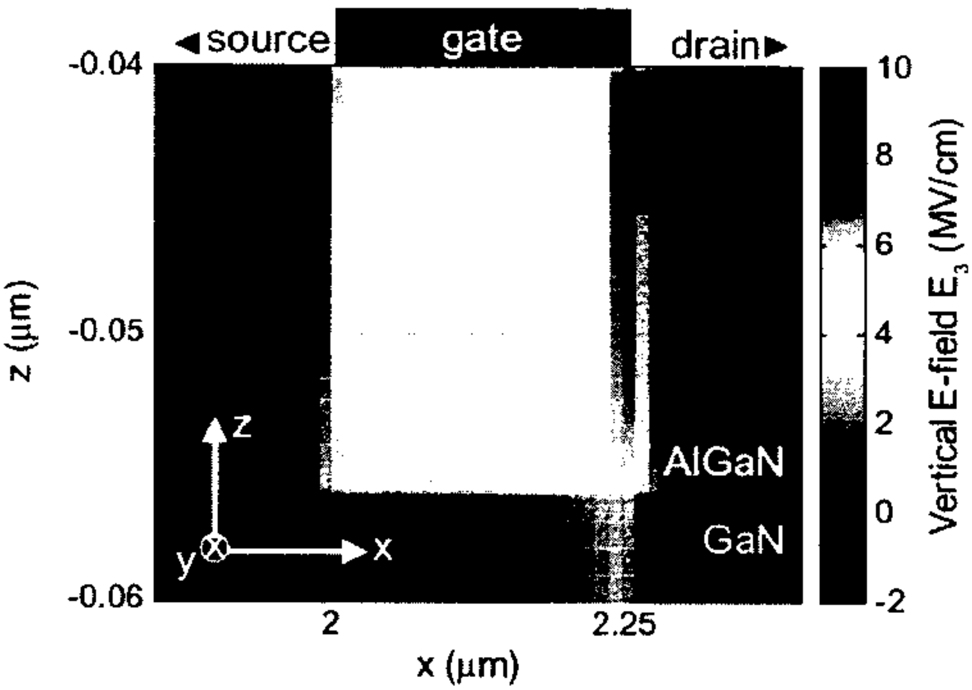


Figure 4.1 (c). Vertical electric field profile.© 2014 Elsevier. Reprinted, with permission, from [29].

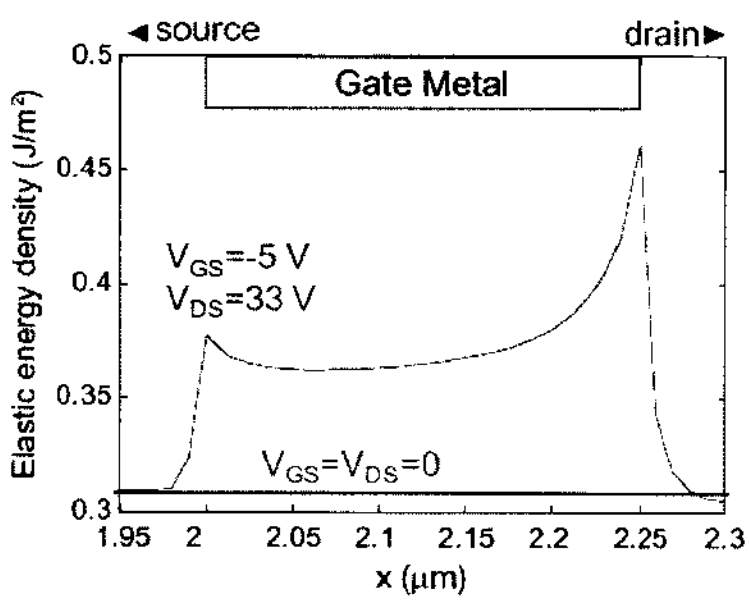


Figure 4.1 (d). Elastic energy density in AlGaN layers.© 2014 Elsevier. Reprinted, with permission, from [29].

Figure 4.1(a) and (b) shows the vertical electric field and elastic energy profiles under gate edge obtained in our simulations. The simulation was done at drain to source voltage of 33V and gate to source voltage of -5V. Figures 4.1 (c) and (d) show the vertical electric field and elastic energy profiles from Ref. [29] at exactly the same drain and gate bias.

From Figure 4.1(a) and (b), it can be seen that both the electric field values and elastic energy density values show sharp peak at the gate edge near the drain side. This predicted response is similar to the results obtained by Joh et al [29]. The elastic energy density value under the gate edge, obtained from our model, is seen to equal about 0.49 J/m^2 which is almost the same as the value shown in Figure 4.1 (c) and (d) from reference [29]. These close agreements between our simulation result and the reported data validate our model and provide confidence in our numerical method and its implementation for treating the electrical response of GaN HEMT structures.

4.2 ELECTRICAL MODELING RESULTS FOR ALGAN/GAN HEMTS

4.2.1 INTRODUCTION

The overall problem of evaluating the degree of induced stress and strain arising from the inverse piezoelectric effect is quite complex because the outcome depends on a range of parameters. More specifically, for the GaN/AlGaN HEMT structure, the internal electric fields that are the root cause of this effect, and influenced by the aluminum mole fraction, the thickness of the Al-layer, the applied external biasing, any variations in the cap-layer such as the possible use of high-*k* dielectric materials on top of the AlGaN layer etc. Hence for completeness, a systematic analyses of all the various factors needs to be carried out. One also needs to evaluate possible stress and strain that could be created internally due to device heating and thermal effects during operation. In the following sections, these various aspects alluded to above, have been examined. The next section provides a baseline study and also focuses on the role of the aluminum composition within the AlGaN layer of the GaN-AlGaN HEMT. The subsequent section examines the role of the cap-layer on GaN, and a variety of possible options are evaluated for their role in influencing the internal electric fields and stress. Includes in the analyses, are the use of a thin GaN cap above the traditional AlGaN layer, the use of different high-*k* dielectric materials, and changes in the AlGaN layer thickness in the presence of high-*k* materials. Finally, the role of heating and its influence on causing stress and strain with the HEMT is evaluated for completeness.

4.2.2 BASELINE RESULTS AND FOCUS ON ALUMINUM MOLE FRACTION VARIATIONS

All the simulation results presented in this section were carried out on the model described in section 3.2 with source voltage set at 0V, gate voltage set at 2V and a variable drain voltage (V_d) that was adjusted in the 5V to 20V range. Figure 4.1(e) shows the 2DEG sheet carrier density (n_s) and polarization charge density (σ) as a function of Al content for AlGaN thicknesses of 16nm and 20nm. Polarization charge density and 2DEG are seen to be augmented with increases in the Al content. The 2DEG densities also increased with increasing AlGaN thickness. With increases in the Al content from 0.26 to 0.3, the polarization charge density σ was seen to increase from 0.0231 C/m^2 to 0.0269 C/m^2. This shows that a higher Al-content or increased AlGaN layer thickness would work towards providing higher currents, and hence, small-signal current amplification in the HEMTs.

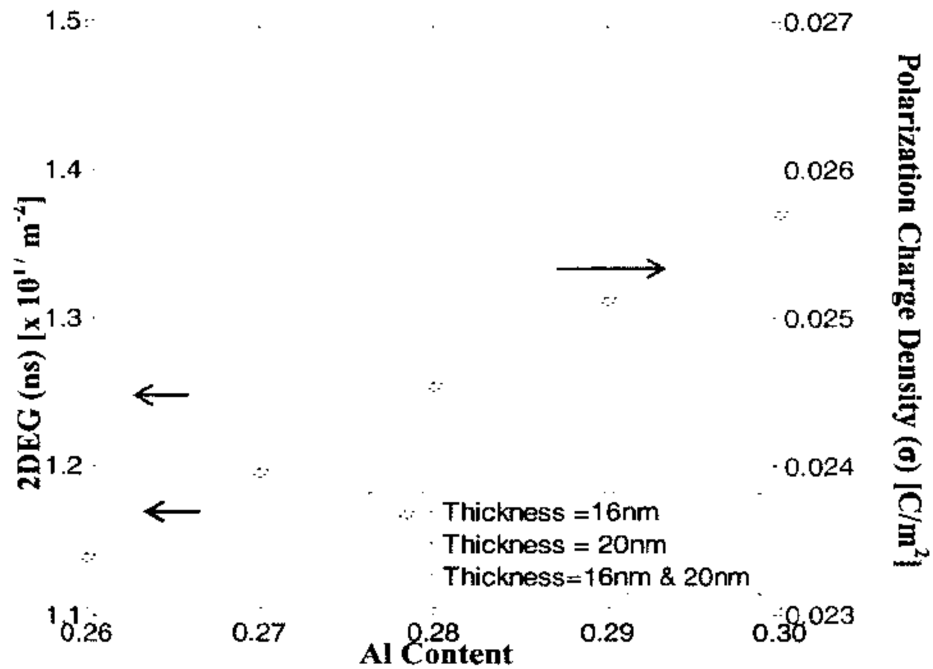


Figure 4.1 (e). 2DEG sheet carrier density (ns) and polarization charge density (σ) as a function of Al content at AlGaN thicknesses.

The breakdown field of Wurtzite crystal structure GaN devices has been reported to be in the ~3-5 MV/cm range [84, 85]. Defect formation in a stressed material is determined by the critical elastic energy per unit area. This latter areal elastic energy density is obtained by integrating the volume elastic energy density calculated using the equations given in chapter 3 along the direction normal to the interface (the y-axis) within the AlGaN layer. The critical elastic energy density value was reported to be about 0.49 J/m^2 [29]. The elastic energy density can be computed from the electric fields inside the device. Hence, as a logical step towards the evaluation of the energy density, electric field distributions in AlGaN/GaN HEMT at different drain biases were calculated. The impact of electric field on stress, strain and in turn elastic energy density in the AlGaN barrier, were then all systematically obtained to analyze the parameter space that can lead to the attainment of breakdown fields and critical energy densities in AlGaN/GaN HEMTs.

Variations of these parameters in the AlGaN/GaN layers for different device configurations are discussed below. Figures 4.2(a)-4.2(i) show the results of electric field distributions, potentials, stress etc. for a AlGaN/GaN HEMT with a 26% Al mole-fraction content (x_{Al}) and AlGaN thickness of 16nm (t_{AlGaN}) at a drain voltage (V_d) of 10V. Figures 4.3(a)-4.3(g) show the results the same Al-mole fraction (of 26%) and AlGaN thickness (t_{AlGaN}) of 16nm, but now at a higher drain voltage of 20V. These two sets of figures are given on the following pages.

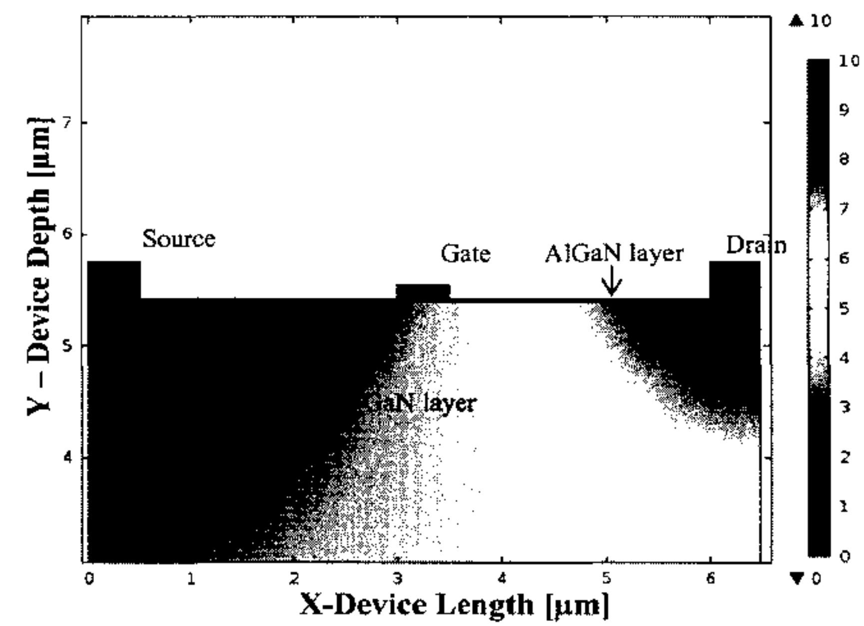


Figure 4.2(a). 2D Electric potential in AlGaN/GaN layers [$x_{Al} = 0.26$, t_{AlGaN} =16nm, V_d = 10V].

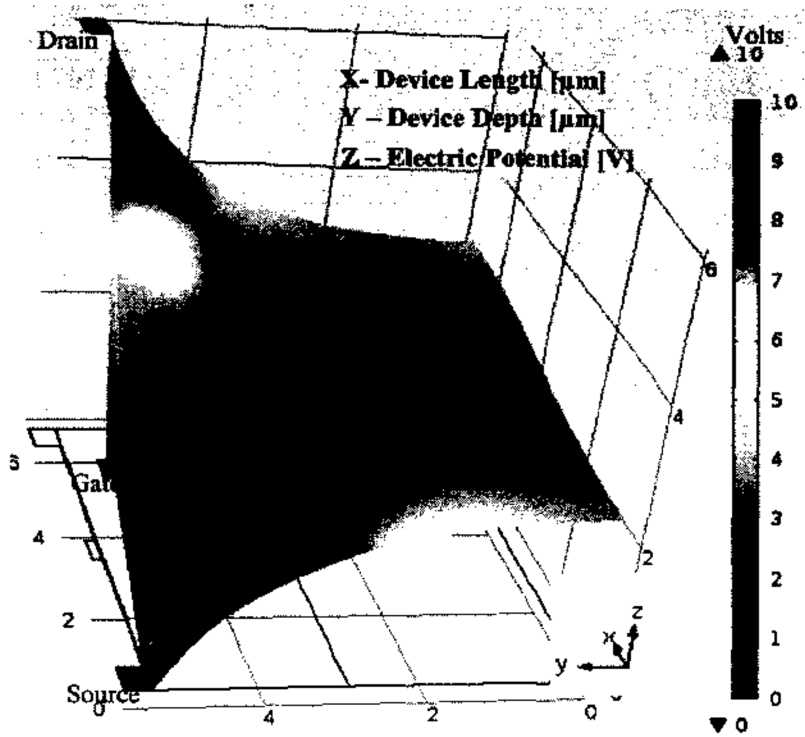


Figure 4.2(b). Electric potential in AlGaN/GaN HEMT [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 10V].

