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Thermo-Piezo-Electro-Mechanical Simulation of AlGaN (Aluminum Gallium Nitride) / GaN (Gallium Nitride) High Electron Mobility Transistor

Lorin E. Stevens
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THERMO-PIEZO-ELECTRO-MECHANICAL SIMULATION OF ALGAN
(ALUMINUM GALLIUM NITRIDE) / GAN (GALLIUM NITRIDE)
HIGH ELECTRON MOBILITY TRANSISTOR

by

Lorin E. Stevens

A thesis submitted in partial fulfillment
of the requirements for the degree

of

MASTER OF SCIENCE

in

Mechanical Engineering

Approved:

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UTAH STATE UNIVERSITY
Logan, Utah

2013
ABSTRACT

Thermo-Piezo-Electro-Mechanical Simulation of AlGaN (Aluminum Gallium Nitride) / GaN (Gallium Nitride) High Electron Mobility Transistor

by

Lorin E. Stevens, Master of Science
Utah State University, 2013

Major Professor: Dr. Leila Ladani
Department: Mechanical Engineering

The objective of this research has been to understand the stress/strain behavior of AlGaN/GaN High Electron Mobility Transistors (HEMT) through multiphysics modeling and simulation. These transistors are at scales of micro/nano meters and therefore, experimental measurements of stress and strain are extremely challenging. Physical mechanisms that cause stress in this structure include thermo-structural phenomena due to mismatch in both coefficient of thermal expansion (CTE) and mechanical stiffness between different materials (e.g. metal traces used as gate, source, and drain; isolation layers; GaN; and AlGaN), piezoelectric effect caused by application of gate voltage, and existence of a two-dimensional electron gas (2DEG) layer in between AlGaN and GaN materials. COMSOL Multiphysics software was used to conduct a finite element (FE) simulation of the device to determine the temperature and stress/strain distribution in the device, by coupling the thermal, electrical, structural, and piezoelectric effects inherent in
the device. The HEMT-unique 2DEG layer has been modeled as a simultaneous localized heat source and surface charge density, whose values are based on experimental results in literature. Select anisotropic material properties reported in literature were used for AlGaN and GaN; all other materials were considered isotropic. A 3D thermal model is initially conducted to obtain a literature-validated temperature distribution which is then applied to a separate 2D model to find the resulting coupled thermo-piezo-structural stress/strain distributions. The contribution and interaction of individual stress mechanisms including piezoelectric effects and thermal expansion caused by device self-heating have been quantified. Critical stress/strain values and their respective locations in the device have been identified as likely failure locations, and have been compared to results in literature. The visualization of stress/strain distribution through FE modeling has assisted in estimating the mechanical failure mechanisms and possible mitigation approaches. Select results include: 1) tensile inverse piezoelectric stress and compressive thermal stress, 2) coupled von Mises stress increased with drain voltage, with a higher rate of increase as gate voltage became more positive, and 3) piezoelectric stress (uncoupled) increased with either higher drain voltage or more negative gate voltage. Mismatch between layers was also a factor which produced stress concentration at interfaces. To decrease the likelihood of device failure due to these mechanisms, it is recommended to utilize substrate materials with high thermal conductivity and also set reasonable gate/drain voltage levels to assist in mitigating overall stress/strain buildup.

(117 pages)
Due to the current public demand of faster, more powerful, and more reliable electronic devices, research is prolific these days in the area of high electron mobility transistor (HEMT) devices. This is because of their usefulness in RF (radio frequency) and microwave power amplifier applications including microwave vacuum tubes, cellular and personal communications services, and widespread broadband access. Although electrical transistor research has been ongoing since its inception in 1947, the transistor itself continues to evolve and improve much in part because of the many driven researchers and scientists throughout the world who are pushing the limits of what modern electronic devices can do. The purpose of the research outlined in this paper was to better understand the mechanical stresses and strains that are present in a hybrid AlGaN (Aluminum Gallium Nitride) / GaN (Gallium Nitride) HEMT, while under electrically-active conditions. One of the main issues currently being researched in these
devices is their reliability, or their consistent ability to function properly, when subjected to high-power conditions.

The researchers of this mechanical study have performed a static (i.e. frequency-independent) reliability analysis using powerful multiphysics computer modeling/simulation to get a better idea of what can cause failure in these devices. Because HEMT transistors are so small (micro/nano-sized), obtaining experimental measurements of stresses and strains during the active operation of these devices is extremely challenging. Physical mechanisms that cause stress/strain in these structures include thermo-structural phenomena due to mismatch in both coefficient of thermal expansion (CTE) and mechanical stiffness between different materials, as well as stress/strain caused by “piezoelectric” effects (i.e. mechanical deformation caused by an electric field, and conversely voltage induced by mechanical stress) in the AlGaN and GaN device portions (both piezoelectric materials). This piezoelectric effect can be triggered by voltage applied to the device’s gate contact and the existence of an HEMT-unique “two-dimensional electron gas” (2DEG) at the GaN-AlGaN interface.

COMSOL Multiphysics computer software has been utilized to create a finite element (i.e. piece-by-piece) simulation to visualize both temperature and stress/strain distributions that can occur in the device, by coupling together (i.e. solving simultaneously) the thermal, electrical, structural, and piezoelectric effects inherent in the device. The 2DEG has been modeled not with the typically-used self-consistent quantum physics analytical equations, rather as a combined localized heat source* (thermal) and surface charge density* (electrical) boundary condition. Critical values of stress/strain and their respective locations in the device have been identified. Failure locations have
been estimated based on the critical values of stress and strain, and compared with reports in literature. The knowledge of the overall stress/strain distribution has assisted in determining the likely device failure mechanisms and possible mitigation approaches. The contribution and interaction of individual stress mechanisms including piezoelectric effects and thermal expansion caused by device self-heating (i.e. fast-moving electrons causing heat) have been quantified.

* Values taken from results of experimental studies in literature
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Lorin E. Stevens
## ABSTRACT

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Contribution of thermal and piezoelectric volumetric strain to coupled solution, as gate and drain voltages were altered.............92
1.1. **Literature review**

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 [1]. One of the main issues being researched in these devices is their reliability.

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 [2, 3]. 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 [4] 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 [5].
Studies conducted by Kisielowski et al. [6] 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 Sarua et al. [7]. Internal strain is induced in material to accommodate the lattice constant mismatch in GaN-AlGaN structures during the fabrication of these devices. Because of the piezoelectric effect, these strains induce electric fields that may strongly affect the carrier distributions near the material interfaces [8]. Over time, relaxation of the strains caused by high temperatures in the device channel (i.e. 2DEG region) 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 a 2009 experimental study performed by del Alamo and Joh [9], it was found that when subjected to a critically-high gate voltage, the HEMT may exhibit electric current leakage defects, generated either within the AlGaN layer or near the gate’s lower edge. The authors of the study were led to believe that the inverse piezoelectric effect was introducing mechanical stress into the AlGaN layer and eventually producing these defects. Because experimental testing of these miniature devices presents various difficulties, many finite element (FE) approaches have also been used to perform reliability analyses.

In Sarua et al. [10], two-dimensional (2D) FE simulation in conjunction with Raman optical spectroscopy were used to show that a source-drain voltage ($V_{ds}$) 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.

Beechem et al. [11] performed a study using both experimental Raman optical spectroscopy and FE analysis to compare/contrast major stress contributors in an HEMT device (thermal, converse piezoelectric, residual). The study found that the dominant residual tensile stress is counterbalanced by the compressive thermal contribution, and also that the 2DEG density is intrinsically linked to the stress level that evolves during device operation.

Sarua et al. [7] performed a study similar to their previous one [10], but this time thermal effects were more closely considered. While in the previous study a gate voltage \( V_{gs} \) of −8 V was used to prevent self-heating by keeping the channel current below 0.3 mA, in this latter study the effect of self-heating generated in operating AlGaN/GaN HEMT devices on mechanical strain/stress was investigated while varying the source-drain voltage \( V_{ds} \). The services of three-dimensional (3D) thermo-mechanical numerical modeling using TAS (i.e. Thermal Analysis System) finite-difference-based software (created by ANSYS) was employed for simulation, and then compared with the Raman optical spectroscopy experimental results. One conclusion made from this study was that the thermal stress generated by non-uniform self-heating in these devices was not only on the same order of magnitude as the piezoelectric stress present, but its opposite sign denoted a potential source for an overall reduction in the net stress experienced in the device during operation.
Benbakhti et al. [12] utilized COMSOL software to create a coupled 2D electro-thermal model of a GaN-based transfer length measurement (TLM) [i.e. gateless HEMT] structure. Electron mobility values were calculated and used to show that for a given electric field, an unfavorable decrease in electron mobility occurs when the 2DEG temperature is raised; thus self-heating in the modeled device was found to decrease overall high-power performance. Additionally, Bertoluzza et al. [13] has performed a 3D thermal simulation of GaN-based HEMT structures using COMSOL to show the complex interaction of device variables including geometry, substrate material, and heat removal strategies, and their contribution to the overall thermal effects.

1.2. Gaps in the literature

Through critical observation of what has already been done in research as well as considering suggestions made in literature, there is much need for additional research of AlGaN/GaN HEMTs. Sarua et al. [10] calls for further investigation of piezoelectric strain fields generated by high bias levels, and the effect of carefully coupling physical processes in the modeling procedure, due to the order-of-magnitude inconsistency between their experimental and simulation stress values in an HEMT device. They point out that at present, little is known about the effect of electric field characteristics on inverse piezoelectric strain, and suggest the future development of full-scale coupled models because of the complex nature of these devices. In addition, they state that the present lack of experimental data describing both the electric and elastic fields is limiting the scholarly progress in understanding the overall device properties during operation. Although Beechem et al. [11] made note of the discrepancy by Sarua et al. [10], and performed a study of their own to see if results would be any different, they used an
isotropic linear elastic assumption for all materials. Though their reasoning for this was that anisotropic properties reported in literature have more discrepancy between them than reported isotropic properties, the alternative anisotropic approach was not considered for comparison. In addition, their outright exclusion of the AlGaN, gate, source, and drain from thermal consideration because of their small size resulted in stress/strain results which lacked data from these regions which are important to analyze, even though their effect on the maximum temperature in the device is undoubtedly negligible. Sarua et al. [7] stated that the effects of non-uniform heating on thermal stresses in AlGaN/GaN devices is much less studied than other well-known device degradation issues such as the inverse piezoelectric effect, and hence the very limited knowledge of its effects on reliability call for more work in the area by willing researchers. Although much has already been done to determine the exact causes of both electrical and mechanical HEMT device degradation, many studies in literature have reiterated the fact that more research needs to be done on the subject.

Because HEMT devices are fabricated on such a small scale (i.e. nano-micro), testing their mechanical behavior is usually very challenging and requires extensive equipment. For example, measuring 2DEG channel temperature using common methods of micro Raman spectroscopy and infrared thermal imaging have limitations of device geometry dependence, difficulty in assessing fully-packaged devices, and vertically averaging temperature in GaN [14]. A multiphysics modeling approach will provide insights to how and if the simultaneous combination effects of temperature and piezoelectricity may activate certain failure mechanisms, and if these mechanisms diminish the reliability of these devices. This physics-based modeling will predict the
stress concentration points and potential damage initiation sites. The modeling will also justify further experimental investigations of these phenomena if necessary.