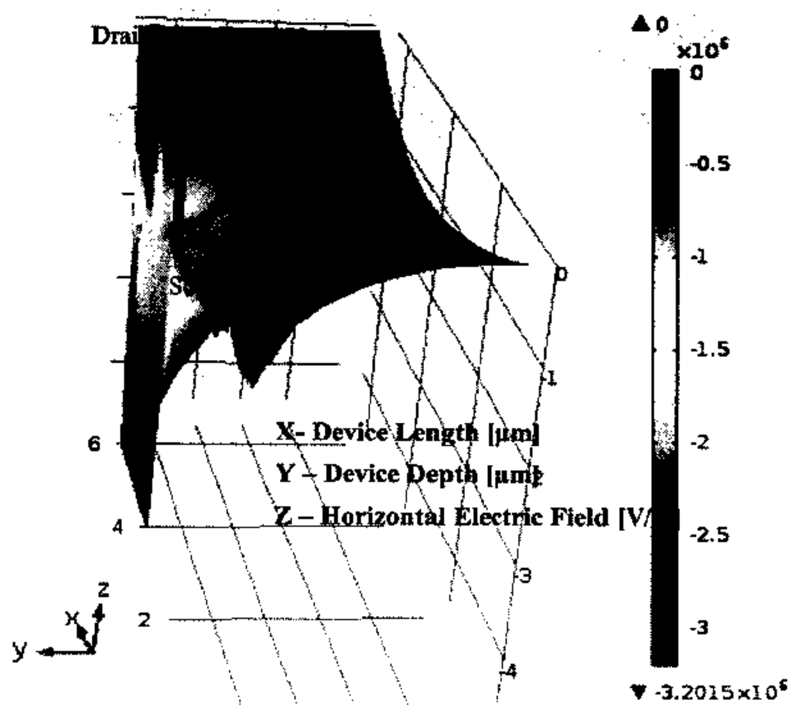


Figure 4.2(c). Lateral electric field in AlGaN/GaN layers [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 10V]. The electric field values are in V/m

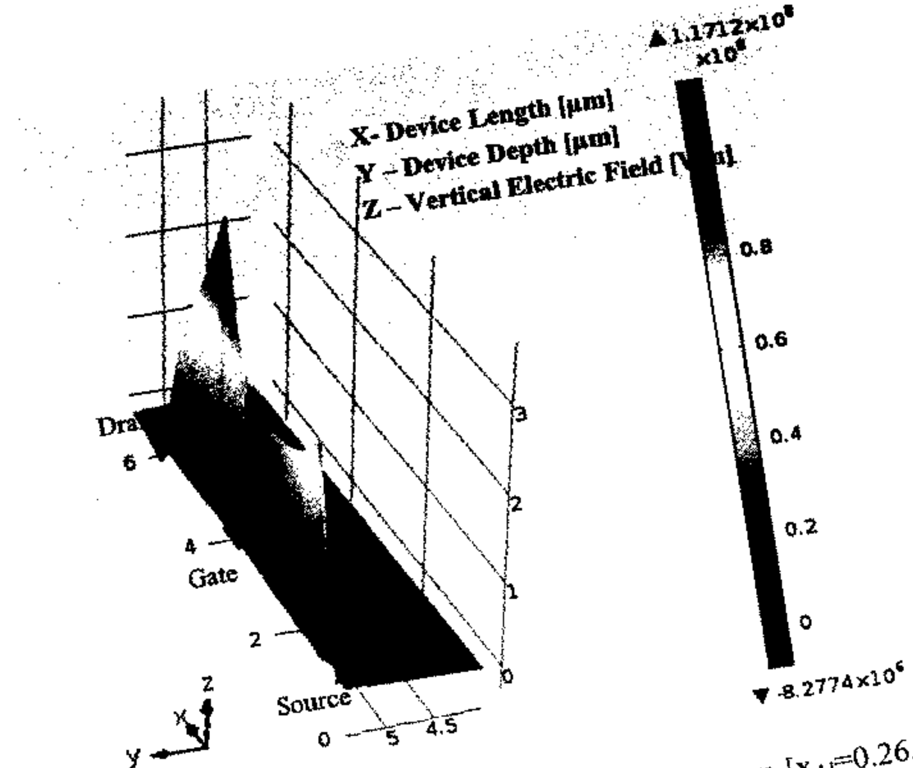


Figure 4.2(d). Vertical electric field (V/m) AlGaN/GaN layers [x_{Al}=0.26, t_{AlGaN}=16nm, V_d=10V].

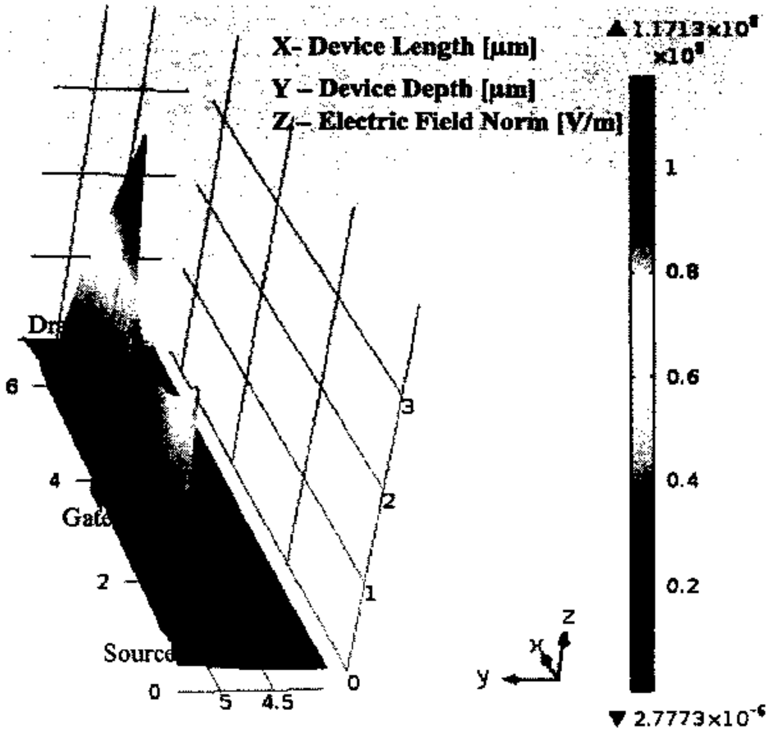


Figure 4.2(e). Electric field norm (V/m) in AlGaN/GaN layers [x_{Al}=0.26, t_{AlGaN}=16nm, V_d=10V].

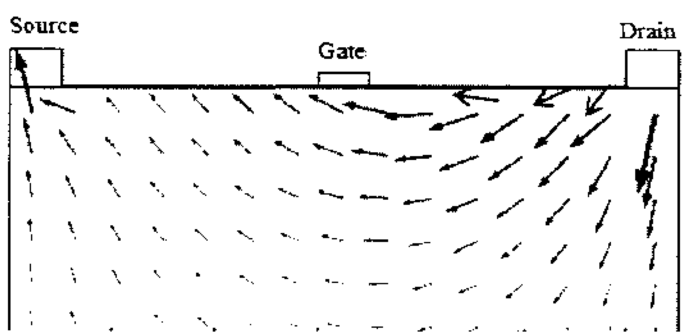


Figure 4.2 (f). Arrow surface showing electric field lines in ALGaN/GaN layers [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 10V].

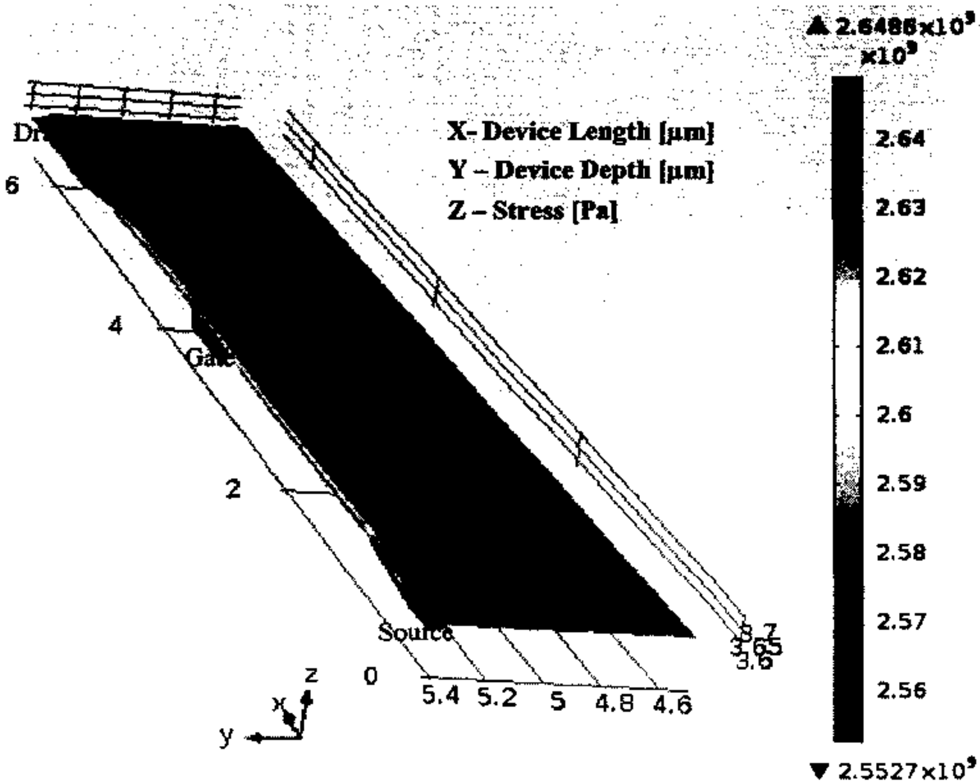


Figure 4.2(g). Planar stress (Pa) in ALGaN/GaN layers [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 10V].

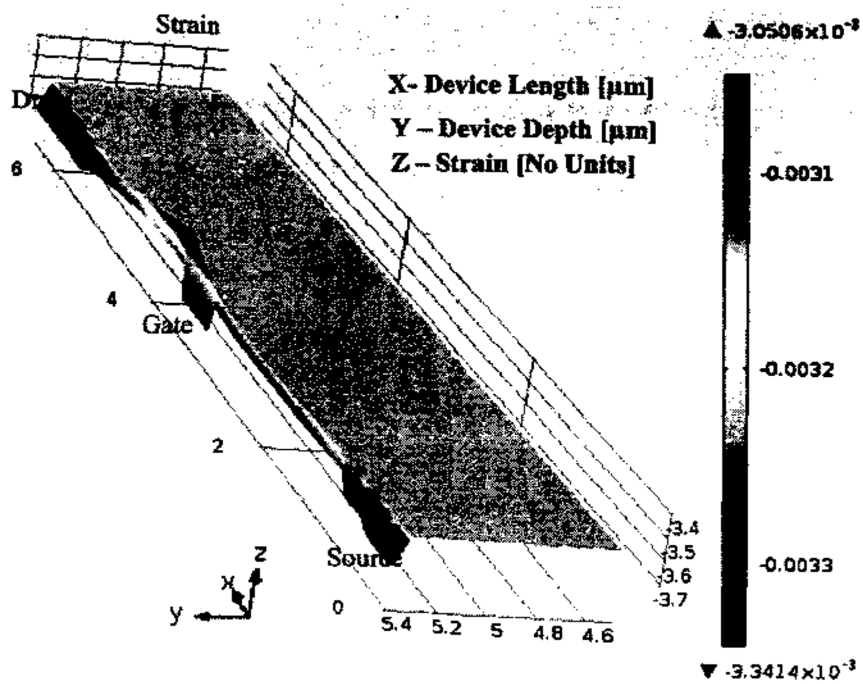


Figure 4.2 (h). Vertical strain in AlGaN/GaN layers [$x_{Al} = 0.26$, t_{AlGaN} =16nm, $V_d = 10V$].

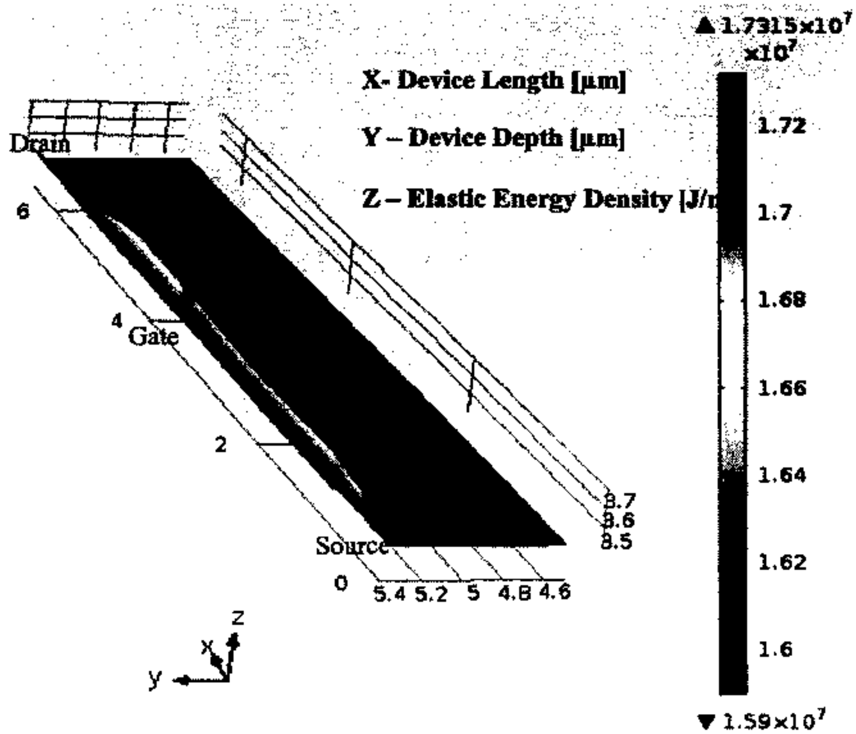


Figure 4.2(i). Elastic energy density (J/m^3) in AlGaN/GaN layers [x_{Al}=0.26, t_{AlGaN}=16nm, V_d=10V].

Though there is a lot of data and the plots may look "busy", useful information can be extracted from the set of figures. From these results, it can be observed that the vertical electric field, as well as the elastic energy density, sharply peak just below the gate edge on the drain side of the device. This location can thus be a potential weak spot for failure. Also as may be expected, it becomes apparent from Figures 4.2 and 4.3 that changes in elastic energy density due to the inverse piezoelectric effect become larger with increasing voltages and can lead to crystallographic defects.

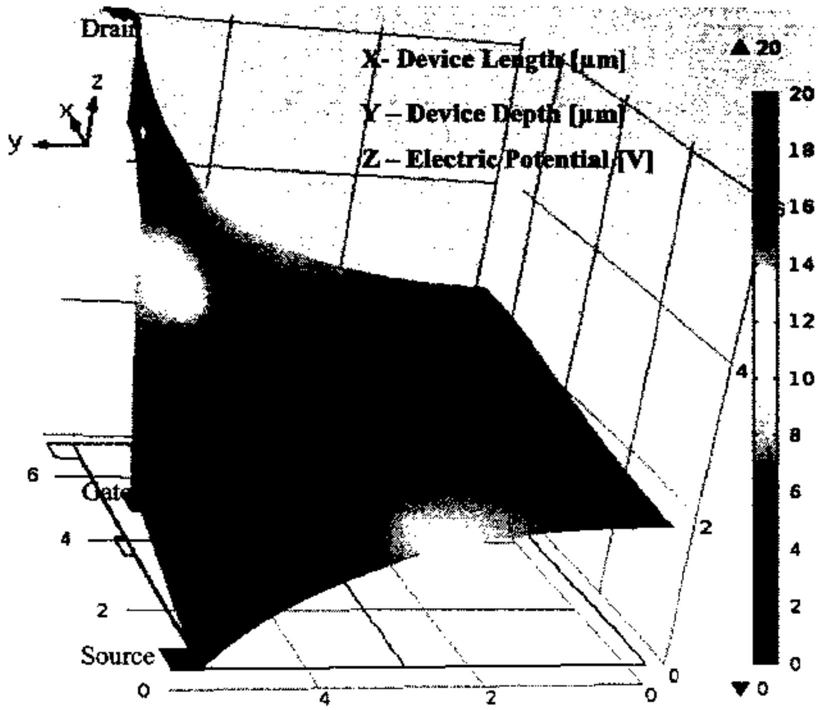


Figure 4.3 (a). Electric potential in AlGaN/GaN HEMT {x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 20V].

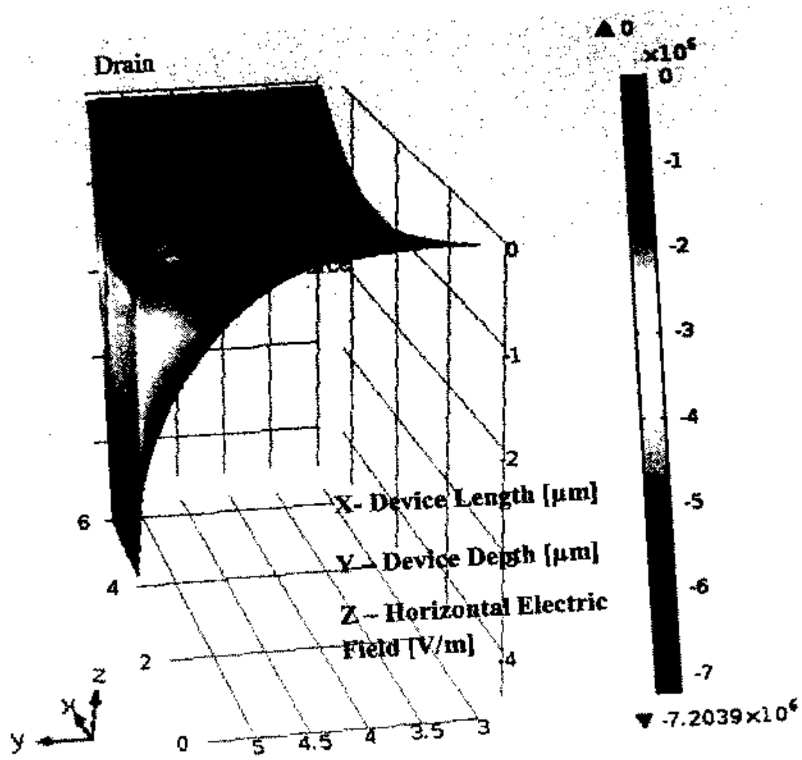


Figure 4.3 (b). Electric field magnitude in AlGaN/GaN layers [x_{Al}=0.26, t_{AlGaN}=16nm, V_d=20V].

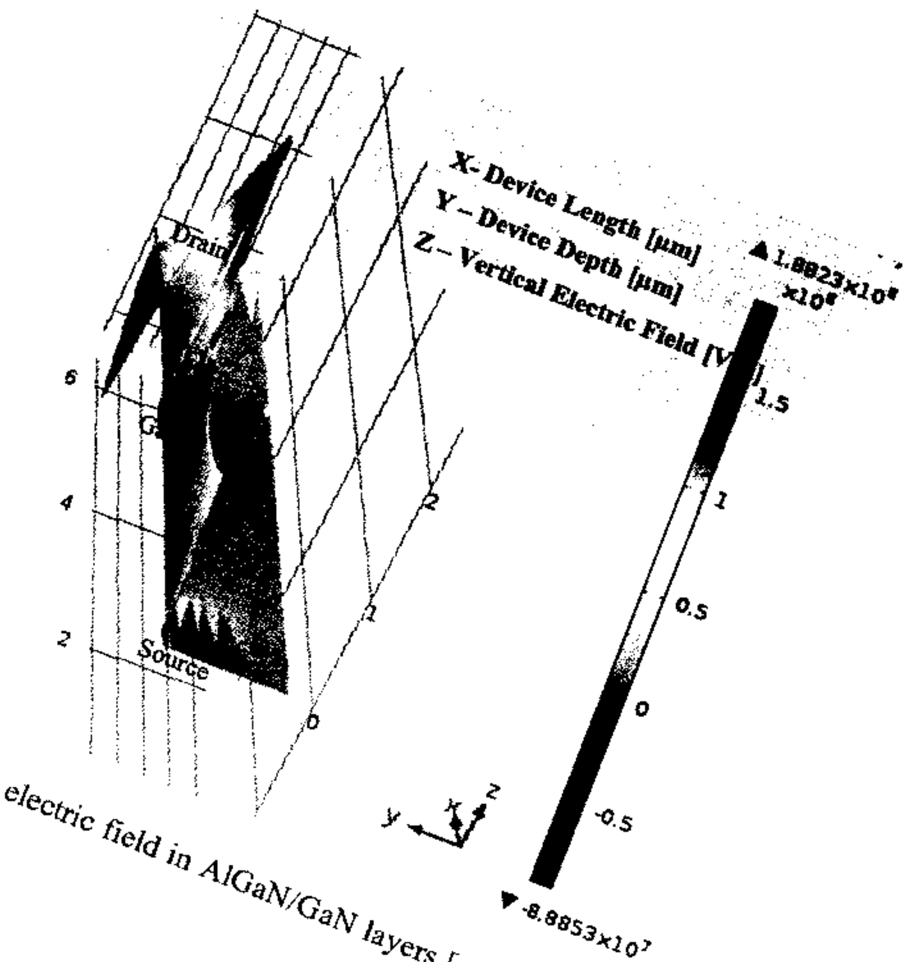


Figure 4.3 (c). Vertical electric field in AlGaN/GaN layers [$x_{Al} = 0.26$, t_{AlGaN} =16nm, V_d = 20V].

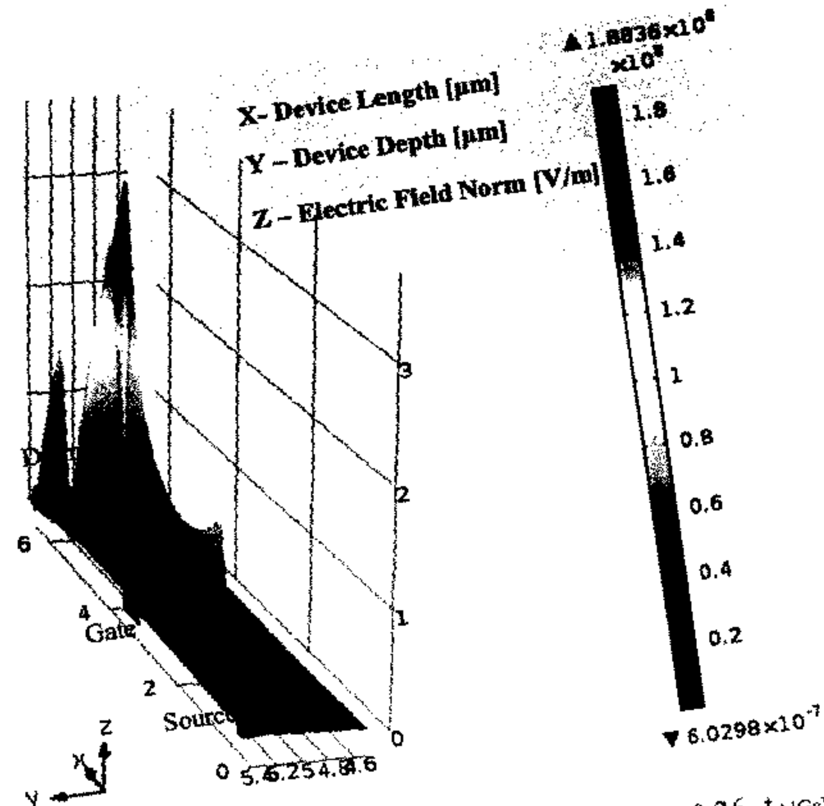


Figure 4.3 (d). Electric field norm in AlGaN/GaN layers [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 20V].

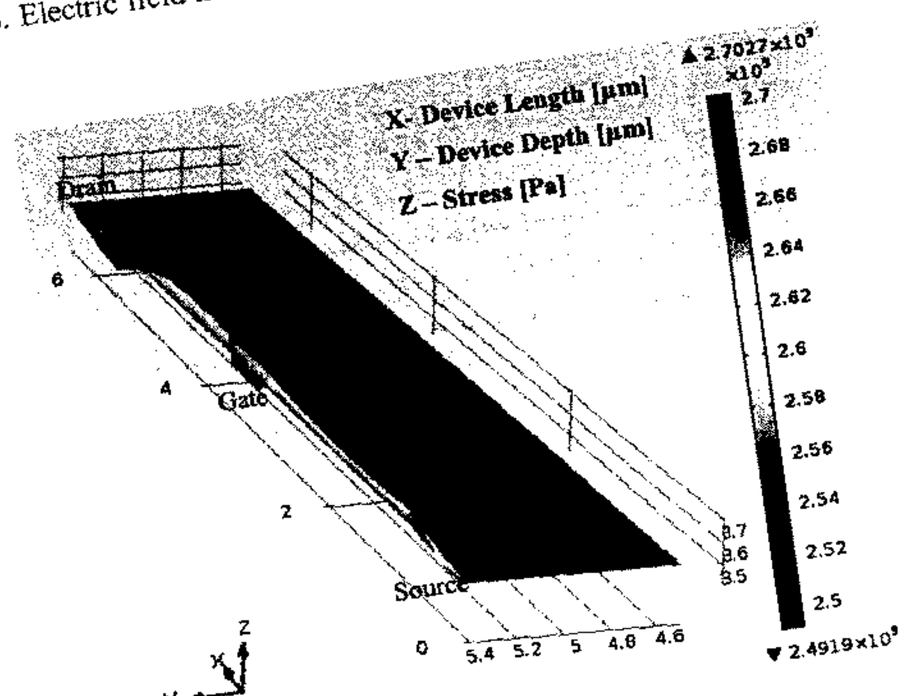


Figure 4.3 (e). Planar stress in AlGaN/GaN layers [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 20V].

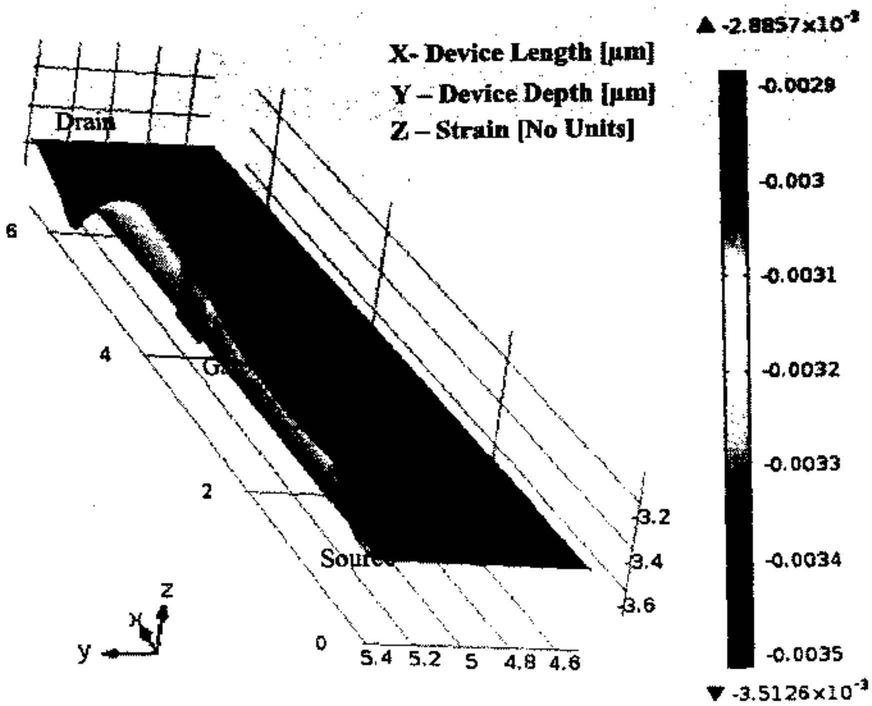


Figure 4.3 (f). Vertical strain in AlGaN/GaN layers [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 20V].

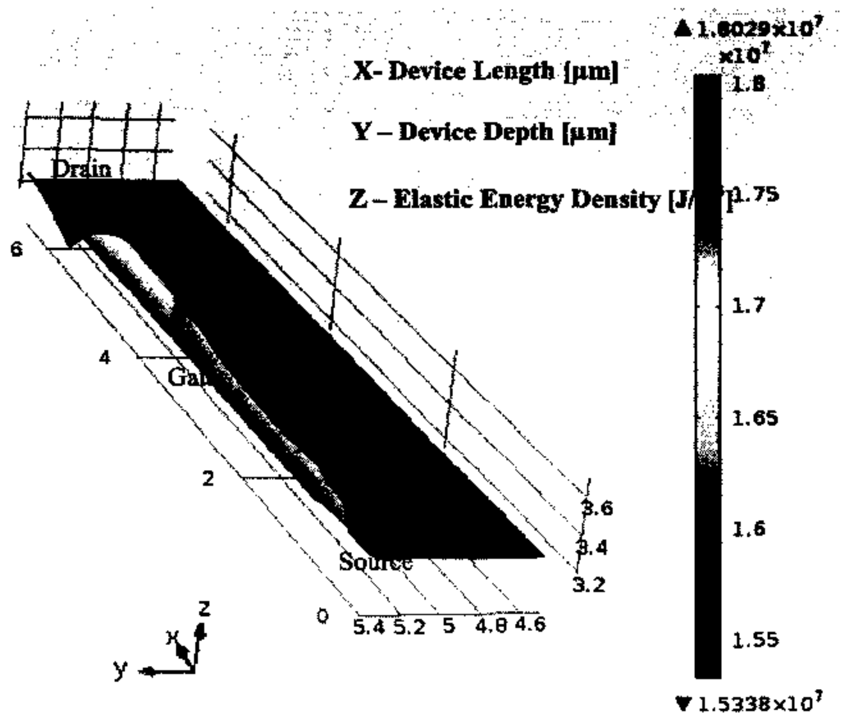


Figure 4.3 (g). Elastic energy density in AlGaN/GaN layers [x_{Al} = 0.26, t_{AlGaN} =16nm, V_d = 20V].

Figures 4.4 and 4.5 show the effect of increased Al content on the electric field and elastic energy density. Figs. 4.4(a) and 4.4(b) are the vertical electric field and elastic energy density profiles for an Al-mole fraction x_{Al} of 0.26, an AlGaN layer thickness t_{AlGaN} of 16nm, and a drain voltage V_d of 20V. The corresponding data for a higher Aluminum mole fraction x_{Al} of 0.3, but the same drain voltage V_D (=20 Volts), and AlGaN layer thickness t_{AlGaN} of 16nm is shown in Figures 4.5(a) and 4.5(b). The vertical electric field and elastic energy density values have increased from 1.9 x 10^8 to 2.1 x 10^8 and 0.29 to 0.38, respectively, with increase in Al content from 0.26 to 0.3 with 16nm AlGaN thickness and 20V drain bias.

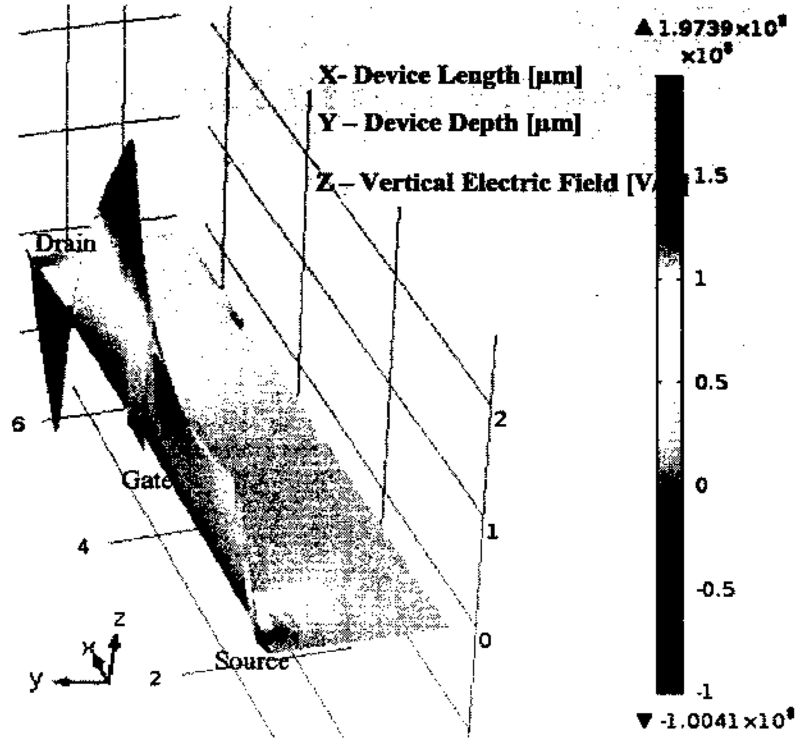


Figure 4.4 (a). Vertical electric field in AlGaN/GaN layers [x_{Al} = 0.28, t_{AlGaN} =16nm, V_d = 20V].