1.3. Thesis statement

This thesis proposes to investigate the stress/strain behavior that occurs in an AlGaN/GaN-based HEMT through the means of multiphysics FE simulation. In contrast to quantum physics-based modeling approaches which are common in literature, this thesis will take a novel mechanical approach of coupling piezoelectric effects, thermal expansion, and electric conditions present on selected model boundaries, in order to mimic the mechanical effects of actual intricate electrical flow through the transistor. The expected outcomes are realistic material deformations along with indications of potential failure sites in the active device deduced from calculated stress values. The specific contribution of each set of modeled physics (i.e. piezoelectric, thermal, structural, electrical) to mechanical behavior in the device will be quantified, with specific analysis of how each affects the other physics present. Thus, the end product of this thesis will be a report detailing: 1) individual and collective mechanical effects of the physical phenomenon that coexist in these devices, 2) a comparison to both simulated stress/strain and experimental behavior results found in literature, and 3) the effectiveness of the modeling approach, with suggestions for future improvement.

1.4. Approach

1.4.1. Mechanical standpoint. A finite element model using only COMSOL Multiphysics software will be developed to determine the stress/strain behavior of a select HEMT device experimented upon in literature. The focus of the overall approach
to this research will be to put emphasis on the mechanical issues in the HEMT device, while making simplifying assumptions for the electrical details, in order to understand the device stress/strain mechanics. In reality, the 2DEG region of an HEMT device has a highly complex quantum nature [15]. 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 two boundary conditions: 1) a heat source value (i.e. power dissipation), and 2) a surface charge density resulting from polarization present in the GaN and AlGaN materials. Both of these boundary conditions will be extracted from experimental values found in literature.

**1.4.2. 3D thermal analysis.** HEMT devices have been modeled in literature as both 2D and 3D structures. However, Menozzi et al. [16] showed that 2D thermal models tend to over-predict the peak temperature in the active device area (i.e. 2DEG region) – more accurately predicted by 3D thermal models. It is well-known that performing a 2D analysis instead of 3D cuts down on computation time due to a lower quantity of meshing elements, but because Menozzi et al. [16] showed the adverse effects of neglecting 3D thermal effects, the author of this thesis report chose to do a 3D thermal analysis, using symmetry where possible to reduce computation time. One consideration needed in taking a 3D approach, however, is whether all domains need to be included in the model. If the relatively thin AlGaN layer and the three superior contacts (see section 2.3.3) are included, the 3D model quickly becomes overburdened with an excessive amount of elements. This is because the meshing step of modeling requires many elements to be produced in these thin domains in order to maintain a reasonable level of element quality and aspect ratios necessary for a reliable model solution to be produced.
Because of this fact, it is common in literature to disregard these relatively thin layers in thermal analysis because their small size (nm) relative to the GaN and substrate (μm/mm) yields them negligible in affecting the peak temperature in the active device area. The author of this thesis report has chosen to remove these superior layers in the 3D thermal analysis, leaving just the GaN and substrate to be analyzed, with the active device area modeled as a heat source value at the location where the AlGaN/GaN heterojunction would be.

1.4.3. 2D coupled analysis. When it comes to including the piezoelectric and other structural effects into a coupled multiphysics model in order to determine the overall stress/strain behavior in the HEMT device, the structural and thermal expansion mismatch of the AlGaN layer and superior contacts as well as the piezoelectric properties of AlGaN all are critical, thus they cannot be disregarded. One way to accommodate for this is to create a 2D model, and carefully take into consideration both the knowledge of how an HEMT functions electrically as well as its overall geometry.

In 2D FE modeling, it is required for the user to define whether a state of plane strain or plane stress is being assumed to represent true 3D geometry. It is very common in literature to see 2D illustrations of HEMT devices (see section 2.3.3), 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, and a plane strain assumption for a 2D model seems most logical. Moreover, Beechem et al. [11] claim select HEMT devices exhibit a “biaxial” state of stress, but only in the plane of the 2DEG. Thus, if the device is to be modeled as the 2D profile most commonly seen
in literature (see section 2.3.3), a state of plane stress would not be realistic. Because of these considerations, a state of plane strain has been chosen for the 2D coupled model.

1.4.4. 2D boundary condition considerations. Using a 2D coupled model requires that the data in the 3D thermal model somehow be imported. Most FE softwares allow a user to extract data along any given edge in the model, most commonly to create plots. However, the author of this thesis will utilize this data extraction capability in COMSOL to extract temperature values at all meshing nodes along select edges in the 3D thermal model (see Fig. 1) and import these data sets of temperature vs. position, into a 2D coupled model, as interpolation functions to be applied as position-dependent temperature expressions assigned to boundary conditions along edges corresponding to a 2D profile (similar to that shown in section 2.3.3) of the 3D model. Because the temperatures found along the active device area are of greatest interest, temperature data extraction will not be necessary on all 3D model edges, rather just those located directly below the active device area, with the rest of the 2D model temperature values being determined by material-dependent thermal conduction. Other crucial boundary conditions applied in the 2D coupled 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 will then undergo a coupled thermal-structural-piezo analysis, including the effects of thermal expansion.

It is important to note here that the voltages applied to the source, drain, and gate will not be applied at the top of the contacts, rather at their base (i.e. at their interface with the underlying AlGaN layer). The reason for this is that the purpose of the voltage in the model is not to create a functioning electrical device, rather to see how it affects the
Fig. 1 – Schematic showing transition from 3D thermal model to 2D coupled model. Edges of temperature data extraction are shown in blue, and the active device area at 2DEG location is shown in red.

Piezoelectric materials which are sensitive to the influence of surrounding charge and voltage levels.

The base of the substrate will possess an isothermal (300 K) boundary condition and all other external boundaries will be considered adiabatic (i.e. insulated) – both conditions being consistent with literature [16]. Geometry as well as material properties will be taken from literature, and where geometry is not explicitly detailed, ratios will be employed by comparing with other relevant studies in literature.

1.4.5. Overview. The overall modeling approach for this thesis report is shown in a flowchart in Fig. 2. Fulfilling what was outlined in the thesis statement, the developed computer model will be able to perform not only a coupled thermal-structural-piezo analysis, but will also be able to isolate the contribution of each physics subset and
analyze how it ends up affecting the others when becoming coupled with them. This will be made possible by the many useful post-processing features of COMSOL which conveniently allows the visualization of both the location and value of maximum temperature and stress/strain. The user can at any time choose to momentarily deactivate a certain physics subset in order to see the contribution of another. In this way it is possible to isolate the contribution of stress/strain from both the piezoelectric and the thermal expansion parts of the model, as well as how bias applied to source, drain, and gate affect piezoelectric stress/strain. The location of critical values will be compared/contrasted with what has been reported in literature. Possible reasons for deviation from results in literature will be stated.

Fig. 2 – Flowchart of thesis research, outlining the overall approach to accomplishing objectives of the thesis
2.1. **Primitive transistors**

The transistor is an electric device that was invented by Bell Laboratories in 1947, followed soon thereafter by Texas Instruments (TI). In its primitive state, the device consisted of two closely-spaced metal points on a germanium surface, and was later given the name of “point contact” transistor. One point was called the “emitter” and the other point the “collector”; a third contact called the “base” was applied to the back side of the germanium. A positive electrical bias applied to the emitter increased the conductivity of the germanium just beneath the collector, and thus the output current to the collector from the base was amplified. Just three years later in 1950, Bell Labs introduced silicon transistors in place of germanium, because of its increased reliability in extreme temperature conditions; TI soon made these transistors on a commercial scale for public use in 1954 [17].

In electronic circuits, the transistor has one of two primary purposes: to act either as an on/off switch or as an amplifier of current, voltage, or power inputs. The basic functioning of the transistor described above can be more fully understood by knowing the basic functioning of its predecessor, the diode (e.g. on/off electrical switch). There are two kinds of semiconductors: p-type and n-type; a diode is made by placing them in direct contact with each other. N-type semiconductors conduct current by producing excess electrons and conversely, a p-type semiconductor conducts current because of its deficiency of electrons, i.e. “holes.” Once united, there is a “pn junction” formed at their boundary, across which electric current can flow in just one direction. As seen in Fig.
3(a), once the positive terminal of a battery is connected to the n-type material, electrons (negatively-charged) in this material are attracted to this terminal; in likewise fashion, the p-type holes move in the direction of the negative terminal of the battery. Another way of seeing this is that the charge carriers in both materials move away from the pn junction, creating a wide space called the “depletion region,” so that negligible electric current can flow; this is called a reverse-biased diode. If the battery terminals are switched (Fig. 3(b)), then the electrons in the n-type material move away from its negative terminal and toward the pn junction; the holes in the p-type material move away from its positive terminal and toward the pn junction. This makes a narrow depletion

Fig. 3 – The two types of pn junction scenarios formed in a semiconductor diode. (a) Reverse-biased pn junction (i.e. switch “off” position). (b) Forward-biased pn junction (i.e. switch “on” position). [17]
region at the pn junction, and the electrons and holes at that location neutralize each other, and thus electric current flows easily through the diode [17].

Although a diode can control the direction of the current, it cannot control the size of current flowing through it – however, a transistor can do both. The way to go from a simple pn junction diode to a transistor is to sandwich two of them together in either “pnp” or “npn” (see Fig. 4) fashion, which function in very similar ways. As mentioned earlier, the simplest transistor has three components: an emitter, collector, and base. In the npn transistor, the emitter is an n-type material with many excess electrons, the base is a thin p-type material having a small amount of holes, and the collector is an n-type material with a moderate quantity of electrons. Since there are two pn junctions in this device (emitter-base boundary and base-collector boundary), then there are two depletion regions belonging to these junctions; these regions are the key to the transistor being able to act as an amplifier [17].

In essence, a transistor can amplify an input signal by first applying a variable small voltage between the base and emitter, which in turn acts as the control for the size of the larger (i.e. “amplified”) output current between base and collector. Because the emitter-base diode is forward-biased by a voltage source (e.g. battery), then electrons can freely flow from the emitter to the base. Conversely, the base-collector diode is reverse-biased, such that no holes flow into the base (because of the wide depletion region); this prevents them from intercepting any electrons in the emitter-base forward-biased diode, which would block the current from flowing in the device. Thus, the current running through the transistor, only from the emitter to collector, is controlled solely by the depletion region at the emitter-base junction. When this depletion region is thick, the
Fig. 4 – The basic junction transistor is created by putting two pn junction diodes back-to-back in either pnp or npn fashion; the case of the npn junction transistor is shown here. (a) Illustration of the effect of the forward-biased emitter-base diode on both the flow of electrons and holes. (b) Illustration of complete npn transistor function under active electronic conditions. [17]

Important to understand is that on the other hand when this depletion region is thin, electrons shoot quickly across the emitter-base junction, but they are not blocked by the wide depletion region surrounding the base-collector junction. This is because the base itself is designed to be narrow compared to its two counterparts, allowing the momentum of the electrons originating from the emitter to bring them close to the base-collector junction. Once there, most of the electrons are drawn into the collector by the positive voltage on its backside terminal, passing through the gate-collector junction and associated depletion region, and eventually flowing into the collector to the signify the circuit’s output signal [17].

Although the vast majority of the electrons reach the output signal, a few electrons are lost inside the base because they move into the vacant holes present there.
Hence, electrical engineers design transistors so that a very thin base requires the electron flow from emitter to collector to be extremely sensitive to the input current placed on the base contact, keeping the mainstream electrons from straying far on their path towards the collector. Low levels of dopants are also often included in the design to fill many of the vacant holes that deviant electrons would like to fill. The electric field driving the electrons from the base into the collector is created by the applied voltage across the emitter-base junction. Since this junction is forward-biased, then its varying input voltage changes not only the size of its associated depletion region, but also the size of the large (relative to the input) current flowing in the device [17].