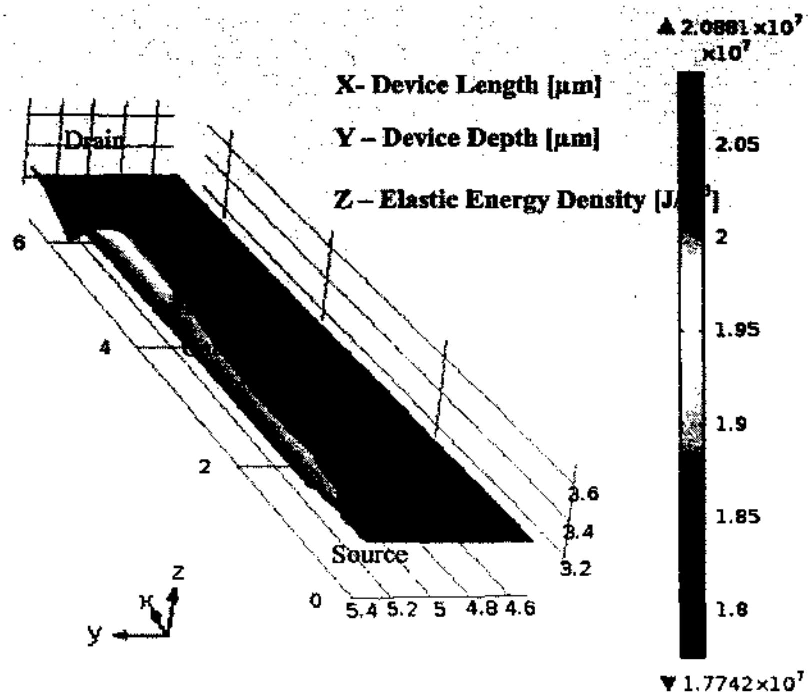


Figure 4.4 (b). Elastic energy density in AlGaN/GaN layers [xAl = 0.28, tAlGaN =16nm, Vd = 20V].

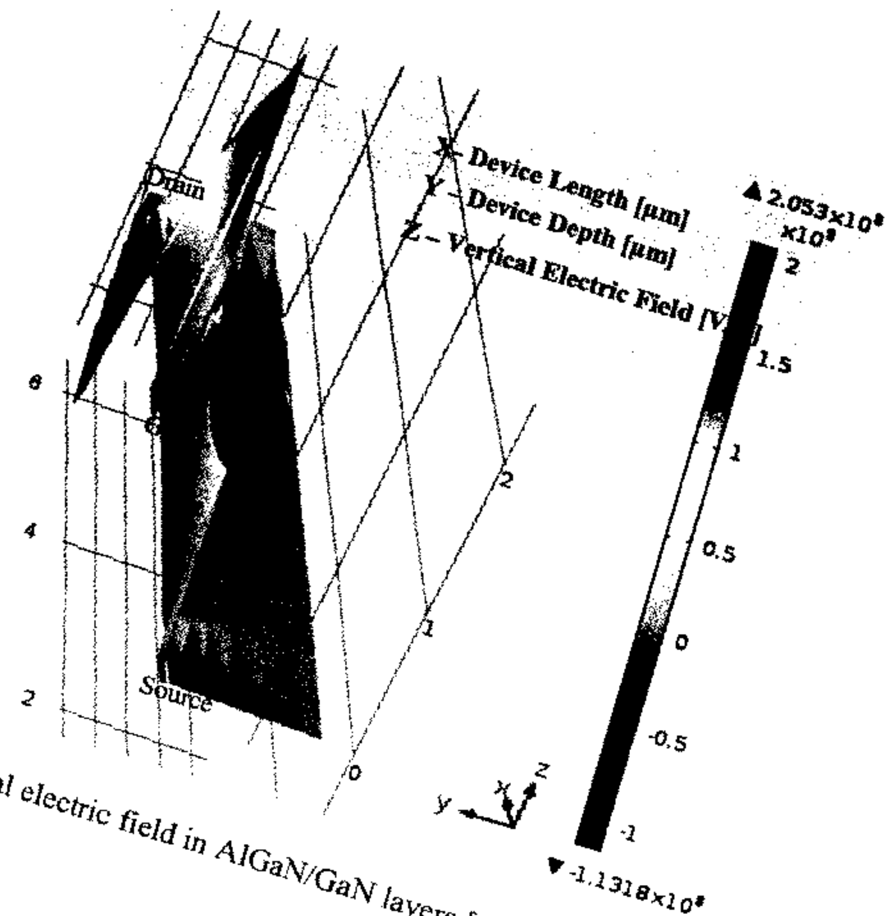


Figure 4.5 (a). Vertical electric field in AlGaN/GaN layers [$x_{Al} = 0.3$, t_{AlGaN} =16nm, V_d = 20V].

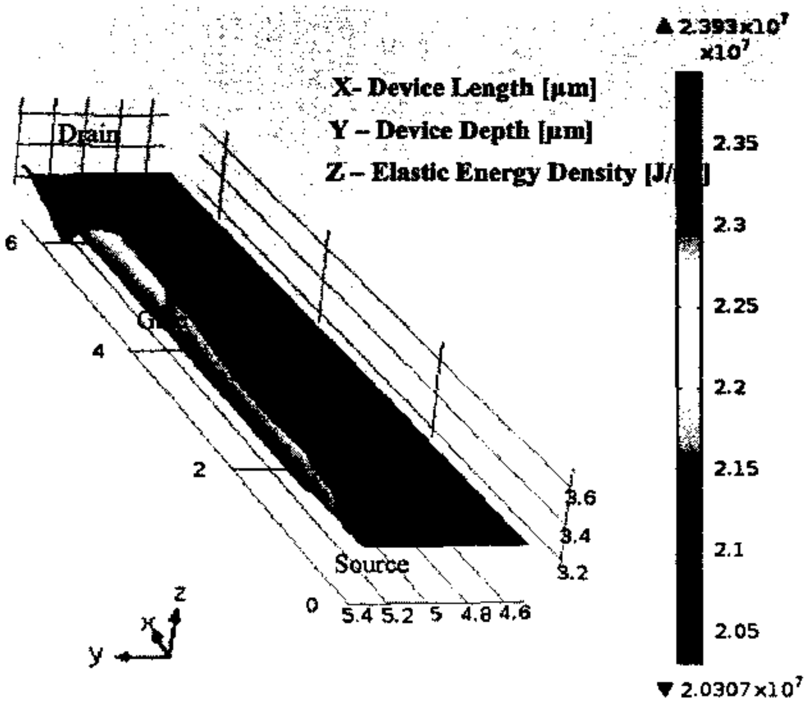


Figure 4.5 (b). Elastic energy density in AlGaN/GaN layers [x_{Al} = 0.3, t_{AlGaN} =16nm, V_d = 20V].

Figures 4.6, 4.7 and 4.8 show planar stress, vertical strain and eleastic energy density, respectively, as a function of distance between source to drain in AlGaN layer at Al contents of 0.26, 0.28 and 0.3 for a 16nm AlGaN layer thickness and 20V drain bias. Figures 4.9 and 4.10 show the maximum values of planar stress and elastic energy density, respectively, in AlGaN layer as a function of drain voltage at Al contents of 0.26, 0.28 and 0.3 with 16nm AlGaN layer thickness. The maximum values of stress or elastic energy density located at the gate edge of drain side were observed to increase with increasing drain bias. In theory, this can lead to defect creation under the gate edge at high voltages which can furthur lead to gate leakage currents via a feedback machanism.

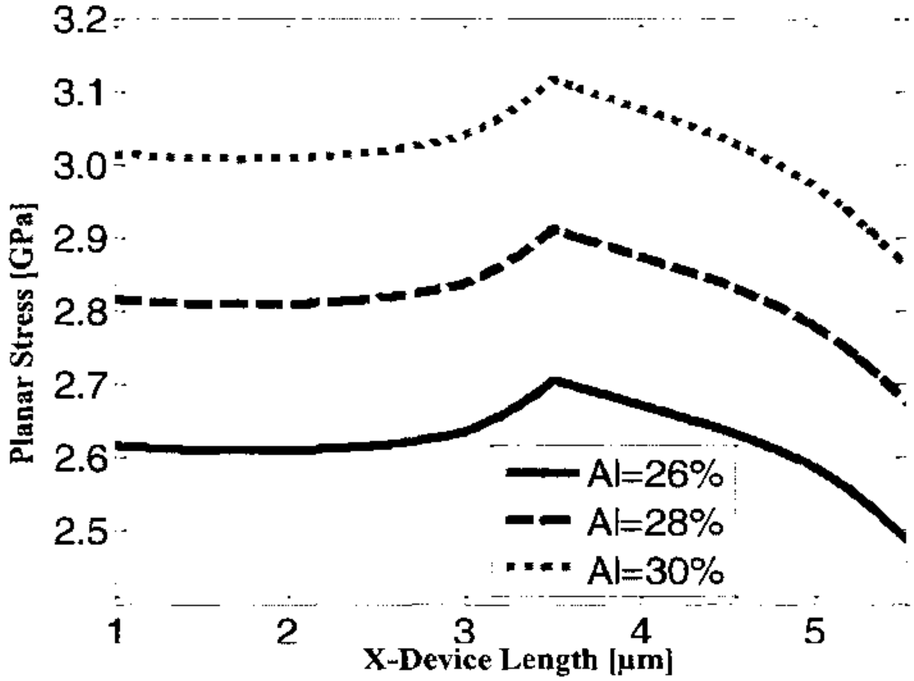


Figure 4.6. Planar stress in AlGaN layer at different Al content [t_{AlGaN} =16nm, V_d = 20V].

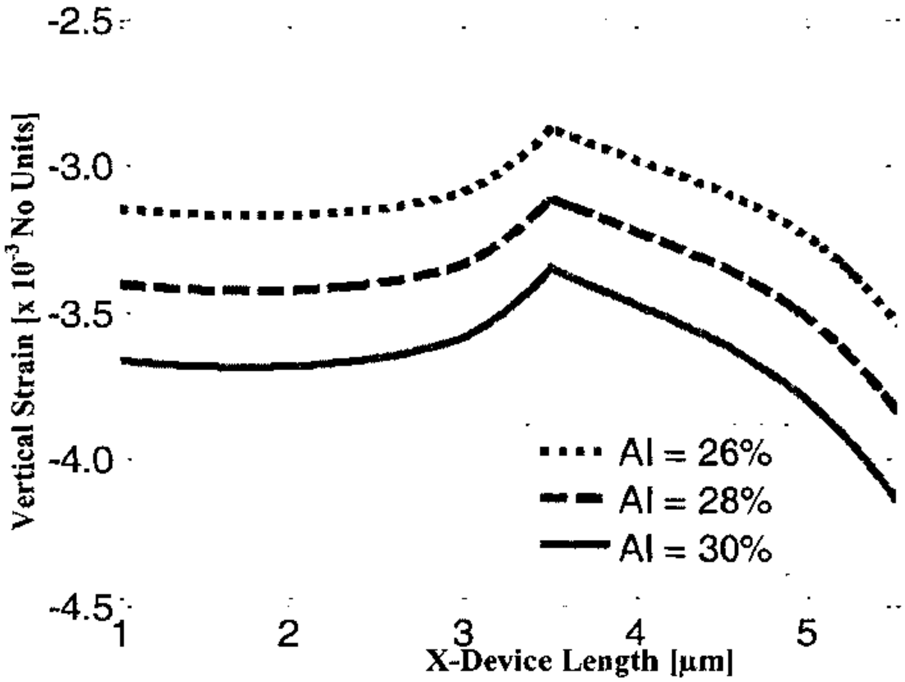


Figure 4.7. Vertical strain in AlGaN layer at different Al content [t_{AlGaN} =16nm, V_d = 20V].

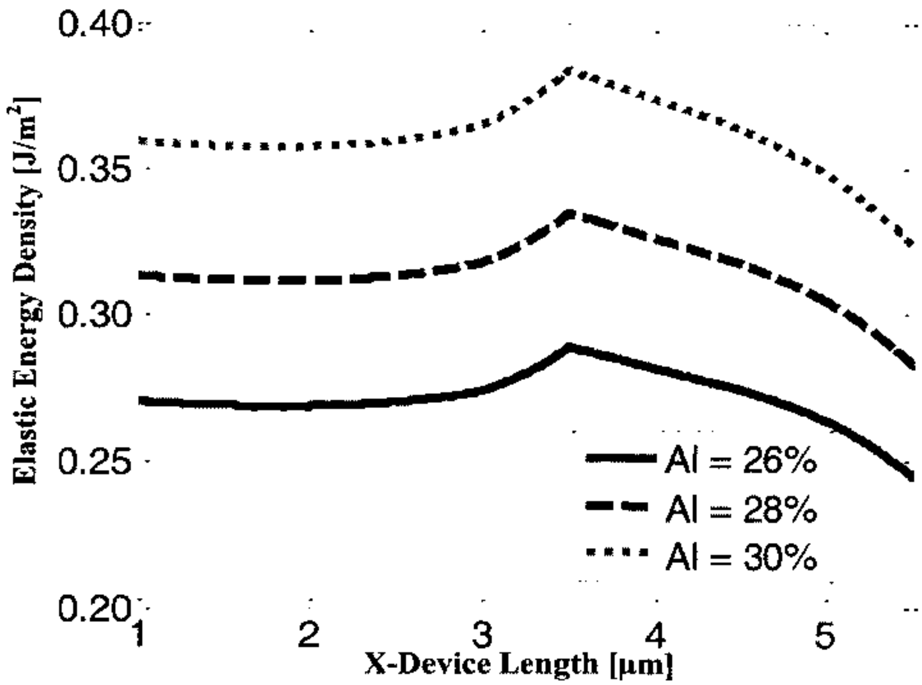


Figure 4.8. Elastic energy density in AlGaN layer at different Al content [t_{AlGaN} =16nm, V_d = 20V].