Simple additions to this basic transistor change its amplifying function. As an example, the inclusion of a load resistor in the collector circuit makes the small variable emitter input produce an even larger varying collector voltage (instead of a larger current) by amplifying the signal at the base. Although these transistors (i.e. “bipolar junction” transistors), used to amplify current/voltage/power, have long since been improved upon by modern field-effect transistors (FET) in various forms, they still are widely used in high-frequency signal applications, and can still be found in many electronic devices such as broadband Internet modems, cable boxes, and CD/DVD players [17].

2.2. **Field-effect transistors (FET)**

Field-effect transistors (FET) were first developed in 1962, and have since become a very important component in the modern electronic industry. There are two basic types of transistors: bipolar and unipolar. The latter is more commonly referred to as FET, and has shown superior performance to bipolar transistors in many circuit applications. The basic idea behind an FET is that by using semiconducting materials,
the conduction of a one-way “channel” or pathway between source and drain terminals is
controlled by an electric field induced by a gate terminal. The channel may use either n-
type or p-type charge carriers, and the electric field which controls channel conduction
enters the device in two ways: by a p-n junction (for a “junction” FET, i.e. JFET) or by a
metal plate separated from the semiconductor channel by an oxide dielectric (for a metal-
oxide-semiconductor FET, i.e. MOSFET or “insulated gate” FET). A combination of
these two electric field introduction methods can be employed as well. The polarity
(positive or negative) of the controlling electric field is dependent on the type of carriers
(n- or p-type) found in the conducting channel [18].

JFET devices can be of either n- or p-channel types, both operating in a similar
fashion but differing in polarity, with the former type having higher channel conductance
and lower current leakage. For the n-channel JFET (see Fig. 5), between source and
drain contacts an n-type “channel” for carriers is embedded in a p-type semiconducting
substrate. Because the two p-n junctions form sidewalls for the current flow through the
channel, then the channel conduction is dependent on the channel geometry and also the
carrier flow density and mobility. Charge carriers will always flow from the lowest to the
highest potential, thus the current flow in the device can go just as easily from source to
drain as it can from drain to source, since the drain potential may be set to be positive or
negative with respect to the source [18].

MOSFET devices can also be of either n- or p-channel types. In an n-channel
MOSFET (see Fig. 6), the channel conduction is manipulated either by a voltage applied
between the gate and source or by a voltage applied between the substrate (i.e. body) and
source, or by a combination of the two. One key identifying characteristic of a MOSFET
is that the gate is separated from the conducting channel by a dielectric (often silicon oxide) which has low current leakage properties. This dielectric component allows the gate-channel voltage to be either positive or negative. For the n-channel MOSFET, a positive gate-source voltage increases the channel conduction, whereas a negative one decreases channel conduction. Since there is not an existing conducting path between the controlling gate and the remainder of the device structure (due to the dielectric presence), there is a gate-to-channel resistance developed, regardless of positive or negative voltage placed at the gate location. One key difference of a MOSFET from a JFET is that the former is capable of on-state operation with either positive or negative gate voltage,

![Fig. 5 – Typical n-channel junction field-effect transistor (JFET) on a p-type silicon substrate [18]](image1)

![Fig. 6 – Basic schematic of an n-channel metal-oxide-semiconductor (MOSFET) device [18]](image2)
whereas the latter operates only in the positive spectrum [18]. Later variations on the general MOSFET device include CMOS (complementary MOS), DMOS (double-diffused MOS), and VMOS (V-groove MOS) [19].

2.3. **High electron mobility transistors (HEMT)**

2.3.1. **Operation mechanism.** High electron mobility transistors (HEMT) also known as heterostructure field effect transistors (HFET), the modulation doped field effect transistor (MODFET), two dimensional electron gas field effect transistor (TEGFET), and selectively doped hetero-junction transistor (SDHT) utilize the difference in band gap between two different materials to form a two-dimensional electron gas (2DEG), which is used as the channel for electrons in the device. This 2DEG uniquely facilitates electron movement while avoiding collision of electrons with any dopants that may be present in the materials.

The meaning of a material’s band gap is the energy required to excite and free an outer shell electron from its orbit (in the valence band of electrons) about the nucleus; the electron thus becomes a mobile charge carrier (in the conduction band). A heterostructure is a structure that consists of two or more layers of different semiconducting materials (and differing band gaps), and the interface between any two of these layers is called a heterojunction, or heterointerface. Each semiconducting material has its own unique conduction and valence electron bands, thus their band gaps are different and there exist discontinuities (i.e. conduction and valence band offsets) at the heterojunction; the sum of these two offset types equal the band gap difference. Both band gap difference and band offsets are crucial factors contributing to the performance of heterostructure devices like HEMTs. In addition to these electric-based offsets at the
heterojunctions, “pseudomorphic” heterostructures are those that also experience a
mismatch in structural lattice constants at the same locations [20].

**2.3.2. GaN vs. 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 (2×10⁶ Vcm⁻¹ comparing with 4×10⁵ Vcm⁻¹ of GaAs),
high peak and saturation carrier velocity (3×10⁷ cm/s and 2×10⁷ cm/s comparing with
2×10⁷ cm/s and 10⁷ cm/s of GaAs) and good thermal conductivity (1.3 Wcm⁻¹K⁻¹
comparing with 0.55 Wcm⁻¹K⁻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 (operation at higher frequencies) [21]. A typical
AlGaN/GaN HFET device is shown in Fig. 7.

**2.3.3. Fabrication.** In manufacturing the device, a nano-scale layer of AlGaN
is grown on a comparatively larger micro-scale GaN layer, which is built on an even
larger micro-scale substrate. For example, Benbakhti et al. [22] used 21 nm AlGaN, 2
μm GaN, and 500 μm substrate of multiple material choices. The choice of substrate is
an important one; typical substrate materials are sapphire (Al₂O₃), Si, or SiC [13, 23].
SiC is generally considered to have the best thermal dissipation properties [22] which
take undesired heat away from the active device area. Sapphire substrates are thermally
outperformed by both SiC and Si ones, but are much cheaper, and it should be noted that
Fig. 7 – Typical AlGaN/GaN HFET – with source, gate, and drain metallization contacts, and SiC substrate included (illustration not to scale). The approximate location of the two-dimensional electron gas (2DEG) is depicted, just below the heterojunction of AlGaN and GaN. [23]

the growth of general HEMT templates on sapphire is more mature than on Si. In addition, recent reports show how the problem of poor thermal conduction via the substrate can be disregarded when using front-side cooling techniques as a supplement [16]. 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 $10^8$-$10^9$/cm$^2$ [23]. 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.

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 [11]. 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 [11], 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 [20]. 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.

2.3.4. Doping and polarization. Often dopants, such as silicon or iron, are added to GaN and AlGaN materials in order to increase the high-power capability of the device [28]. Doping of the AlGaN layer has little effect on the 2DEG density in the HEMT (15% maximum increase) [29]. However, with or without doping, the high polarization that is naturally present at a heterojunction of these two materials creates a powerful 2DEG region nonetheless. AlGaN/GaN HEMTs are generally considered to have better high-power application performance than the more veteran AlGaAs/GaAs HEMT due to the favorable larger 2DEG density [28]. In an AlGaN/GaN HEMT of wurtzite lattice structure (most common type), both the AlGaN and GaN have high polarization present, with that of AlGaN being stronger [20]. 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 [30]. This occurs because the change (i.e. difference) in polarization at the AlGaN/GaN junction is greater than for AlGaAs/GaAs [20].

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 [20].

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 [20]. Spontaneous polarization is the polarization that exists in each material when in its individual bulk (i.e. “free”) state [31], or at zero strain [1]. 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 [20]. At that point in time, the spontaneous and piezoelectric polarizations present are parallel and all act in the same direction [1]. The overall polarization effect is what allows the 2DEG to have such a high electron density even when the AlGaN does not contain dopants [23].
3.1. Introduction

Although AlGaN/GaN HEMT devices are capable of creating a significant amplified output power signal, dissipated (i.e. wasted) power originating from the 2DEG creates unwanted “self-heating” which results in high temperatures, decreasing the electrical performance of the device [32]. Progress has been made in mitigating this issue [33], but it still continues to be a subject of research, not only because of the electrical connotations but also because the higher temperatures result in thermal expansion which creates strain and thus thermo-mechanical stress within the device. Experimental [22], analytical [34], and FE [12] approaches have been taken in research to determine the effect that self-heating exerts in an AlGaN/GaN HEMT. One choice of FE modeling software is COMSOL Multiphysics, which has been proven as a reliable tool in HEMT applications [22, 35-36], and thus has been chosen as the tool of choice for this thesis.

3.2. COMSOL thermal application

For a given thermal modeling problem, there exists the Heat Transfer module in COMSOL. This module contains a few different application modes, the most general of which is the General Heat Transfer application mode. 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. For heat transfer analysis, the governing equation [37] is:
\[ \rho C_p \left( \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = - (\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} - \frac{T}{\rho} \left( \frac{\partial p}{\partial T} \right) \left( \frac{\partial p}{\partial t} \right) + (\mathbf{u} \cdot \nabla) p + Q \]  

(Eq. 1)

where:

- \( \rho \) is the density (kg/m\(^3\))
- \( C_p \) is the specific heat capacity at constant pressure (J/(kg·K))
- \( T \) is absolute temperature (K)
- \( \mathbf{u} \) is the velocity vector (m/s)
- \( \mathbf{q} \) is the heat flux by conduction (W/m\(^2\))
- \( p \) is pressure (Pa)
- \( \tau \) is the viscous stress tensor (Pa)
- \( \mathbf{S} \) is the strain rate tensor (1/s): \( \mathbf{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \)
- \( Q \) contains heat sources other than viscous heating (W/m\(^3\))

Equation 1 includes viscous heating and pressure work terms, which are excluded in the General Heat Transfer application mode, and is reorganized into:

\[ \rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q - \rho C_p \mathbf{u} \cdot \nabla T \]  

(Eq. 2)

where \( k \) is the thermal conductivity (W/(m·K)). If both radiation and convection effects are excluded from Eq. 2, only conduction effects remain, and the governing equation becomes:
\[ \rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q \]  
(Eq. 3)

3.3. **Thermal contribution to coupled model**

In a study done by Chattopadhyay [34], a self-consistent analytical model was developed to compare static I-V (Current vs. Voltage) characteristics (see Fig. 8) for an AlGaN/GaN HEMT on sapphire substrate against experimental results from Gregušová et al.[25] for matching geometry dimensions and materials. Since the analytical results shown in Fig. 8 bore close resemblance to the experimental results and was thus validated, Chattopadhyay [34] then reported the estimated device 2DEG channel temperature (i.e. maximum device temperature) as a function of drain voltage, for three different applied gate voltages (see Fig. 9). Using COMSOL, an FE approach was taken by the author of this thesis to model this same HEMT device originally fabricated by Gregušová et al. [25].

The tasks in this thermal modeling process were to obtain an FE solution of the temperature distribution in the device, identify the 2DEG channel temperature, and then validate the FE model results by superimposing simulation results on the data found in Fig. 9. Because thermal conduction was the only type of heat transfer considered in the analytical model by Chattopadhyay [34], and no ambient conditions were specified in the experimental study done by Gregušová et al. [25], the author of this thesis modeled accordingly, resulting in Eq. 3 becoming the governing equation for the FE analysis.
3.4. Thermal modeling

3.4.1. 2D vs. 3D. HEMT devices have been modeled in literature as both 2D and 3D structures. Bertoluzza et al. [13] reported that 3D effects in a thermal HEMT model can be very significant and should not be ignored. They reported that if a 2D model is used instead, the calculated peak temperatures in the active device area may be incorrectly estimated as significantly higher than its 3D counterpart. It is well-known
that performing a 2D analysis instead of 3D cuts down on computation time due to a lower quantity of meshing elements, but heeding the warning of Bertoluzza et al. [13], the author of this thesis has chosen to construct a 3D model instead of 2D for thermal analysis.

One caveat of taking this 3D approach, however, is the fact that including the relatively thin AlGaN layer and the three superior contacts (see Fig. 7) would overburden the 3D thermal model with an excessive number of elements. Because of this fact, it is common in literature to disregard these because their small size (nm) relative to the GaN and substrate (μm/mm) yields them negligible in the thermal analysis, which leaves just the GaN and substrate to be analyzed [16].

3.4.2. Device configuration and dimensions. As shown in Fig. 7, HEMT illustrations are typically shown in 2D format. Thus it is important to first understand the HEMT dimensioning terminology used in literature, as follows:

1) “Length” signifies the left-to-right dimension (e.g. the space between source and gate varies in length).
2) “Width” signifies the dimension pointing into the page; HEMT geometries do not change (i.e. uniform) with respect to this dimension.
3) “Thickness” signifies the top-to-bottom dimension (e.g. as you travel through the “thickness” direction, you pass through the AlGaN, GaN, and substrate layers).

The simulated AlGaN/GaN HEMT for this thesis is based on a device defined by Gregušová et al. [25]. Regarding the thermal modeling for finding 2DEG channel temperatures, the only specifications explicitly given by Gregušová et al. [25] for the two
domains (i.e. GaN and substrate) were: 1) 3-μm thickness of GaN, 2) the substrate is made of sapphire (Al$_2$O$_3$), and 3) the device active area width is 50 μm. Personal correspondence [38] made with one of the authors of Gregušová et al. [25] resulted in specifying an active device area length of 97.5 μm. The substrate dimensions decided on by the author of this thesis were based on Menozzi et al. [16], in which an FE model was used to compare simulated channel temperature results to experimentally measured values. A schematic of the model built by Menozzi et al. [16] is shown in Fig. 10.

Menozzi et al. [16] modeled the GaN layer as spanning the entire substrate in length and width directions, so the author of this thesis has done the same. Since one of the main purposes of the substrate, as stated in section 2.3.3 of this report, is to take heat away from the active device area by thermal conduction, its dimensions can have a great effect on the device channel temperature. Using the GaN-to-substrate thickness ratio in Fig. 10 for a GaN thickness of 3 μm gave a resultant substrate thickness of 390 μm.

![Fig. 10 – 3D FE model used in Menozzi et al. [16], where the shaded area represents a quarter of the active device area since symmetry was employed to minimize computation time. Both isothermal (T = 300 K) and adiabatic (i.e. insulated) boundary condition cases were considered in that study.](image-url)
The same substrate-to-GaN thickness ratio of about 100:1 is approximately what is also used in another study \cite{13}. Menozzi et al. \cite{16} provided a square-shaped area (400 x 400 μm) in length and width directions for the substrate, thus the author of this thesis used the same approach, and used a ratio of their active device area vs. substrate length-width areas to determine the analogous dimensions for the model used in this thesis. For the full active device area length-width dimensions used in this thesis (97.5 μm and 50 μm, respectively), a resultant quarter-symmetry substrate length and width identical dimension of 2.28 mm was calculated, or 5.56 mm without symmetry. The thermal model geometry, using quarter symmetry, is shown in Fig. 11.

![Schematic of 3D thermal model](image)

Fig. 11 – Schematic of 3D thermal model, illustrating only a quarter of the active device area since symmetry was employed to minimize computation time. Thicknesses of the two layers include 3 μm GaN and 390 μm Al₂O₃ substrate.
3.4.3. **Material properties.** All thermal material properties required to run this thermal model (see Eq. 3) are found in Table 1. All thermal properties used for GaN were found in literature, but most sapphire thermal properties were already stored in COMSOL and were thus utilized. The only overriding thermal property for sapphire to come from literature was its thermal conductivity.

Table 1 – Required material properties used in 3D thermal model

<table>
<thead>
<tr>
<th>Material</th>
<th>Density, ( \rho ) [kg m(^{-3})]</th>
<th>Thermal conductivity, ( k ) [W m(^{-1}) K(^{-1})]</th>
<th>Heat capacity at constant pressure, ( C_p ) [J kg(^{-1}) K(^{-1})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>6095 [39]</td>
<td>160(T/300)(^{-1.4}) [40]</td>
<td>Interpolation function taken from extrapolated values [41] - see Fig. 12</td>
</tr>
<tr>
<td>Sapphire (Al(_2)O(_3))</td>
<td>3965 [42]</td>
<td>49(T/300)(^{-1}) [34]</td>
<td>730 [42]</td>
</tr>
</tbody>
</table>

3.4.4. **Thermal boundary conditions.** All thermal boundary conditions were assigned similar to the boundary conditions in the FE model created by Menozzi et al. [16] (see Fig. 10). The bottom substrate surface was maintained at a constant 300 K (i.e. isothermal). The top GaN surface and the remaining exterior model boundaries were considered adiabatic (i.e. insulated). It should be noted that the two boundaries of symmetry in the thermal model (see Fig. 11) were also considered adiabatic since a symmetry boundary condition in COMSOL is treated identically to an adiabatic boundary condition.

The most crucial boundary condition applied in the thermal model was that of the power dissipation value applied to the active device area (AlGaN/GaN interface), where the 2DEG is present (see section 2.3.1). The method for determining the dissipation value \( P_{\text{diss}} \) to apply at this location was taken from the classic electronic theory equation of
Fig. 12 – GaN heat capacity at constant pressure ($C_\text{p}$) interpolation function produced in COMSOL using extrapolated data values in literature [41]. In the plot, cubic spline interpolation was incorporated for the data range (see blue line) and linear extrapolation was used for temperature values outside the data range (see red dashed lines).

$P = IV$, where in the case of an HEMT transistor, $I$ is the measured drain current ($I_d$) and $V$ is the measured drain voltage ($V_d$) [34]. Thus, by extracting both $I_d$ and $V_d$ values (at 1-V $V_d$ intervals) along the static I-V characteristic curve reported experimentally by Gregušová et al. [25] as well as the analytical approximation by Chattopadhyay [34] (see Fig. 8), power dissipation values were calculated.
In order to apply a power dissipation (i.e. boundary heat source/heat flux) value to a 2D surface, COMSOL calls for an input value in units of W/m$^2$, but this $I_dV_d$ calculation results in units of mW/mm, or W/m. Bertoluzza et al. [13] used the same approach of stating that the power dissipation is concentrated in the active device area. They also stated that, for example, a power density of $3.5 \times 10^9$ W/m$^2$ corresponds to 3.5 W/mm, when normalized to a unit gate periphery. Thus the power density unit of W/mm is a normalized form of W/m$^2$. The technique of normalization is commonly used in research so that although different studies may have different experimental/simulated geometries, their results may be effectively compared on a basic (i.e. “normalized”) scale. Such is the case with reporting power density output and dissipation values in HEMT devices.

In a comprehensive overview of modern microwave transistors, Schwierz and Liou [20] provide a table of output power densities for different HBT (Heterojunction Bipolar Transistor) devices, in both W/mm and W/μm$^2$ representations. The per-unit lengths therein are associated with the device emitter length and area (length · width), respectively. The term “emitter” in the HBT is analogous to the term “drain” in an HEMT. Thus this alludes to the fact that the per-unit length part of the “W/mm” units in the case of HEMT power dissipation can be associated with the drain’s length, and thus to calculate its corresponding “W/m$^2$” units, one must divide by the drain width dimension, resulting in a per-drain-area representation. One characteristic of an HEMT device is its ability to convert DC (direct current) electric signal to RF (radio frequency) electric signals. However, this signal conversion implies that a fraction of the supplied power is lost, and actually dissipated on the active power device. Colantonio et al. [43]
report that the major part of such loss is located at the active device output, meaning the drain, and thus how it is dissipated depends on the drain geometry. This more definitely confirms the convictions of the author of this thesis that the “/m²” term of the power dissipation value required as a COMSOL input refers to the drain area (length*width).

Thus, the final conclusion on this matter from literature is that the per-unit-length indication (“/m”) on the calculated Pₚₐₑₛ value (=Iₐ Vₐ) units refers to the drain contact length. Since COMSOL calls for units of W/m², then the above-calculated Pₚₐₑₛ value must also be divided by the drain contact width (same as the active device area width): 50 μm.

3.4.5. **Meshing principles.** COMSOL software gives the user various options of mesh element types and meshing techniques prior to computing a solution. Available element types include Lagrange 1ˢᵗ order (linear) through 5ᵗʰ order (quintic), where each progressively higher order requires greater memory storage but smoother derivatives. Because the governing equation for this 3D thermal model does not have higher order derivatives (see Eq. 3), elements of the Lagrange 2ⁿᵈ order (quadratic) type were chosen for meshing, which is also the default option provided by the software. Available meshing techniques in COMSOL include free triangular/quadrilateral/mapped meshing on 2D boundaries, free tetrahedral meshing in 3D domains, and swept meshes of a boundary mesh through an associated 3D domain. With all of these available model meshing options, the consequences of one’s choice of element type and meshing technique should not be trivialized. The most important factor in what decision is made by the user in these areas of consideration should always be the accuracy of the solution, and more especially the accuracy of the solution in critical areas (e.g. high temperature
areas in this 3D thermal model). In FE modeling, once these critical areas are identified, the mesh should be refined in these areas until convergence is achieved.

For convergence purposes, one can attempt to manually refine the mesh in the critical areas, but COMSOL also offers a feature called “Adaptive Mesh Refinement.” Using this feature, an initial solution is found for the quantities of interest (e.g. temperature in the thermal model) 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 there, and then proceeds to solve the model once again. This process undergoes a user-defined amount 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. For the 3D thermal model in this thesis, the author has chosen to build a 3D tetrahedral mesh, and manually refining the 2D triangular mesh in the active device area (i.e. the region of highest temperature). The Adaptive Mesh Refinement feature was not used for the thermal model since the location of highest temperature was already known intuitively; this meshing feature was likewise unused for other application modes in the modeling process, mainly for purposes of eliminating excessive elements by refining the mesh manually only in areas of interest.

To test model convergence, the highest power dissipation ($P_{\text{diss}}$) case, calculated from the analytical $I_d$ and $V_d$ values in Fig. 8 and divided by the active device area width (50 μm), was applied to the active device area in the thermal model. Maximum temperature results for this case, using progressively finer manual mesh sizes in the
active device area, are found in Table 2. A plot of the temperature distribution in the model for this highest power dissipation case is shown in Fig. 13.

Table 2 - Convergence of maximum temperature in the thermal model as mesh size in the active device area was gradually decreased shows that 1-μm-sized mesh was sufficient.