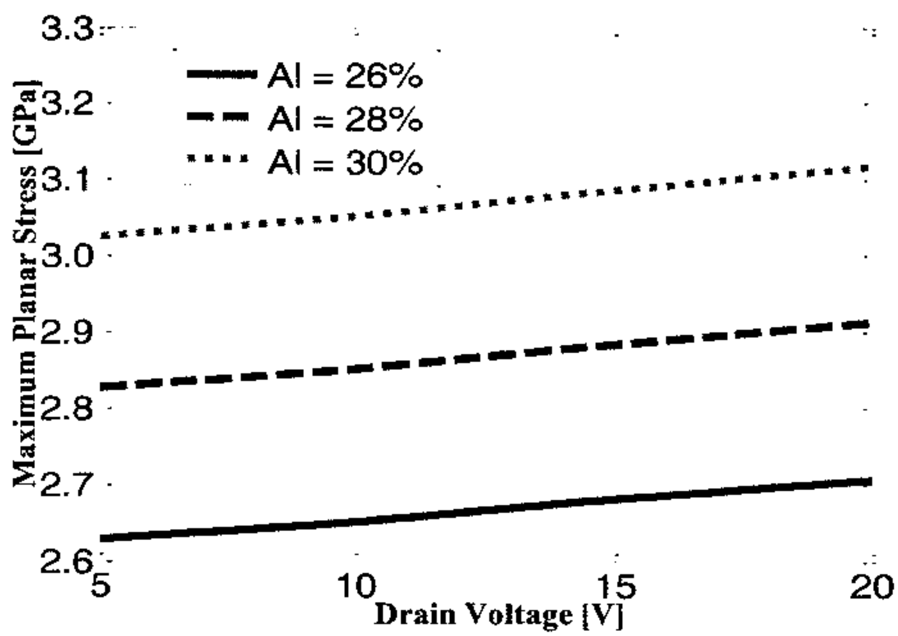


Figure 4.9. Maximum stress as a function of drain voltage.

Figure 4.9 shows the maximum stress as a function of drain voltage in the AlGaN layer at different Al content. The AlGaN later thickness was set to 16nm and a drain voltage V_d of 20V was used.

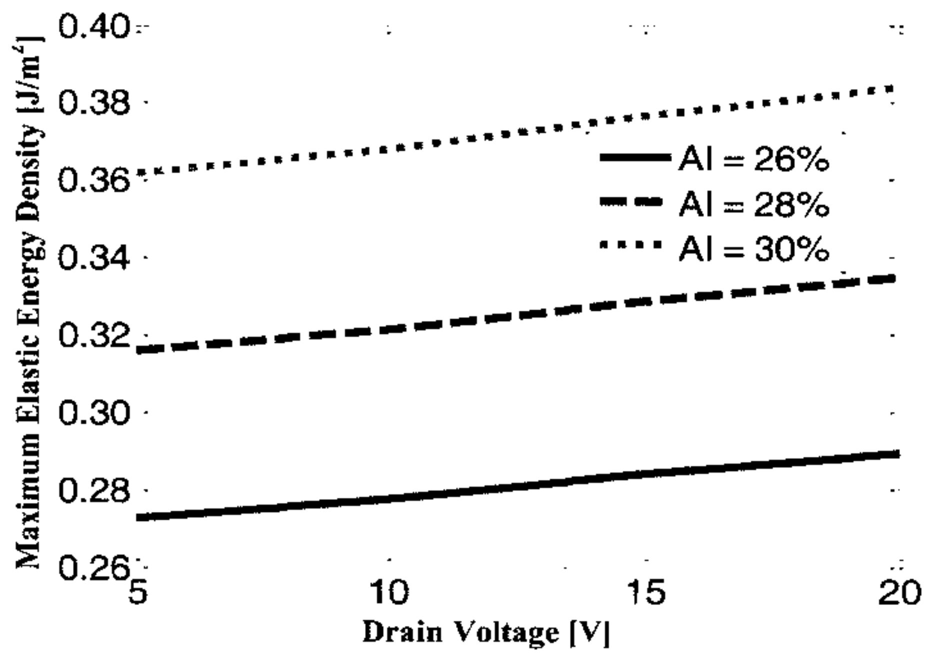


Figure 4.10. Maximum elastic energy density as a function of drain voltage in AlGaN layer at different Al content [t_{AlGaN} =16nm, V_d = 20V].

From the Figures 4.4-4.10 above, it can be observed that increases in Al content increase the vertical electric field in the AlGaN layer. Under an increasing positive field, the planar stress increases which results in an increased elastic energy. Also, the vertical strain is increased in magnitude with increasing fields and Al content. For AlGaN/GaN structure with AlGaN barrier layer grown pseudomorphically on GaN buffer, there exists an unchanged as-grown (i.e., inherent) planar strain equal to 0.0068. From equation 3.5(b) in section 3.2, even in the absence of electric field, there exists a vertical strain that dependes on the Aluminum content. As the Aluminum content increases from 0.2 to 0.3, the magnitude of the vertical strain increases from 0.0025 to 0.0039, and the stored elastic energy density increases from 0.152 to 0.344. Therefore, the elastic energy already present increases with increasing fields due to inverse piezoelectric effect that can lead to degradation if the stored elastic energy reaches the critical value.

4.2.3 FOCUS ON ALGAN THICKNESS VARIATIONS

AlGaN layer thickness is an important parameter that can change the sheet carrier concentration, electric fields and energy density in the AlGaN layer. There exists a critical thickness for strain relaxation in AlGaN/GaN heterostructures beyond which the stored elastic energy in AlGaN layer leads to the formation of dislocations.

Figure 4.11 (a) shows the result of elastic energy density and Figure 4.11 (b) shows the result of vertical field values at two different AlGaN thickness values as a function of drain voltage. Figure 4.12 shows the results for planar stress and vertical strain for AlGaN layer thickness of 22 nm. 20V of drain bias is applied in both the cases. The stress values have observed to decreased as the AlGaN thickness is increased from 16nm to 22nm. The vertical electric field are seen to have decreased from 2.08×10^8 V/m to 1.7×10^8 V/m. Also, the elastic energy density values have increased from 0.33 to 0.41, respectively, with an increase in AlGaN thickness from 16nm to 22nm at an Aluminum content of 0.28 and a 20V drain bias.

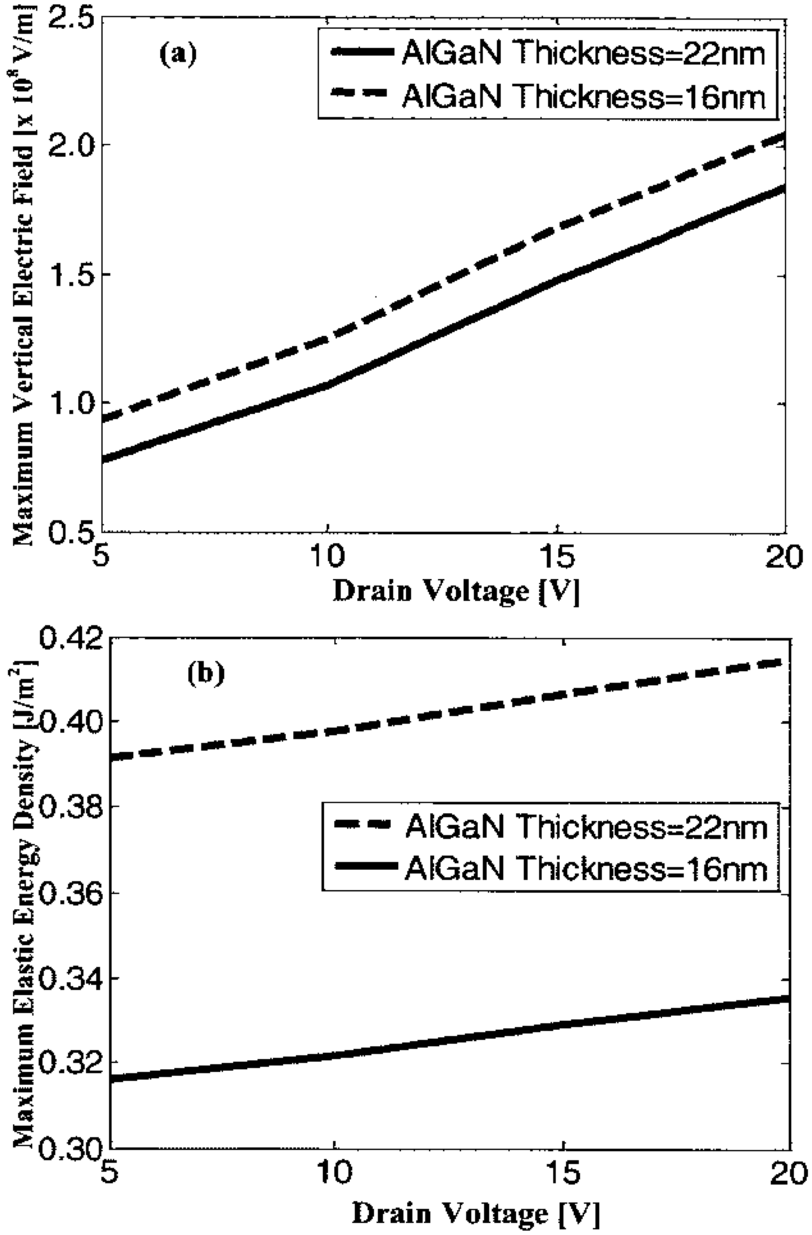


Figure 4.11. Simulation results for different AlGaN thickness [$x_{Al} = 0.28$, $V_d = 20V$]. (a) Vertical electric field, and (b) Elastic energy density.

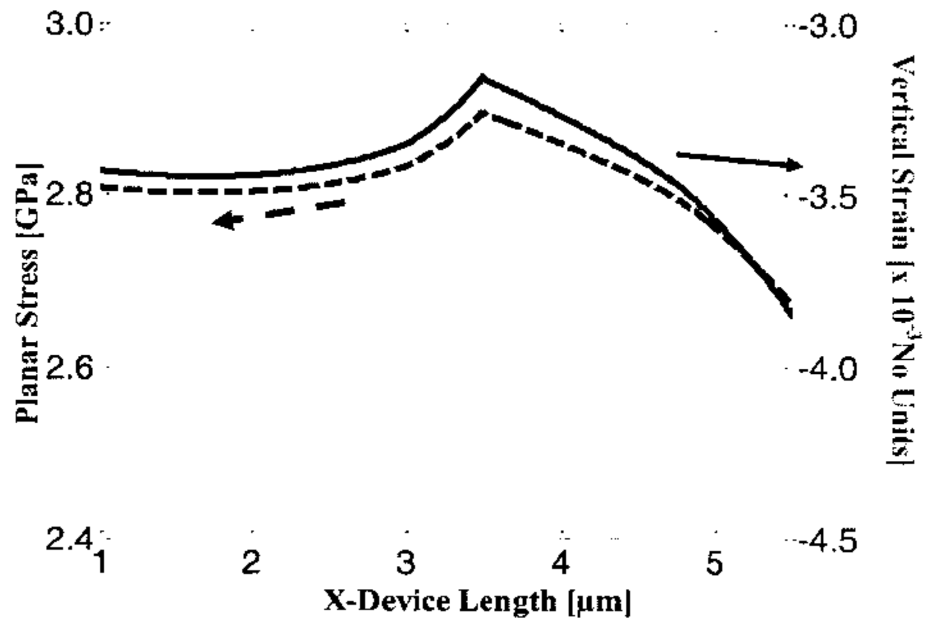


Figure 4.12. Planar stress and vertical strain in AlGaN layer [x_{Al} = 0.28, t_{AlGaN} =22nm, V_d=20V].

4.2.4 EVALUATING THE ROLE OF HIGH-*K* DIELECTRICS

In this section, the effects of a cap layer on electric field values, as well as the elastic energy in AlGaN are discussed. High-*k* dielectric materials have been used as the cap layers on AlGaN layer to study different scenarios.

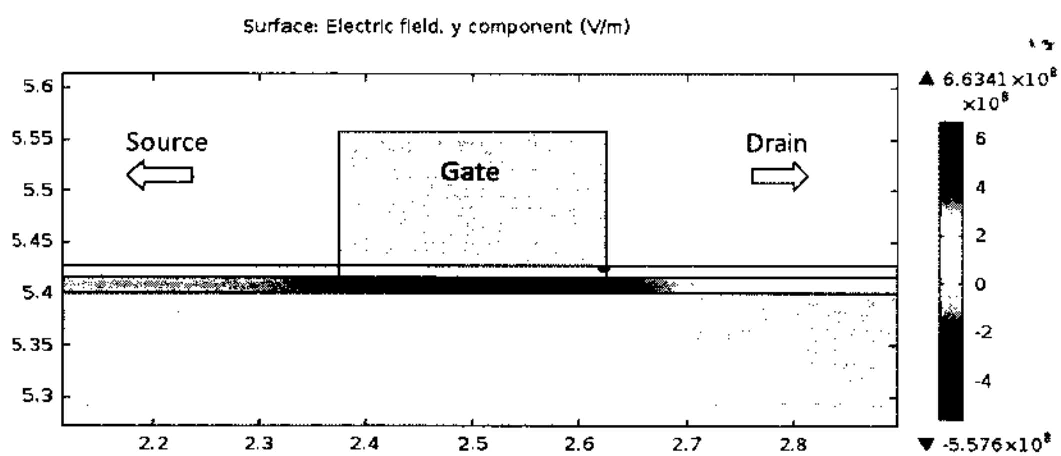


Figure 4.13. 2D Electric field profile in AlGaN/GaN HEMT with high-*k* cap layer.

High-*k* dielectrics have been used as insulating layers between gate electrode and the semiconductor to improve the forward leakage current in AlGaN/GaN HEMTs operating under large input signal conditions [82]. HfO_2 and Ta_2O_5 have been the commonly used high-*k* dielectrics. Given their use, these same materials were chosen here as a test for evaluating and possibly mitigating device failure in the GaN HEMTs.

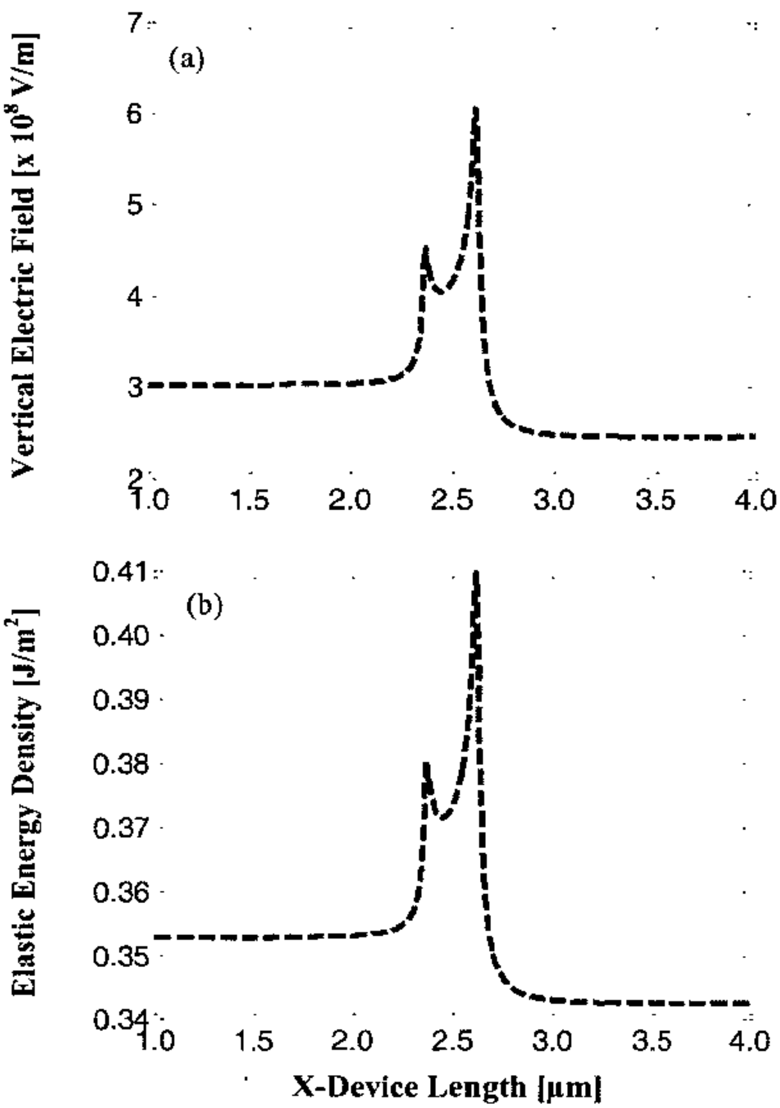


Figure 4.14. (a) Electric field, (b) Elastic energy density profiles under gate in AlGaN layer.