<table>
<thead>
<tr>
<th>Mesh size (μm) on active device area</th>
<th># of elements in entire mesh</th>
<th>Maximum Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>51832</td>
<td>400.11</td>
</tr>
<tr>
<td>3</td>
<td>54472</td>
<td>400.21</td>
</tr>
<tr>
<td>1</td>
<td>59766</td>
<td>400.38</td>
</tr>
<tr>
<td>0.8</td>
<td>62685</td>
<td>400.37</td>
</tr>
<tr>
<td>0.6</td>
<td>71264</td>
<td>400.38</td>
</tr>
</tbody>
</table>

Fig. 13 – Temperature distribution at and near the active device area for the highest power dissipation ($P_{\text{diss}}$) case, calculated from the analytical $I_d$ and $V_d$ values in Fig. 8 and divided by the active device area width (50 μm). Maximum temp. @ device center.
Not only was convergence considered in solving the model, but also element quality. COMSOL documentation [44] states that element quality in a tetrahedral mesh should not go below 0.1 (where 1 is represents 100% quality), or else the user risks compromising the quality of the model’s solution. This quality criterion is most important in the critical areas where the accuracy of results is absolutely necessary. Figure 14 shows the mesh quality in the active device area at the point of maximum temperature.

![Mesh Quality](image)

Fig. 14 – Measure of mesh quality in the thermal model ranges from 0.047 to 0.9986. Although some elements in the model fall below the recommended tetrahedral element quality value of 0.1, because they are not at the location of highest temperature in the thermal model (shown in figure), their presence does not affect the accuracy of the overall solution.
3.4.6. **Eliminating excessive domain.** Modeling dimensions for the 3D thermal model were specified in section 3.4.2. However, one key principle of FE modeling is to avoid modeling excessive amounts of any material if analysis results cease to change in that domain as it extends in any one direction, figuratively, towards infinity.

Incorporating this principle into the modeling process eliminates excessive amounts of elements that would unnecessarily augment model solution times. Figures 15-16 conjointly show the temperature distribution in each global coordinate direction on the model edges leading to the point of highest temperature in the active device area. Figure 16 clearly shows that some domain can be eliminated to speed up model solution times without adversely altering the thermal solution itself. The resulting reduced geometry is shown in Fig. 17. The mesh of this reduced-size thermal model contained only 18875 elements compared with 59766 elements for the original unreduced thermal model.

![Diagram](image)

**Fig. 15** – To explore how much domain may be considered thermally excessive, one-dimensional line plots of lines A, B, and C were generated for the case of highest temperature from high power dissipation ($V_g = 1$ V and $V_d = 20$ V).
Fig. 16 – Temperature vs. position along model edges shown in Fig. 15 illustrate that domains along lines B and C, outside of 1 mm from the point of highest temperature, can be eliminated; the original insulated boundary conditions applied to the new surfaces.
3.5. **Channel temperature verification**

After excessive domain was eliminated from the quarter-symmetry thermal model, its solution was calculated for the wide range of power dissipation values (resulting from the analytical IV characteristic curves in Fig. 8) applied to the active device area. The maximum temperature (i.e. 2DEG “channel temperature”) results, at the same maximum location shown in Fig. 13, are displayed in Fig. 18. The maximum deviations from channel temperatures reported in literature [34] were -5.1 K (-1.48%), 7 K (2%), and 9 K (2.94%) for gate voltages \( V_g \) of 1 V, -1 V, and -3 V, respectively. Thus, the 2DEG channel temperatures calculated in FE analysis were just under-approximated for the positive gate voltage (1 V) and just over-approximated for the negative gate voltages (-1 V and -3 V), in relation to the analytical comparison. It should be noted that although it was important to verify that the power dissipation values used in FE modeling would produce similar results to the analytical channel temperature results [34] in order to give credibility to the thermal approach used in this thesis, it was still
necessary to utilize experimental $I_d$ and $V_d$ data (scantily shown in Fig. 8) in developing temperature profiles closer to reality. Experimental data was taken from Gregušová et al. [25], power dissipation values were calculated, and thermal solutions were calculated in identical fashion as what was done using analytical data; the results of which are shown in Fig. 19.

3.6. Temperature profile extraction

As previewed in section 1.4.4, the main purpose of the 3D thermal model was to extract the temperature profiles along the boundaries of interest (see Fig. 1) and export them to the coupled 2D model. The thermal analysis done up until this section of the report has been done with a quarter-symmetry model for the purpose of verifying channel temperature values and validating the thermal approach. However, the author of this thesis chose to use a half-symmetry model (see Fig. 1) for temperature profile extraction for ease of data transfer. In order to proceed with this newly-formed half-symmetry thermal model, however, it was first necessary to verify that: 1) the mesh near the area of maximum temperature was of adequate quality (see section 3.4.5), and 2) the mesh contained within the four boundaries of interest in Fig. 1 was relatively fine so that representative temperature profiles could be extracted. Using a tetrahedral mesh size of 1 μm (same as in quarter-symmetry model) in both of these key areas, a mesh consisting of 41473 elements was built. A zoomed-in image of the mesh in the active device area is shown in Fig. 20. Once the quality of this mesh was verified to be sufficiently high at the point of highest temperature as well as in the temperature extraction region, line graphs were generated for the four boundaries of interest in Fig. 1, and corresponding data files were saved for use in the 2D coupled analysis.
Fig. 18 – Comparison of COMSOL 3D thermal model results of the 2DEG channel temperature, as a function of applied gate voltage (1/-1/-3 V) and measured drain voltage, to the analytical results reported by Chattopadhyay [34].

Fig. 19 – Channel temperature FE results using experimental data taken from Gregušová et al. [25] to calculate power dissipation values applied to the active device area.
Fig. 20 – Mesh of half-symmetry thermal model in both the active device area as well as the GaN portion from which temperature profiles were extracted for data transfer to the coupled 2D model. The mesh size in both of these areas was set to be 1 μm.
CHAPTER 4
PIEZOELECTRIC MODELING OF HEMT TRANSISTOR

4.1. Piezoelectricity basics

GaN and AlGaN are both piezoelectric materials. As such, they are capable of exhibiting both the direct piezoelectric effect and the inverse/converse piezoelectric effect (see Fig. 21). The former occurs when a material experiences a buildup of electric charge when a direct mechanical stress is applied to it. The latter is just the opposite, when a material experiences strain, and hence stress, from a bias applied across it [45]. The interesting thing is that in an HEMT, both kinds (direct and inverse) are experienced simultaneously, which makes for an interesting analysis. Firstly, the direct piezoelectric effect occurs when high channel temperatures create thermal stress throughout the device, which in turn creates electric charge to be developed. Secondly, the inverse piezoelectric effect occurs when the electric field applied across the device, characterized by the source-drain bias and gate voltage, inherently creates mechanical stress. Proper characterization of the piezoelectric effects occurring in HEMT devices is crucial in design, and has a great effect on electrical performance.

Fig. 21 – Visual representation of both kinds of the piezoelectric effect. (a) Inverse/converse piezoelectric effect, and (b) Direct piezoelectric effect. [46]
4.2. Piezoelectric constitutive equations

The constitutive equations governing piezoelectric behavior within any given material can be written in either “strain-charge” form or “stress-charge” form, both of which are supported by COMSOL, and yield identical results. The author of this thesis chose to enter in material properties in the “stress-charge” form [47].

Strain-charge form:
\[
\varepsilon = s_e \sigma + d^T \mathbf{E} \tag{Eq. 4}
\]
\[
\mathbf{D} = d \sigma + \varepsilon_0 \varepsilon_r \mathbf{E} \tag{Eq. 5}
\]

Stress-charge form:
\[
\sigma = c_e \varepsilon - \varepsilon_0 \varepsilon_r \mathbf{E} \tag{Eq. 6}
\]
\[
\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E} \tag{Eq. 7}
\]

where:
- \(\varepsilon\) = strain (unitless)
- \(s_e\) = compliance (Pa\(^{-1}\))
- \(c_e\) = stiffness (Pa)
- \(\sigma\) = stress (Pa)
- \(d\) = direct coupling matrix (C/N)
- \(e\) = indirect coupling matrix (C/m\(^2\))
- \(\mathbf{E}\) = electric field strength (V/m)
- \(\mathbf{D}\) = electric charge density displacement (C/m\(^2\))
- \(\varepsilon_r\) = relative electrical permittivity (unitless)
- \(\varepsilon_0\) = electrical permittivity of free space = 8.854187817e-12 (F/m)
- \(\rho\) = density (kg/m\(^3\))
4.3. Modeling

The geometry and materials in the piezoelectric model are based on an HEMT device studied by Gregušová et al. [25]. Although the AlGaN layer was excluded from the thermal model, it is crucial in the piezoelectric analysis. A 2D illustration of the modeled device is shown in Fig. 22. Identical to Gregušová et al. [25], the model consisted of a 30-nm Al$_{0.25}$Ga$_{0.75}$N (i.e. compound made of 25 % AlN and 75 % GaN) layer atop a 3-μm GaN layer. The source, gate, and drain were all excluded from piezoelectric consideration because none of them contained any piezoelectric materials [38]; however their x-dimensions (i.e. lengths) were important for boundary condition purposes (discussed later in section 4.4.2). The sapphire (Al$_2$O$_3$) substrate was also excluded from piezoelectric consideration for being a non-piezoelectric material.

Fig. 22 - Model schematic for piezoelectric analysis. The source, gate, and drain domains were excluded from this analysis, but their x-dimensions (i.e. lengths) were important for boundary condition purposes. Geometries are not drawn to scale.
The material properties used in the piezoelectric analysis are found in Table 3.

For a 2D piezoelectric analysis in COMSOL, the default material coordinate plane is X-Y. However, because GaN and AlGaN are both “z-polarized” materials according to their various piezoelectric coefficients, the spontaneous and piezoelectric polarization in each of them acts strictly in the Z-direction (perpendicular to the 2DEG plane). Hence, in the modeling process it was necessary to specify that the material coordinate systems of both these materials be either the X-Z or Y-Z (each yield the same result).