Figures 4.13-4.19 show the simulation results of the MIS HEMT with HfO_2 and Ta_2O_5 high-*k* cap layers as insulators. At first, simulation of AlGaN/GaN HEMT with 12nm high-k cap layer was done with the device in the OFF state with a 33V drain bias and a -5V gate bias. Here, fixed positive and negative charges are placed at the AlGaN/GaN interface and at the top of the AlGaN surface, respectively. Figure 4.13 shows the electric field profile and Figures 4.14 (a) and (b) show the peak electric field and energy density values under the gate in the AlGaN layer. The peak values are observed under gate edge towards the drain side within the AlGaN layer. But, if we compare these peak values with the values observed in Figure 4.1 (a) and (b) for the AlGaN/GaN HEMT *without a high-k cap layer*, it can be observed that the peak electric field value reduced from 9.8 MV/cm to 6.6 MV/cm. Furthermore, the elastic energy density value reduced from 0.49 MJ/m^2 to 0.41 MJ/m^2 with inclusion of the high-*k* cap layer.

The gate bias is now changed from -5V to 2V. Figure 4.15 shows vertical field and elastic energy density in AlGaN/GaN layers with 6nm Ta_2O_5 (ε_r =22) cap layer 16nm AlGaN thickness, a 0.28 Aluminum content at 20V drain bias. Figure 4.16 shows vertical field and elastic energy density in AlGaN/GaN layers with 6nm HfO_2 (ε_r =25) cap layer, 16nm AlGaN thickness, a 0.28 Aluminum content at 20V drain bias. Figure 4.17 compares the vertical electric field values and elastic energy density values in AlGaN layer with and without a high-*k* cap layer. The vertical electric field and elastic energy density values have decreased from 2.08×10^8 to 1.9×10^8 and 0.335 to 0.333, respectively, with addition of high-k cap layer of 6nm for a 16nm AlGaN thickness, a 0.28 Aluminum content and a 20V drain bias.

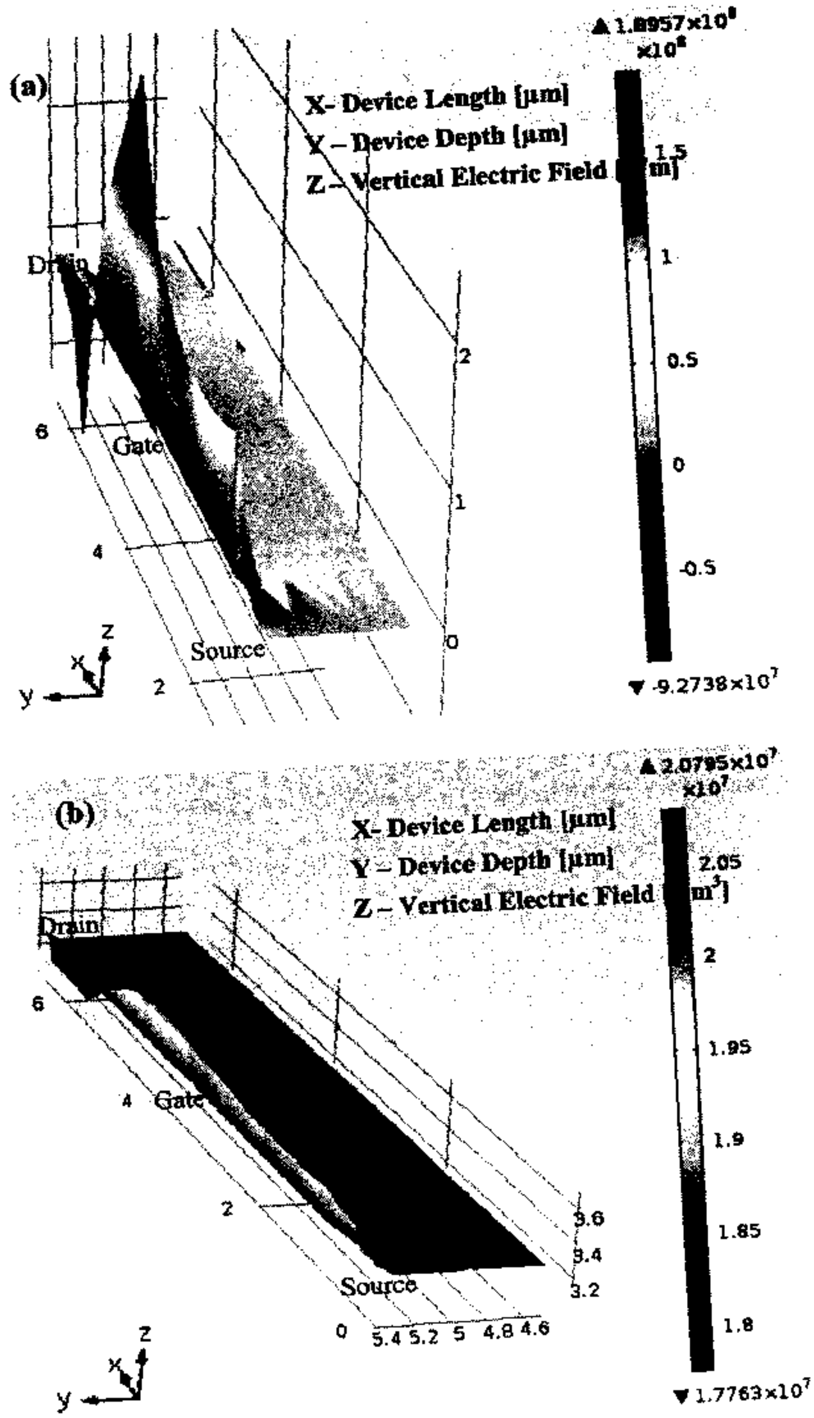
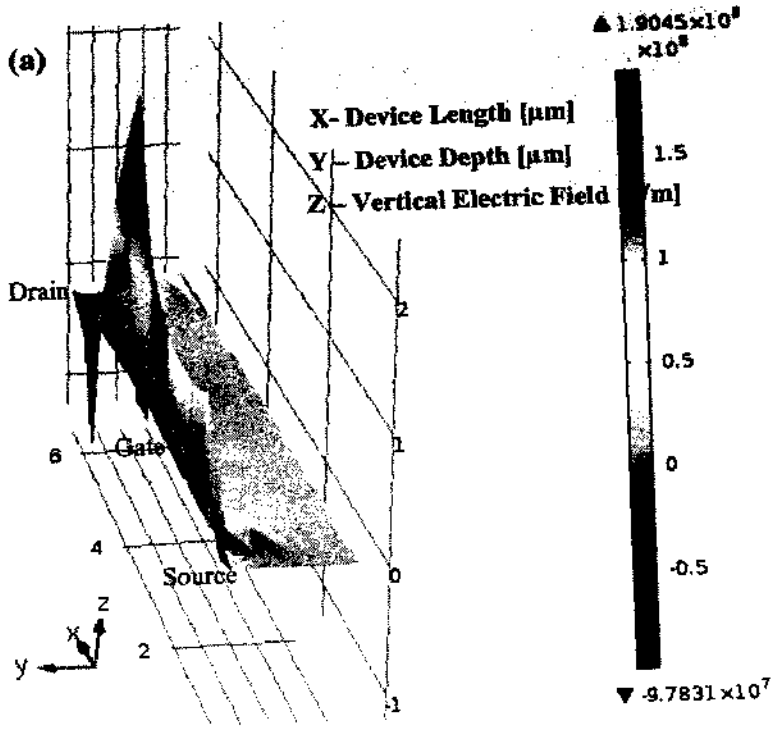


Figure 4.15. Simulations of AlGaN/GaN HEMTs with 6nm Ta_2O_5 cap [x_{Al} = 0.28, t_{AlGaN} =16nm, V_d = 20V]. (a) Vertical electric field, (b) Elastic energy density in AlGaN/GaN layers.

Reduction in both the electric field values and elastic energy density values at the gate edge were observed for HEMTs with high-*k* layer. However, not much difference was observed in electric field values between device having HfO_2 and Ta_2O_5 cap layers. Figure 4.18 shows vertical electric field and elastic energy density values in AlGaN/GaN layers with AlGaN thickness of 22nm which is equivalent to the case of AlGaN thickness of 16nm and high-*k* cap layer thickness of 6nm. This simulation was carried out to compare the results of increasing the thickness of AlGaN layer to the combined total layer with the high-*k* cap structure. As can be observed from the results, the vertical electric field values have significantly decreased and energy density values have significantly increased due to increased thickness of AlGaN layer. Figure 4.19 show the results due to increased thickness of high-*k* cap layer. As the high-*k* layer thickness increases, the electric fields, and in turn elastic energy density, were observed to decrease. Figures 4.20 and 4.21 show results that compare a HEMT with a high-*k* layer with another HEMT without high-*k* layer but with increased AlGaN layer thickness. As it can be seen from the results, increases in AlGaN thickness reduce the electric fields in AlGaN layer, but as the thickness increases critical energy also increases. The elastic energy value increased from ~0.33 J/m^2 at 16nm thickness to ~0.46 J/m^2 at 22nm thickness at drain bias of 20V. This value can also increase with increased drain bias. The value is close to the critical energy density (0.49 J/m^2) beyond which the crystallographic defects start to occur. So, instead of increasing the AlGaN thickness, a thick high-*k* layer proves to be advantageous (and a better option) in reducing the stored elastic energy as well as gate leakage current.



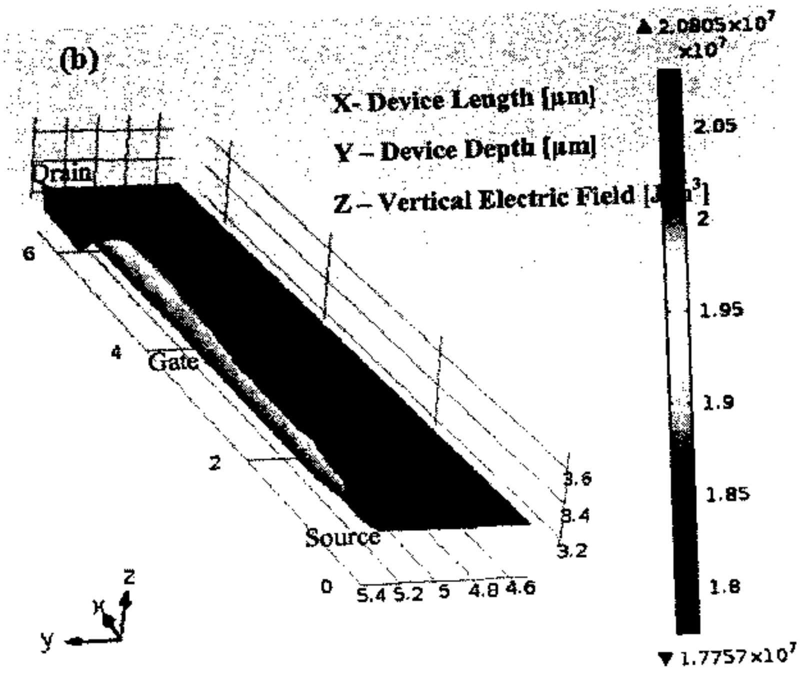


Figure 4.16. Simulation results for AlGaN/GaN layers with 6nm HfO_2 cap [x_{Al} = 0.28, t_{AlGaN} =16nm, V_d = 20V]. (a) Vertical electric field, and (b) Elastic energy density.

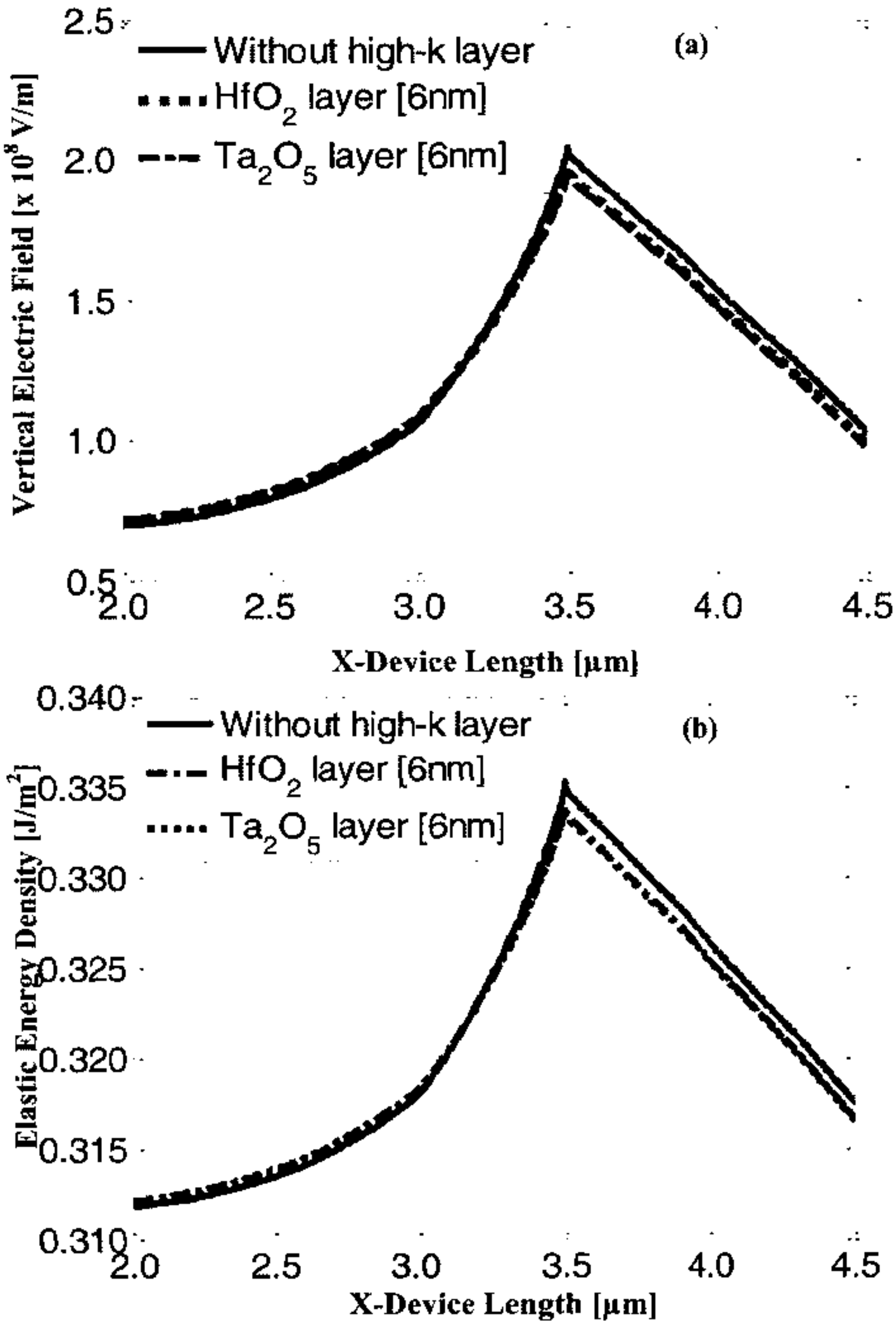
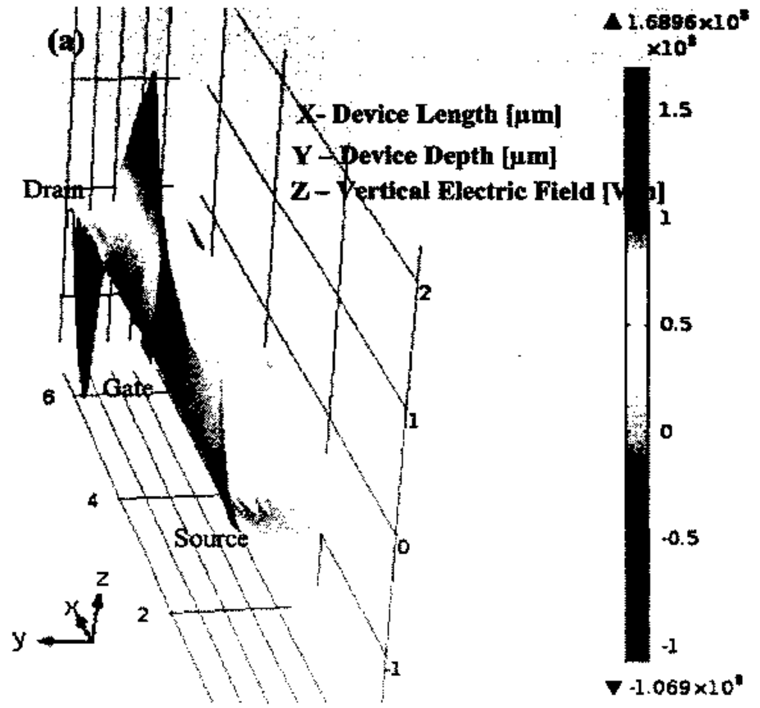


Figure 4.17. Simulations in AlGaN layer with and without high-*k* cap layers [x_{Al} = 0.28, t_{AlGaN} =16nm, V_d = 20V]. (a) Vertical electric field, and (b) Elastic energy density.



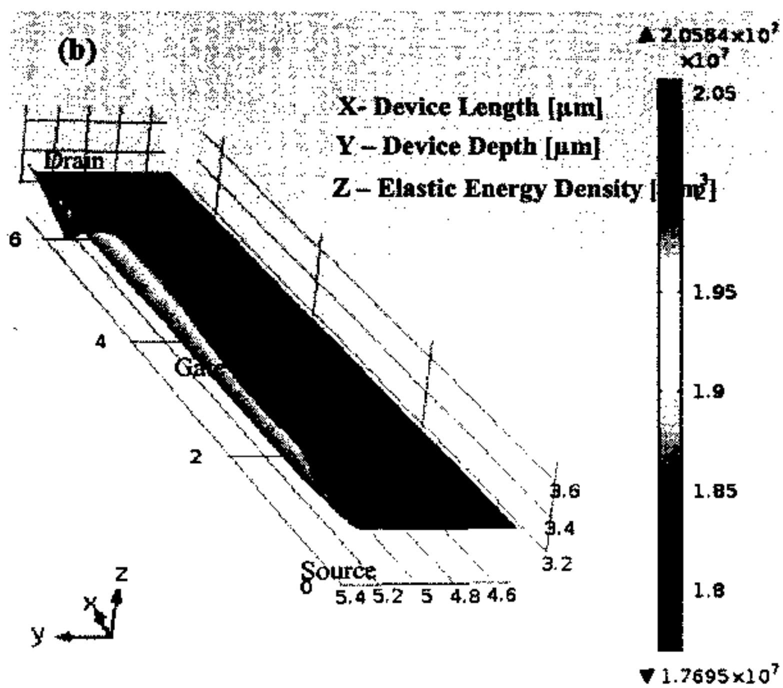


Figure 4.18. Results in AlGaN/GaN layers [x_{Al} = 0.28, t_{AlGaN} =22nm, V_d = 20V]. (a) Vertical electric field, and (b) Elastic energy density.

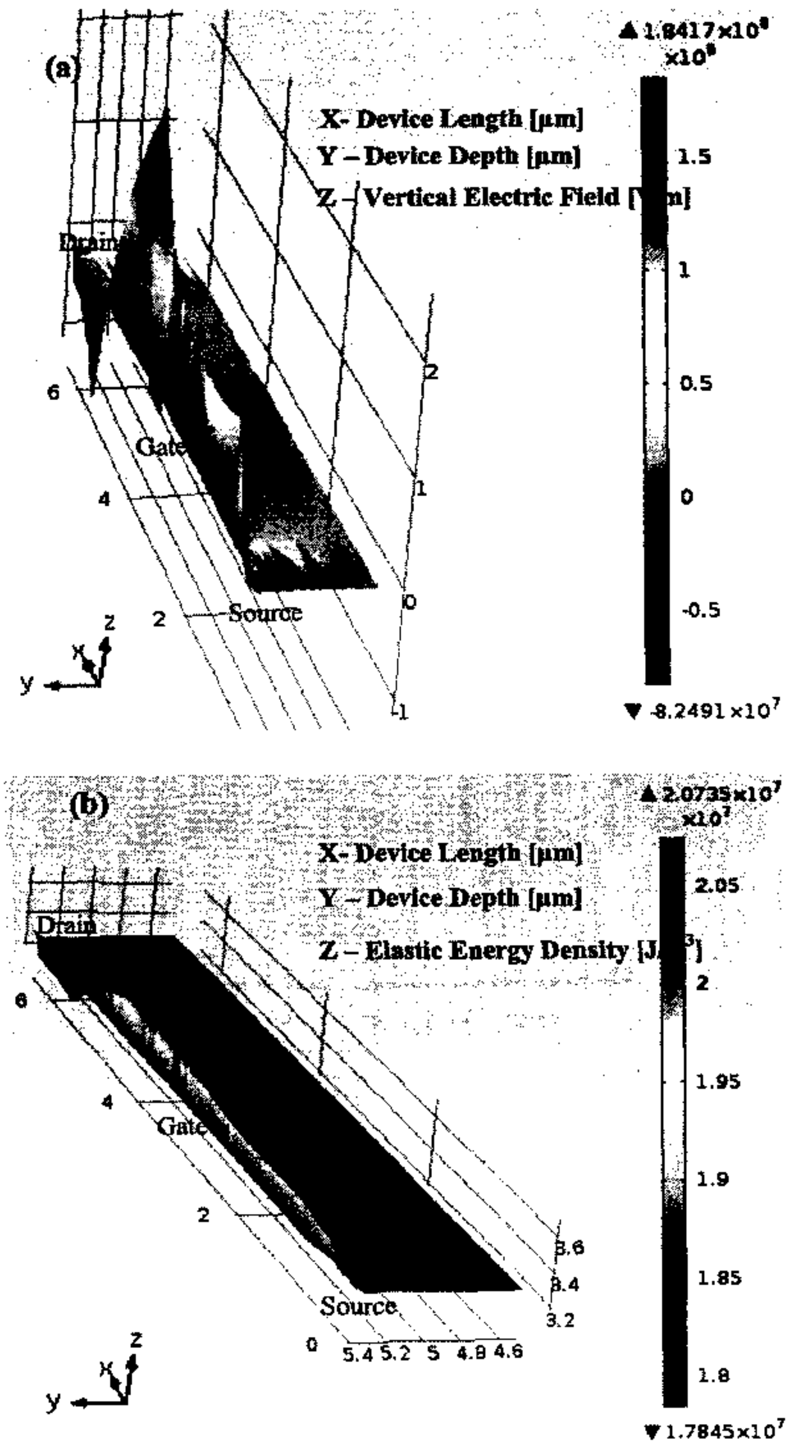


Figure 4.19. Simulations in AlGaN/GaN layers with HfO_2 (high-*k*) cap layer of 12nm [x_{Al} = 0.28, t_{AlGaN} =16nm, V_d = 20V]. (a) Vertical E-field, and (b) Elastic energy density.

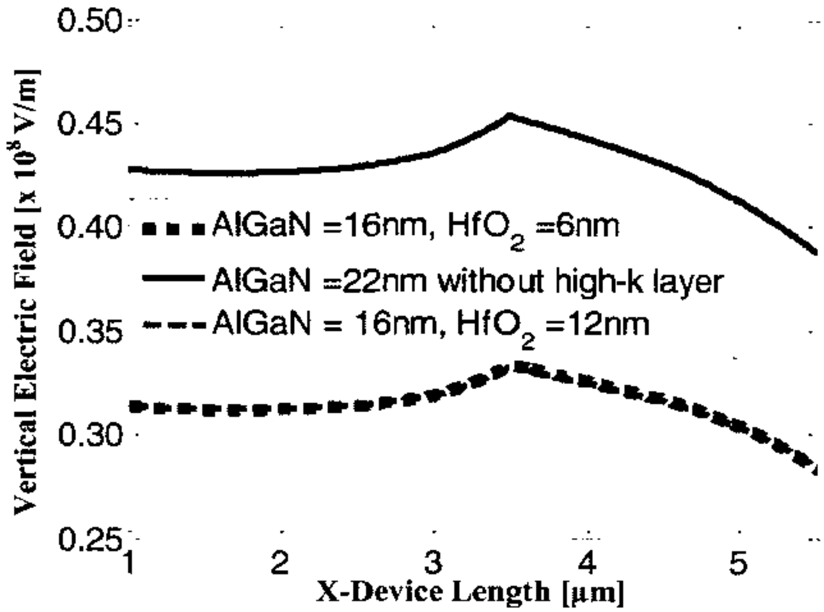


Figure 4.20. Elastic energy density in AlGaN layer with high-*k* (t_{AlGaN} =16nm) and without high-*k* (t_{AlGaN} =22nm) cap layer [x_{Al} = 0.28, V_d = 20V].

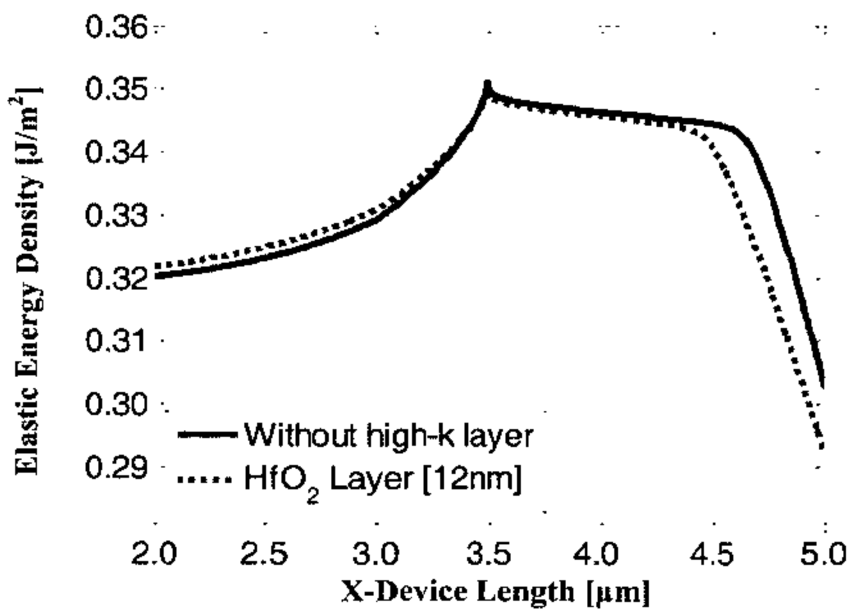


Figure 4.21. Elastic energy density in AlGaN layer with and without high-*k* cap layer [x_{Al} = 0.28, t_{AlGaN} =16nm, V_d = 40V].

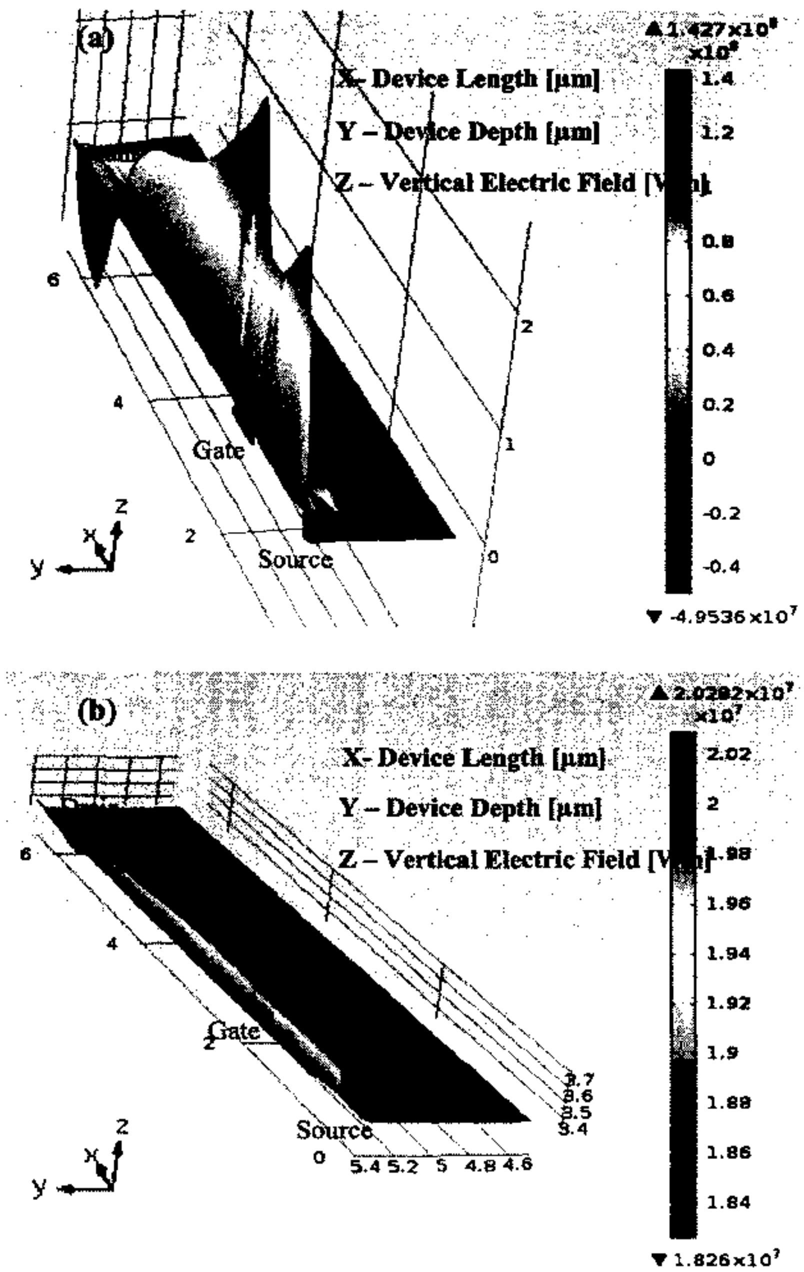


Figure 4.22. Results in AlGaN/GaN layers [x_{Al} = 0.28, V_d = 20V, t_{AlGaN} =16nm, Source to Gate width=1 μm gate-to-drain width = 4 μm]. (a) Vertical electric field, and (b) Elastic energy density

Figure 4.21 show the elastic energy density plot in the AlGaN layer with and without a high-*k* cap layer of 12nm at higher drain bias (40V). The elastic energy is maximum at the gate edge on the drain side, similar to the results for the case with a drain bias of 20V. However, the results show a nearly flat line up to 1μm after the gate edge with high stored elastic energy. It also shows a decrease in the elastic energy density value due to high-*k* cap layer.