Table 3 – Material properties used in piezoelectric model

<table>
<thead>
<tr>
<th>Material Properties</th>
<th>GaN</th>
<th>Notes</th>
<th>Al_{0.25}Ga_{0.75}N</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stiffness matrix, ( C_\varepsilon [\text{GPa}] )</td>
<td>( C_{11} = 390 ); ( C_{12} = 398 ); ( C_{16} = 105 ); ( C_{13} = 123 ); ( C_{15} = 145 ); ( C_{13} = 106 ) [39]</td>
<td>( C_{11} = C_{22} ); ( C_{33} = 398 ); ( C_{44} = 105 ); ( C_{66} = 123 ); ( C_{12} = 145 ); ( C_{13} = 106 ) [48]</td>
<td>( C_{11} = C_{22} ); ( C_{33} = 398 ); ( C_{44} = 105 ); ( C_{66} = 123 ); ( C_{12} = 145 ); ( C_{13} = 106 ) [48]</td>
<td></td>
</tr>
<tr>
<td>Piezoelectric Coupling matrix, ( d [\text{pm V}^{-1}] ) i.e. [pC N^{-1}]</td>
<td>( d_{33} = 2.8 ); ( d_{31} = -1.4 ); ( d_{13} = -3.1 ) [49]</td>
<td>( d_{33} = -0.5d_{33} ) [49]; ( d_{31} = d_{32} ); ( d_{13} = d_{24} ) [50]</td>
<td>( d_{33} = -0.5d_{33} ) [49]; ( d_{31} = d_{32} ); ( d_{13} = d_{24} ) [50]</td>
<td></td>
</tr>
<tr>
<td>Piezoelectric Coupling matrix, ( e [\text{C m}^{-2}] )</td>
<td>Calculated by ( e = d \cdot C_\varepsilon ) [47]: ( e_{31} = -0.4522 ); ( e_{15} = 0.8176 ); ( e_{13} = -0.3255 )</td>
<td>( e_{31} = -0.496 ); ( e_{15} = -0.331 ) [31]</td>
<td>( e_{31} = -0.496 ); ( e_{15} = -0.331 ) [31]</td>
<td></td>
</tr>
<tr>
<td>Relative permittivity, ( \varepsilon_{rs} )</td>
<td>9.5 [52]</td>
<td>9.375 [53]</td>
<td>Dependent on ( x )-content of Al (25%)</td>
<td></td>
</tr>
<tr>
<td>Density, ( \rho [\text{kg m}^{-3}] )</td>
<td>6095 [39]</td>
<td>5386.25 [39,54]</td>
<td>Linear interpolation between 75% GaN and 25% AlN</td>
<td></td>
</tr>
</tbody>
</table>

4.4. Boundary conditions

4.4.1. 2DEG representation. The 2DEG region of an HEMT is of a highly complex nature and its physics are defined on the quantum level. It is theoretically considered to be two-dimensional (in the length-width plane – see section 3.4.2), yet has an actual thickness on the order of Angstroms (Å). According to Golio [55], the centroid
location of the 2DEG is normally 80-100 Å below the AlGaN/GaN interface. However, it is more commonly modeled in literature exactly at the interface itself [32]. Cole [15] presents one way to mathematically represent the 2DEG phenomenon by showing that the Schrödinger equation can be solved self-consistently with three derived moment-based equations from the Boltzmann Transport Equation (BTE), namely: the carrier concentration equation, the momentum conservation equation, and the energy transport equation, along with the separate Poisson equation. The same study then outlines how to incorporate these derivations into forming functional numerical algorithms for successfully modeling the device heterostructure.

Due to the mechanical- rather than electrical/quantum physics-based emphasis of this thesis, the self-consistent 2DEG-characterizing algorithms discussed above were not employed. When the AlGaN layer in an AlGaN/GaN HEMT is undoped, the 2DEG channel is induced by polarization effects [20]. Thus, one may assume an electric boundary condition at the AlGaN/GaN interface simulating a 2DEG presence to be represented as a “surface charge density” of electrons, resulting from the combined effect of the spontaneous and piezoelectric polarizations present (see section 2.3.4 of this report).

During HEMT device operation, the quantity of electrons (i.e. current) can fluctuate substantially depending on both the electrical bias applied to the source and gate, as well as the overall design and enhancements of a given transistor. Faqir et al. [2] performed numerical simulations of various AlGaN/GaN HEMTs to determine the effects of a high electric field application, and compared the results against experiments on the same devices under the same conditions. In these simulations, a fixed and uniformly-
distributed charge was applied at the AlGaN/GaN interface to represent the polarization present, and any changes in the polarization charge due to the electric field applied by way of bias (i.e. voltage) were neglected. Hence, the author of this thesis has chosen the 2DEG-representative approach of applying a fixed, uniformly-distributed, and electric-field-independent surface charge density at the AlGaN/GaN interface. This constant value was based upon an interpolation of reported values by Ambacher et al. [30] for the maximum 2DEG sheet carrier concentration (i.e. the concentration of electrons in the active device area) present when Al$_{0.25}$Ga$_{0.75}$N is deposited on GaN. Combined with knowing the coulombic charge on an electron (1.602 e-19 C), a resultant surface charge density of 0.02219771 C/m$^2$ was calculated.

4.4.2. Voltage. 4.4.2.1. Location of application. In reality, voltage (i.e. bias or potential difference) is applied to the source and gate in HEMT devices, resulting in an electric potential distribution throughout the device and resultant values at the drain contact including potential difference ($V_d$), output current ($I_d$), and output power ($P_{out}$). In accordance with the mechanical approach of this thesis, voltage levels from Fig. 19 were applied to gate and drain, with the source grounded (i.e. 0 V), as boundary conditions meant to control distribution of electric charge rather than the actual flow (i.e. current) of electrons, in order to view how the charge affected the GaN and AlGaN piezoelectric materials.

The location of these applied voltage boundary conditions was of interest. Ideally, these boundary conditions would be applied to the top of the three contacts. However, the approach taken in this thesis report was to not apply the voltage at the top of the contacts, rather at their base (i.e. at their interface with the underlying AlGaN
layer). The reason for this was that due to the mechanical thesis approach, charge distribution within the source, gate, and drain was not of interest since it does not affect their mechanical stress levels (i.e. they are not piezoelectric). Additionally, the I-V (i.e. Current-Voltage) characteristic curves in Fig. 8 used to calculate the dissipated power ($P_{\text{diss}}$) for the heat source values applied at the 2DEG location are static (i.e. @ 0 Hz frequency) rather than frequency-dependent characteristic curves. HEMT devices are frequently called RF (i.e. radio frequency) or microwave devices because their electric characteristics are dependent on the frequency at which they are operated. If the purpose of this thesis were to do a functional electrical analysis (which it is not), the ohmic (i.e. source and drain) and Schottky (i.e. gate) contacts would need to have specified relative permittivities (i.e. dielectric constants) related to their electric conductivity. The relative permittivity of gold (Au), for example, varies widely as the electromagnetic wavelengths of electric current change [56]. The same holds true for titanium (Ti) and nickel (Ni) materials as well [57].

4.4.2.2. Electric potential distribution continuity. Using the 2DEG and voltage electric boundary conditions outlined in sections 4.4.1 and 4.4.2.1 of this thesis report, along with a standard “zero charge” condition applied to all other boundaries of the model, a 2D model version (see Fig. 22) having a quadratic-type element triangular mesh conforming to the element quality standards outlined in section 3.4.5 of this thesis report was run as a test to see the electric potential distribution in the device. The result of the case of $V_g = 1$ and $V_d = 20$ from Fig. 8 is shown in Fig. 23. It is evident from this figure that the calculated voltage buildup in the source-gate and gate-drain regions of the model was excessive.
Sources in literature [58-61] give examples of what the potential distribution should look like in an HEMT device. Kaneko et al. [59] performed an experimental study to investigate the cross-sectional potential distribution in AlGaN/GaN HEMTs by using Kelvin probe force microscopy. The potential distribution in one of the HEMT devices investigated by that study is shown in Fig. 24. In that displayed potential distribution, it can be seen that not only are there no large spikes of voltage in the source-gate or gate-drain regions as was experienced in Fig. 23, but also the overall distribution is relatively continuous and gradual in transition from its source (@ 0 V) to its drain (@ 40 V). The fact that voltage levels in an HEMT strongly affect the piezoelectric

![Image](image_url)  

**Fig. 23** – Excessive voltage buildup in source-gate and gate-drain regions. [Case: \(V_g = 1 \text{ V}, V_d = 20 \text{ V}\)
deformation makes it impossible to disregard any significant deviation from what the potential distribution should be in the device.

The approach taken by the author of this thesis in order to overcome the issue of adverse voltage spikes in the device was to force a gradual transition of voltage within the source-gate and gate-drain regions along the top AlGaN edge. This was done by applying a boundary condition in those two regions which resulted in a linear transition of potential. To illustrate this approach, the voltage boundary condition along the entire top AlGaN edge for the same $V_g = 1\, \text{V}$, $V_d = 20\, \text{V}$ case are shown in Fig. 25, and the potential distribution throughout the device are shown in Fig. 26. Although not perfect, the results were much more acceptable than those of Fig. 23, with a smooth transition from one region to the next and no undesirable spikes in voltage.
Fig. 25 – Voltage distribution along the top AlGaN edge where voltage is applied, with a linear transition in the source-gate and gate-drain regions. [Case: $V_g = 1\, \text{V}, V_d = 20\, \text{V}$]

Fig. 26 – Voltage distribution in model when linear transition voltage is applied on top source-gate and gate-drain gaps. [Case: $V_g = 1\, \text{V}, V_d = 20\, \text{V}$]
CHAPTER 5
COUPLED THERMO-PIEZO-ELECTRO-MECHANICAL MODEL

5.1. **Addition of ohmic and Schottky contacts**

Neither the thermal model (see chapter 3) nor the piezoelectric model (see chapter 4) included the actual ohmic and Schottky contacts’ domains in their analyses because their presence would not have had any influence on the thermal and piezoelectric results. However, these contacts do affect the mechanical behavior in the device through their thermal expansion and mechanical stiffness mismatch contributions, thus they must be included in the overall coupled model for final analysis.

As mentioned earlier, personal correspondence [38] was made with one of the authors of Gregušová et al. [25] to assist in completing the overall model dimensions. However, even after this correspondence, the specific layering configuration (see section 2.3.3) of the ohmic Ti/Al/Ni/Au and Schottky Ni/Au contacts was still undefined. What occurs during the deposition of the ohmic contacts (i.e. source and drain) in AlGaN/GaN HEMT devices is that the metallization of stacked layers is deposited on the AlGaN layer, then evaporated for solidification purposes, and finally experiences a rapid thermal annealing at 850 °C for 30 s in a N₂ ambient [25]. Ruvimov et al. [62] showed that after the annealing is completed, the structure of the contact is drastically changed (see Fig. 27). Not only does the overall contact structure decrease in thickness, but new inner alloys are formed (i.e. diffusion of Au through Ni forms Au-Al alloy; expansion of Al–Ni alloy at the top surface).

The obvious complexity of the finalized contact configuration persuades many in the FE research community to simply exclude all contacts from their models. For
example, Beechem et al. [11] performed an experimental study of stress contributors within AlGaN/GaN HEMTs having Ti/Al-based ohmic contacts for source and drain, and an Ni Schottky gate contact. However, when they employed FE analysis to verify the results of the thermal portion of stresses, they excluded not only the contacts but also the entire AlGaN layer, claiming that due to their extreme thinness, they contribute little to the mechanical response. Their approach appeared justified when the FE results showed close coincidence with the experimental thermal stresses in the GaN domain.

Because the approach to this thesis report is not strictly electrical in nature, but also mechanical, replacing the physical contacts with only the electric boundary conditions they incur (i.e. voltage) on the bordering AlGaN layer could result in inaccurate mechanical response in the coupled model. Since the author of this thesis predicts that including the physical contacts in the coupled model increases the accuracy of the results, a simplifying assumption was requisite in order to include them. From personal correspondence [38] with an author of Gregušová et al. [25], it was discovered that prior to evaporation, the overall ohmic contact thickness was 350 nm. However, its
overall configuration after evaporation and annealing was considered questionable due to similar issues faced by Ruvimov et al. [62]. Thus, the first assumption made was that the pre-evaporation contact thickness value would be used in conjunction with layer ratios designated in a conventional alloyed Ti/Al/Ni/Au ohmic contact structure used in literature [63] to arrive at an ohmic contact of Ti/Al/Ni/Au (20.6/226.5/56.6/46.3 nm), respectively. Also from this same personal correspondence [38], it was discovered that the overall thickness of the double-layer Ni/Au gate contact was 130 nm. Thus, by using the layer ratios designated by the Ni/Au Schottky gate used in the same literature source [63] as was used for the ohmic contacts, a resultant Schottky gate configuration of Ni/Au (11.8/118.2 nm), respectively, was defined for usage in the model.

5.2. 3D vs. 2D coupling

When adding the piezoelectric and other structural effects to the already-calculated 3D thermal results in order to determine the overall stress/strain behavior in the HEMT device, the same approach of excluding the AlGaN layer and superior contacts (i.e. source, drain, and gate) which was used in the 3D thermal model was not acceptable for two reasons. First, the structural and thermal expansion mismatches of these layers are important. Second, the piezoelectric response of AlGaN cannot be ignored. Choosing to include these additional layers adds both considerably more elements to the model, which when combined with the fact that both the thermal and piezoelectric application modes in COMSOL are running simultaneously for the coupled analysis, error messages indicating short-term memory limitations began to come, thus the model could not be solved given the computer’s standard capability. The following potential techniques were examined to overcome these issues:
1) Change the model element type from the default quadratic-Lagrange to linear-Lagrange. According to basic FE principles, a decrease in element order results in less degrees of freedom (DOF) for each node; thus models consisting of linear-elements (i.e. the least DOF possible) generally give solutions that are overly-stiff compared to reality. Moreover, even with this one change, the standard computer memory was still insufficient.

2) Change the 3D coupled model into an approximated 2D coupled model. This was made possible by extracting temperature results from the 3D thermal model and importing them to a 2D coupled model (see Fig. 1). Since the key electronic charge and voltage components of the piezoelectric-structural model portion did not affect the temperature in the device, this 3D-to-2D dimensional alteration requiring a one-way coupling (instead of simultaneous coupling) between thermal and piezoelectric-structural did not decrease the soundness of the overall coupled solution.

To further justify option (2) as being an acceptable approach, it was important to take into consideration both the knowledge of how an HEMT functions electrically as well as its overall geometry. As stated in section 3.4.2 of this report, it is very common in literature to see 2D schematics of HEMT devices because their geometry is unchanged in the “width” direction (i.e. into the page). From an electrical standpoint, this 2D representation is significant as well since the profiles of electrical flow do not change in this direction either. Additionally, Beechem et al. [11] claims select HEMT devices to exhibit a “biaxial” state of stress, meaning in the plane of the 2DEG. Thus if the device is to be modeled as the 2D profile most commonly seen in literature (see Fig. 7), a state
of plane stress would not be suitable, thus it would have to be modeled in a state of plane strain. The plane strain condition in solid mechanics can be applied when one dimension is considerably larger than the other two. This dimensional situation happens to be very commonly-found in HEMT devices, since the “width” dimension (i.e. into the page) of an HEMT device is commonly a factor or two larger than the other two modeled length and thickness (not including substrate) dimensions. Thus, the option to change from a 3D-model to a 2D-model was structurally compatible in the case of the modeled HEMT device. Figure 28 illustrates the approach that was taken.

Fig. 28 – (repeat of Fig. 1) – Schematic showing transition from 3D thermal model to subsequent coupled 2D model. Extracted temperature profiles on the 3D highlighted GaN portion were applied to the similarly-dimensioned GaN portion in coupled 2D model. 2DEG location is shown in red.
5.3. **Boundary conditions**

The foundation of the coupled 2D model was to first extract temperature profiles from four edges of the 3D GaN portion highlighted in Fig. 28, and apply them as boundary conditions to the identically-XZ-plane-dimensioned GaN portion in the 2D model. The method used for extracting these temperature profiles was to create a line plot of the temperature values along the four boundaries of interest in the 3D thermal model, export them to a text file, and then import these text files to the coupled 2D model to be used as a basis for thermal interpolation functions applied on the same four GaN boundaries.

Other key boundary conditions applied in the coupled 2D model were voltage (see section 4.4.2), a surface charge density of 0.02219771 C/m$^2$ resulting from polarization at the 2DEG location (see section 4.4.1), and a fixed (no translation/rotation) boundary on the bottom of the Al$_2$O$_3$ substrate to allay any rigid-body motion.

5.4. **Material properties**

All material properties required for creating the 3D thermal and 2D piezoelectric models were given previously in Table 1 and Table 3, respectively. However, additional material properties were necessary when creating the coupled model; these properties are found in Table 4.

5.5. **Thermal expansion**

The equation for thermal expansion (i.e. thermal strain) in thermo-mechanical situations is: $\varepsilon = \alpha \Delta T$, where $\alpha$ is the coefficient of thermal expansion of the given material and $\Delta T$ is the change in temperature from the reference temperature (typically
Table 4 – Additional material properties needed for coupled model

<table>
<thead>
<tr>
<th>α: Coefficient of thermal expansion [K⁻¹]</th>
<th>Sapphire (Al₂O₃)</th>
<th>Al₉₀₂₅Ga₀₇₅N</th>
<th>GaN</th>
<th>Ti</th>
</tr>
</thead>
<tbody>
<tr>
<td>α: 6.5e-6 [42]</td>
<td>α: see Fig. 29 and Fig. 30</td>
<td>α: see Fig. 31 and Fig. 32</td>
<td>α: see Fig. 29 and Fig. 30</td>
<td>α: 8.6e-6 [42]</td>
</tr>
<tr>
<td>Cₚ: Heat capacity at constant pressure [J kg⁻¹ K⁻¹]</td>
<td>Cₚ: 6.5e-6 [42]</td>
<td>Cₚ: 492.62 (Linear interpolation between 75% GaN and 25% AlN @ 300 K) [41, 64]</td>
<td>Cₚ: 522 [42]</td>
<td>Cₚ: 522 [42]</td>
</tr>
<tr>
<td>k: Thermal conductivity [W m⁻¹ K⁻¹]</td>
<td>k: 0.22 [42]</td>
<td>k: see Fig. 33</td>
<td>k: 21.9 [42]</td>
<td>k: 21.9 [42]</td>
</tr>
<tr>
<td>v: Poisson’s ratio</td>
<td>v: 0.33 [42]</td>
<td>v: 0.44 [42]</td>
<td>v: 0.36 [42]</td>
<td>v: 0.36 [42]</td>
</tr>
<tr>
<td>εᵣ: Relative permittivity</td>
<td>εᵣ: 5.7 [42]</td>
<td>εᵣ: 0.33</td>
<td>εᵣ: 5.7 [42]</td>
<td>εᵣ: 0.33</td>
</tr>
</tbody>
</table>

Fig. 29 – Temperature-dependent variation of the in-plane thermal expansion coefficient (αₐ) of GaN [65]
Fig. 30 – Temperature-dependent variation of the out-of-plane thermal expansion coefficient ($\alpha_c$) of GaN [65]

Fig. 31 – Linearly-interpolated (between 75% GaN and 25% AlN), temperature-dependent variation of the in-plane thermal expansion coefficient ($\alpha_a$) of Al$_{0.25}$Ga$_{0.75}$N [65, 66]
Fig. 32 – Linearly-interpolated (between 75% GaN and 25% AlN), temperature-dependent variation of the out-of-plane thermal expansion coefficient ($\alpha_c$) of Al$_{0.25}$Ga$_{0.75}$N [65, 66]

Fig. 33 – Interpolation function of temperature-dependent thermal conductivity of Al$_{0.25}$Ga$_{0.75}$N, based on extracted values from literature [67]
300 K). The most user-friendly way to include thermal expansion consideration in COMSOL software when piezoelectric materials are present is to include an “initial strain” ($\varepsilon_o$) in every material domain, whether piezoelectric or not. Although the $\alpha$ coefficient for some of the modeled materials is already stored in the software material library, all $\alpha$ coefficients (except for GaN and AlGaN) were copied as renamed global parameters in the model for ease of use.

As outlined in Table 4, the coefficient of thermal expansion for GaN and AlGaN are not just constant values, rather a non-linear temperature-dependent expression. These expressions were developed in the modeling software as interpolation functions based on imported text files of extrapolated values from coefficient of thermal expansion data in literature. Moreover, the way these two materials expand is unlike the other materials in the model in that in the case of each these two materials, their non-linear thermal expansion is different in the “c-lattice” direction (i.e. perpendicular to the 2DEG plane) than in the “a-lattice” direction (i.e. parallel to the 2DEG plane). Because of this difference, it was necessary to define a different expression for $\varepsilon_o$ in these two directions for these two materials.

The modeling software calls for the $\varepsilon_o$ input structure as a 3x3 matrix. Since thermal expansion was assumed to act in the three global directions (XYZ), then the expressions for thermal expansion needed only to be inputted in as a diagonal $\varepsilon_o$ matrix. In the case of GaN and AlGaN, their $\varepsilon_o$ matrix was inputted as:

$$\begin{bmatrix} \alpha_{a} & \alpha_{c} \\ \alpha_{c} & \alpha_{a} \end{bmatrix}\Delta T,$$

according to the global coordinate system, since x-y is the default work plane in a 2D analysis in COMSOL.
5.6. **Meshing**

Just as in the 2D piezoelectric model (see section 4.4.2.2), the mesh used for this 2D coupled model was a triangular mesh of quadratic-Lagrange type. However, just as in the 3D thermal model (see section 3.4.5), refinement of the mesh was employed until satisfactory convergence was experienced for stress values near the active device area (i.e. 2DEG location) which was the area initially expected to exhibit the most interesting mechanical response to all the coupled physics present in the model. Although experimentation with a mapped mesh was also found to give reasonable results, a triangular mesh was chosen since it offered greater ability to localize a refined mesh at critical locations, without excessively increasing the total model element quantity. It should be noted that due to the thinness of the AlGaN layer as well as the thinness of select layers within the ohmic and Schottky contacts, it was necessary to first mesh the thin nickel layer within the gate contact, whereupon all additional meshing was possible.

5.7. **Coordinate systems**

As discussed in section 4.3, for a 2D piezoelectric analysis involving GaN and AlGaN, the working plane must be set to either X-Z or Y-Z for polarization purposes. However, in a 2D coupled arrangement with thermal physics present as well, only the piezoelectric materials in the piezoelectric application mode need this setting, whilst all others may be represented in the default global coordinate system with X-Y as their working plane. This seemingly conflicting situation did not complicate the interpretation of the model solution, since all results were reported in the global coordinate system.
CHAPTER 6
RESULTS AND SUMMARY

6.1. Static analysis

To avoid confusion, those reading this report should be reminded that the simulation in this thesis has been a static (i.e. stationary), rather than transient (i.e. time-dependent) analysis. Although long-term reliability of these HEMT devices is important, this thesis has not touched on this subject. For more information on long-term reliability, refer to other literature [5].

6.2. Solution convergence

For any FE model, the convergence of the software to the most accurate solution form is crucial. For this thesis report the convergence criteria referred to by COMSOL as “relative tolerance,” which is a tolerance-based termination of iterative solver processes, was chosen as $1 \times 10^{-6}$, which is the default value in COMSOL v. 3.5a. Convergence of the solution was also dependent on the mesh elements themselves. As mentioned earlier, different-ordered Lagrange elements are available for each application mode in the software. The effect of the choice of this element order is shown in Fig. 34, which is shown as a representative case for this study. Because of the results shown in the figure and also solution time efficiency, it was decided to utilize quadratic Lagrange elements throughout because of their sufficient accuracy with adequate mesh refinement, and also moderate speed of solution convergence.
Fig. 34 - Plot showing how varying order of Lagrange elements affect the solution. This plot includes the von Mises stress (for $V_g = 1$ V and $V_d = 19$ V) located in AlGaN at the drain-side edge of the gate, where it was common to see high piezoelectric stress buildup. Since each progressively higher element order results in more degrees of freedom, this leads to higher deformation and higher stress calculation in any given FE model. As seen in the figure, linear elements exhibited higher element rigidity as expected. Quadratic, cubic, and quartic elements all reached a similar solution; however, the higher the element order, the quicker convergence occurred.