4.2.5 FOCUS ON POSITION OF GATE

The position (i.e., relative placement) of the gate electrode was observed to influence the magnitude of electric fields in AlGaN layer as well. In figure 4.22, the effect of gate shift towards the source side. As the gate moves towards the source, the values of electric fields and elastic energy density were observed to decrease strongly. The vertical electric field and elastic energy density values have decreased from 2.08 x 10^8 V/m to 1.46 x 10^8 V/m and 0.335 to 0.325, respectively, with gate shifted toward source by 1.5 μm from center. The AlGaN thickness was taken to be 16nm, with a 0.28 Aluminum content and a 20V drain bias. Table 4.1 summarizes the maximum values of vertical electric field and elastic energy density for all the cases discussed above for comparison.

Table 4.1. Maximum values of vertical electric field and elastic energy density in AlGaN layer.

Parameter	x_{Al}=0.26 t_{AlGaN}=16 V_d=20	x_{Al}=0.28 t_{AlGaN}=16 V_d=20	x_{Al}=0.3 t_{AlGaN}=16 V_d=20	x_{Al}=0.28 t_{AlGaN}=22 V_d=20	x_{Al}=0.28 t_{AlGaN}=16 V_d=20 HfO_2=12nm	x_{Al}=0.28 t_{AlGaN}=16 V_d=20 (L_{sg}<L_{gd})
Vertical Electric Field	1.9x10^8 (V/m)	2.02x10^8 (V/m)	2.1x10^8 (V/m)	1.75x10^8 (V/m)	1.87x10^8 (V/m)	1.46x10^8 (V/m)
Elastic Energy Density	0.29 (J/m^2)	0.334 (J/m^2)	0.38 (J/m^2)	0.455 (J/m^2)	0.332 (J/m^2)	0.325 (J/m^2)

4.3 THERMAL MODELING RESULTS FOR ALGAN/GAN HEMTS

For completeness, thermal modeling was carried out based on model described in section 3.3.2. The 2DEG channel power density for a given bias and thermal strain due to the change in temperature were observed. Figure 4.25 shows power density calculated across the AlGaN/GaN interface. Figure 4.26 shows the 2DEG channel temperature due the power density values applied across the active device area. The observed temperature increase was insignificant. Figure 4.27 shows the thermal in plane and out of plane strain due to 2DEG channel temperature in AlGaN layer. These results collective underscore the irrelevance of thermal heating. Such temperature increases have been shown to be insignificant, and play no possible role in contributing to internal stresses or degradation of the GaN HEMT structures.

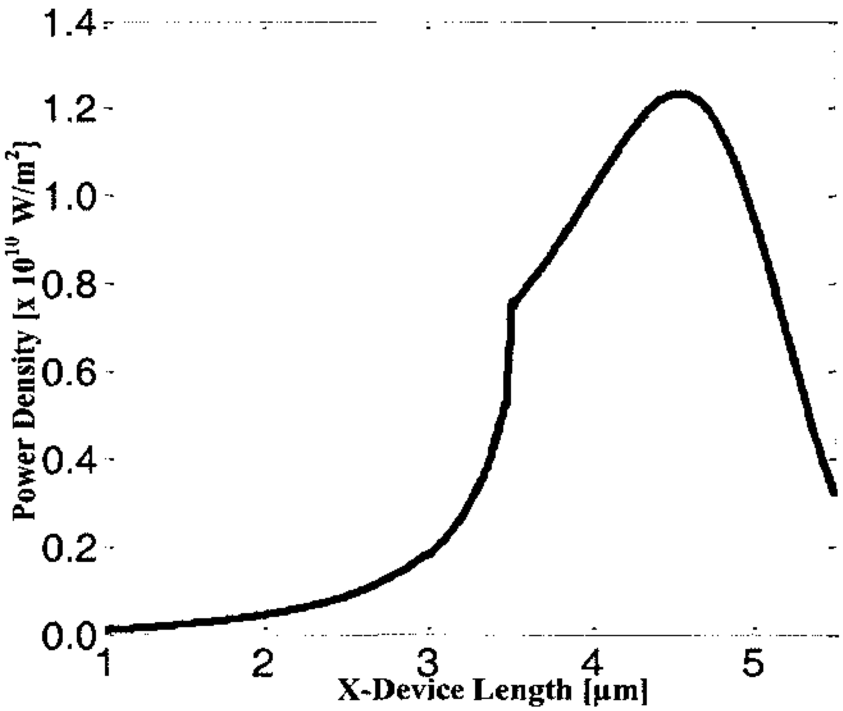


Figure 4.23. Power density across AlGaN/GaN interface [x_{Al} = 0.28, t_{AlGaN} =16nm, V_d = 20V].

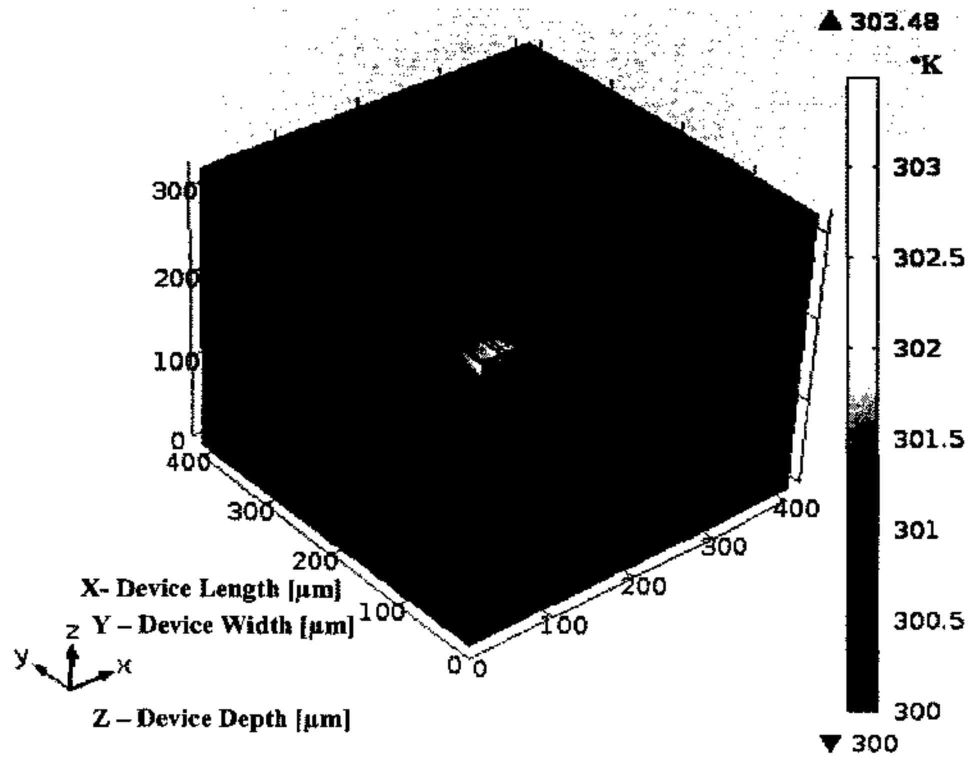


Figure 4. 24. Temperature distribution across GaN/Substrate from a 3D model.

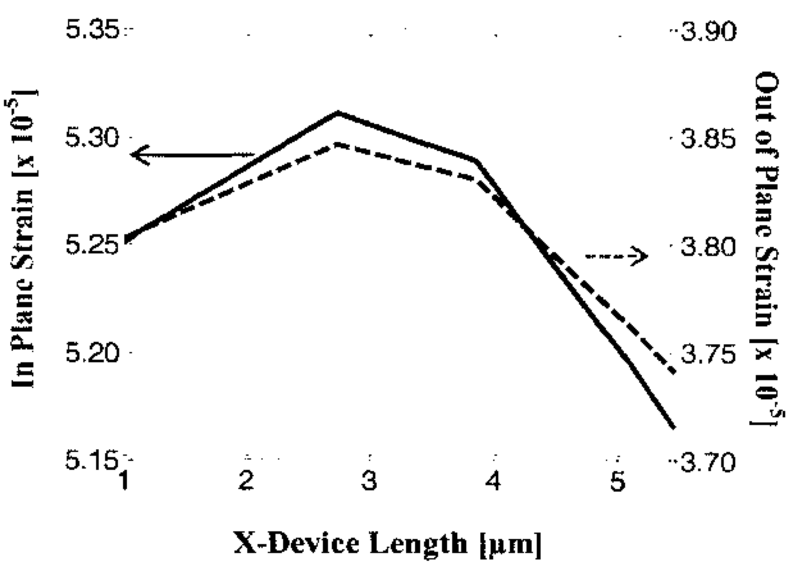


Figure 4. 25. In-Plane and out of plane strain in AlGaN layer [x_{Al}=0.28, t_{AlGaN} =16nm, V_d = 20V].

4.4 CONCLUSIONS

For the design of AlGaN/GaN HEMTs, it is important to understand the role of parameters such as AlGaN thickness and Aluminum content that affect the formation of the 2DEG, and electric fields that drive the inverse piezoelectric effect. The analysis presented in this chapter was based on simulation results that were obtained by varying important design parameters. The 2DEG was observed to increase with larger AlGaN thickness and Aluminum content. But, it is also important to reduce the electric fields in the AlGaN layer which were observed to be present at the gate edge near drain side and were increasing with increasing Aluminum content. The effect of high-k layers were also studied. It was understood from the results that a larger AlGaN thickness can be used to reduce electric fields. However, since this thickness cannot go beyond a critical value (otherwise unstable island formation can occur), high-*k* layer can be used to further reduce both the electric fields and elastic energy densities. Results also suggested that larger the drain-to-gate electrode distance, the lower are the vertical electric field and stored energy density values. Also, strain changes due to temperature changes were studied, and thermal strain due to 2DEG channel temperature changes were observed to be almost insignificant.

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

5.1 CONCLUSIONS

Numerical simulation models were developed to quantitative access and evaluate the role of the inverse piezoelectric effect (IPE) in AlGaN/GaN High Electron Mobility Transistors at high electric fields. The high electric fields arise practically in the scaled down devices that typically have sub-micron dimensions. The goal was to acquire the numerical capability to investigate the parameters that drive the degradation due to the IPE in HEMTs. Another important objective was to assess the relative effect of each parameter in affecting the reliability of the device, and the ways in which detrimental effects could be reduced through a judicious choice of the parameter or geometry or material. These objectives were all successfully achieved. We investigated, electric field distribution, stress, strain and stored energy in AlGaN layer for an AlGaN/GaN HEMT structure in detail. In addition, an optimized parameter space was probed, and for completeness, the role of device heating was also examined.

The model development was initiated by considering the changes in 2DEG density, electric field distributions and stored elastic energy with variations in Al mole fraction in the AlGaN layer, as well as changes in AlGaN thickness and drain biasing. The calculations were discussed in detail in chapter 3 and the results obtained with each set of parameter variation were presented in Chapter 4. It was observed that Al mole fraction and AlGaN thickness play an important role in inducing high electric fields in AlGaN layer. Pseudomorphic AlGaN layers grown on GaN layers have tensile in-plane strains. The elastic energy generated by such strains leads to deformation. With increasing Al mole fraction, the strain present in AlGaN layer was observed to increase significantly. Consequently the critical thickness where dislocations can become detrimental, places an important limit on device design. Although higher 2DEG densities and lower electric fields were observed with the increasing thickness of AlGaN layer, the significant increase observed in elastic energy stored in AlGaN layer were seen to place limit on the barrier layer thickness. Values beyond which dislocations can potentially start to occur were determined. Consequently, a low Al content AlGaN layer and thickness below critical thickness were observed to be important for reducing the device degradation. The effect of capping layers such as high-*k* cap layers on top of AlGaN layers were studied.

The use of high-*k* materials such as HfO_2 and Ta_2O_5 as cap layers was examined. High-*k* materials are commonly used as insulators to reduce the leakage current from gate. It was observed that, electric field magnitudes and stored elastic energy densities could be decreased with the use of high-*k* cap layer, although no significant difference was observed between HfO_2 and Ta_2O_5 materials as cap layers. Therefore, AlGaN/GaN model with high-*k* cap layer were shown to ensure low gate tunneling through traps, sustain much higher critical voltages, and support a larger gate voltage swing. Also, electric field magnitudes were observed to be further reduced with increasing high-*k* cap layer thickness. These high-*k* cap layers are commonly grown using Atomic Layer Deposition method which is used to grow thin uniform layers. In the numerical evaluations, high-*k* layers with 6nm and 12nm thickness were used. Our results thus indicate great potential of high-*k* cap/AlGaN/GaN MOS HEMTs for high power applications. The effects of shifting the gate position were also observed. Results showed that the electric fields and in turn the stored elastic energy densities, could be decreased with increasing distance between gate and drain. For completeness, the effects of power density generated due to 2DEG and its influence on 2DEG channel temperature and in turn thermal strain were also studied. The drain bias applied in the model was in the range of 5 to 20V. In this range, the temperature changes as well as thermal strain were observed to be very low. Therefore, considering the overall results, it can be summarized that a AlGaN/GaN HEMT model with relatively low Al content, AlGaN layer with thickness below critical thickness that generates enough 2DEG density for high power applications, a high-*k* cap layer that suppresses large electric fields, and gate tunneling, gate position towards the source end will form an optimum parameter set for reducing the device degradation.

5.2 FUTURE WORK

The AlGaN/ GaN HEMT model developed for understanding the underlying degradation mechanism based on the inverse piezoelectric effect with different model parameters (such as Al content, barrier thickness, cap layers etc.) is useful. However, this model can be further improved and the methodology can be applied to numerous other applications. A few such tasks for possible future work are presented below.

1. The present model assumed AlGaN layer as the barrier layer. The same model simulation could be used for evaluating different alloy compositions such as InGaN barrier layers. Such evaluations would provide insights into the effects of different alloy composition on device degradation.
2. In this model, a single high-*k* layer was used as cap layer. The model can be expanded by using a passivation layer such as silicon nitride or aluminum nitride layer between the high-*k* cap and the barrier layer.
3. The model as explained in the previous section was simulated with drain bias in the range of 5 to 20V. The model can be simulated at higher drain bias for all different cases to observe the value of critical voltage beyond which the elastic energy density might reach the critical threshold value.
4. Also, the temperature effects could be coupled to the electrical simulation model by adding the thermal strain value as initial strain in the AlGaN layer while calculating the total stress generated. This would make for self-consistent thermal analyses.
5. The model described used sapphire as substrate. The effects of different substrates on temperature changes could also be studied using the model developed in this research.
6. The effects of different Cap layers such as AlN, InGaN and the relation between strain variations in AlGaN layer due to cap layers could also be studied.
7. A uniform positive charge representing the spontaneous and piezoelectric polarization and 2DEG charge was applied at the AlGaN/GaN interface. The effects of additional trapped charges in the AlGaN layer could be studied to better understand the changes in the electrostatics of the device due to trapped charges

in the barrier layer. Such charging can practically result from gate tunneling currents.

8. Finally, a self-consistent, dynamic model towards device failure could be developed. This would need to include leakage currents, charge trapping from the leakage flux, concomitant changes in the local electric field due to variations in the trapped charge, and the positive feedback for subsequent leakage currents. A feedback loop could be constructed for a dynamic development until final device failure with large leakage currents. For greater accuracy and completeness, thermal changes in the material properties, or trapping- or detrapping characteristics could also be included.

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