6.3. Introduction to results

In order to efficiently visualize the stress/strain distribution in the device and be able to adequately identify critical locations in the device where mechanical failure is expected to occur (omitting residual effects), two methods were used consecutively: 1) surface plots highlighted “hot”/“cold” spots, and then 2) linear cross-sectional lines were drawn through these areas of interest to better quantify stress/strain values of interest at a high sampling rate of data density. After several test runs of the model, in both coupled and uncoupled configurations, it was quickly realized the AlGaN layer was undergoing...
the highest and most frequent concentration of stress and strain. Because of this, linear cross-sectional lines were drawn parallel to the AlGaN/GaN interface: one next to the interface, one in the middle of the AlGaN layer, and one next to the top AlGaN surface (adjacent to the contacts). These three lines continued to serve as the referenced potential locations of critical stress and strain values for interpretation of both coupled and uncoupled model results.

The same ranges of gate voltage (\(V_g = 1, -1, -3\) V) and drain voltage (\(V_d = 1-19\) V) were considered for finding mechanical response results as were used previously to obtain the FE channel temperature results (see Fig. 19). FE simulations were run at drain voltages of 1, 10, and 19 V to establish trends, whereupon finer 1-volt steps were taken wherever more investigation was merited based on change in location, magnitude, and/or mantissa of critical stress/strain values.

It needs to be stated at this point that one of the main motives of obtaining stress/strain distribution in the device has been to identify the maximum stress and strain values specifically in the AlGaN, GaN, and sapphire substrate domains of the device – with special attention on the AlGaN layer, per failure locations reported in literature. The presence of the gate, source, and drain contacts has been crucial in creating reasonably realistic stress and strain distributions in the other domains; however the stress and strain distribution and associated critical values within these contacts have been disregarded in and of themselves, even if larger in magnitude than what is observed in the other domains. The reason for stress/strain disregard in these contacts is twofold: 1) the perfectly-layered configuration of the contacts used for the FE simulation is an approximation yet far from real metallurgical configuration (see Fig. 27), and 2) there...
have been no reports in literature of concern over mechanical failure in these contacts which would cause the HEMT device to degrade.

On a similar note, because of the mechanical approach to this thesis report, in using electric boundary conditions to imitate actual electron flow, not all of the mechanical results were realistic – more specifically on the extreme peripheral edges of the AlGaN layer, where abnormal results of both high tension and compression were observed, but disregarded since there have been no reports in literature of mechanical failure in these HEMT devices at these peripheral locations where temperatures are lower and electric fields are less influential.

6.4. Eliminating unnecessary stress concentration

As seen in Fig. 1, the bottom two corners of the gate contact as well as the bottom inner corners of the source and drain contacts are theoretically square corners. However, in FE modeling design, it is common to use filleting of sharp inner corners in order to eliminate unwanted stress concentration. This is the approach the author of this thesis has taken, since piezoelectric and thermal stress/strain in the AlGaN and GaN layers are of greatest interest, which is in harmony with what has been reported in literature. Figure 35 shows a fillet used in the model (radius of curvature: 10 nm), and Fig. 36 and Fig. 37 show how the insertion of fillets influenced the thermal stress distribution results. The magnitude of piezoelectric stress/strain results were not influenced by the presence of fillets due to the exclusion of the gate, source, and drain contacts in the uncoupled piezoelectric model. However, fillets caused a very minor shift ($\leq$ 10 nm) in location of these piezoelectric values, which was similarly experienced in the thermal model.
Inserted fillets at the bottom corners of the gate contact as well as the bottom inner corners of the source and drain contacts were necessary to eliminate unwanted stress concentrations at these locations which cause mechanical noise in the solution.

Pictured is the thermal stress contribution $\sigma_x$ for the case of $V_g = 1$ V and $V_d = 19$ V, in AlGaN near its interface with the source (shown at left), gate (shown at center), and drain (shown at right) contacts when fillets were NOT included at sharp inner corners in the model; because of this, notable stress concentrations were experienced.
Fig. 37 – Pictured is the thermal stress contribution \( \sigma_x \) for the case of \( V_g = 1 \text{ V} \) and \( V_d = 19 \text{ V} \), in AlGaN near its interface with the source (shown at left), gate (shown at center), and drain (shown at right) contacts when fillets were included at sharp inner corners in the model (in contrast to Fig. 36); because of these inserted fillets, the stress concentrations at these locations were greatly diminished.

### 6.5. Coupled thermal-piezoelectric results

By using the principles outlined in section 6.3, the locations with highest von Mises stress (\( \sigma_v \)) and volumetric strain (\( \varepsilon_{\text{vol}} \)) were identified in the coupled model (Figs. 38 and 39). Individual stress and strain tensor components in the coupled model were quantified at these same locations (see Table 5 and Table 6). The critical locations of von Mises stress and volumetric strain were not identical, but were always located within the AlGaN layer of the device, and most often near the top of this layer near the contacts. The case tested which had both highest von Mises stress and volumetric strain was that of \( V_g = 1 \text{ V} \).
and \( V_d = 19 \) V; stress and strain surface plots of this case are shown in Fig. 40 and Fig. 41, respectively.

6.6. Piezoelectric stress/strain contribution

When thermal contribution was neglected (i.e. no thermal expansion included), only piezoelectric contributions were considered. Under these simulated conditions, only the GaN and AlGaN layers were active participants in the stress/strain analysis because of their piezoelectric natures. Using the principles outlined in section 6.3, the locations

Fig. 38 – The gate and drain voltage had a great effect on the maximum von Mises stress experienced in the coupled model, which was found in the AlGaN layer near the contacts. This maximum value was found to be located at the drain-side of the gate for most cases, with a few exceptions >>> Case 1 \((V_g = 1 \) V; \( V_d = 1 \) V): maximum von Mises stress located at gate-side of source; Case 2 \((V_g = 1 \) V; \( V_d = 14-19 \) V): maximum von Mises stress located at source-side of gate.
Fig. 39 – The gate and drain voltage had a great effect on the maximum volumetric strain experienced in the coupled model, which was found in the AlGaN layer near the contacts. Locations of highest volumetric strain were as follows: Case 1 ($V_g = 1$ V): just to the left of gate-side of source; Case 2 ($V_g = -1, -3$ V): just to the left of drain-side of gate. Volumetric strain increased as drain voltage was increased. As gate voltage became more positive, volumetric strain increased at a faster rate with increased drain voltage.

of maximum piezoelectric von Mises stress ($\sigma_v$) and volumetric strain ($\varepsilon_{vol}$) were identified (see Fig. 44 and Fig. 45); see Table 9 for respective values. Individual piezoelectric stress and strain tensor components at the previously-identified locations of critical stress/strain in the coupled model were also identified (see Table 7 and Table 8). The critical locations of von Mises stress and volumetric strain were not identical, but were always located within the AlGaN layer of the device, and most often near the top of
this layer near the contacts. Figures 42 and 43 show surface plots of the worst-case scenarios of piezoelectric stress and strain, respectively. The following are general observations of the results:

- High stress and strain were only present in AlGaN layer, whose values were nearly uniform throughout the entire AlGaN domain. Maximum values were generally located at the drain-side of the gate contact; the only exception to this was the cases of $V_g = 1$ V and $V_d = 1, 2$ V, in which case the maximum values were experienced at the gate-side edge of the source contact.

Fig. 40 – Surface plot of von Mises stress in the coupled model for the worst case scenario of $V_g = 1$ V and $V_d = 19$ V at the location of highest von Mises stress in the AlGaN layer (542.15 MPa), at the source-side of the gate contact. Note mismatch in stress between layers consisting of different materials.
Fig. 41 – Surface plot of volumetric strain in the coupled model for the worst case scenario of $V_g = 1\,\text{V}$ and $V_d = 19\,\text{V}$ at the location of highest volumetric strain in the AlGaN layer (1.835E-3), just to the left of the gate-side of the source contact. Note mismatch in strain between layers consisting of different materials.

- Virtually no $\sigma_y$ was present (see Table 7); the author of this thesis concluded the reason for this was likely because the piezoelectric materials (AlGaN and GaN) are only polarized in the x- and z- directions of their individual material property coordinate systems. Thus, a biaxial state of stress, where $\sigma_x = \sigma_z$, was produced – which is consistent with literature [11].

- Virtually no $\varepsilon_x$ was present; the author of this thesis concluded the reason for this was because the polarization between the GaN and AlGaN layers – which causes
piezoelectric strain – is only ever present in the global y-direction (i.e. perpendicular to the AlGaN/GaN interfacial surface).

- The maximum stress and strain experienced in the device varied linearly with drain voltage for negative gate voltages; Fig. 44 and Fig. 45 clearly illustrate this trend.

Table 5 – Effect of gate and drain voltage on stress in coupled model; values listed below were found at location of maximum von Mises stress ($\sigma_v$), and their respective x- and y-locations are also shown (Note: $x = 0$ is at the centerline / axis of symmetry in the 2D geometry, which passes through the gate contact). All other stress tensor components were zero. Only the case of $V_g = 1$ V and $V_d = 1$ V had its maximum in the middle of the AlGaN layer instead of next to the top surface. Although the magnitude of $\tau_{xy}$ for the listed case of $V_g = 1$ V and $V_d = 19$ V was consistent with the trend established, its negative sign was connected with its maximum von Mises stress being located on the opposite side of the gate contact (i.e. source-side) which was unlike most of the cases with same gate voltage and less drain voltage; immediately adjacent cases of $V_g = 1$ V and $V_d = 14$-18 V also experienced this change in location of maximum von Mises stress, as well as a change in sign for the shear stress.

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>$y_{av}$</th>
<th>$x_{av}$</th>
<th>$\sigma_v$</th>
<th>$\sigma_x$</th>
<th>$\sigma_y$</th>
<th>$\sigma_z$</th>
<th>$\tau_{xy}$</th>
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<tbody>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 1$ V</td>
<td>middle</td>
<td>-3.7540</td>
<td>192.58</td>
<td>187.59</td>
<td>-5.010</td>
<td>187.520</td>
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<td></td>
<td>$V_d = 10$ V</td>
<td>top</td>
<td>1.2537</td>
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<td>-145.930</td>
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<tr>
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<td>$V_d = 19$ V</td>
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<td>170.74</td>
<td>-38.770</td>
<td>168.550</td>
<td>32.026</td>
</tr>
</tbody>
</table>
Table 6 – Effect of gate and drain voltage on strain in coupled model; values listed below were found at location of maximum volumetric strain ($\varepsilon_{\text{vol}}$), and their respective x- and y-locations are also shown. All other strain tensor components were zero. As drain voltage increased, locations of maximum volumetric strain gradually shifted to the left (i.e. drain-to-source direction); see values for $x_{\varepsilon,\text{vol}}$ below.

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>$y_{\varepsilon,\text{vol}}$ (AlGaN: top/middle/bottom)</th>
<th>$x_{\varepsilon,\text{vol}}$ (µm)</th>
<th>$\varepsilon_{\text{vol}}$</th>
<th>$\varepsilon_x$</th>
<th>$\varepsilon_y$</th>
<th>$\gamma_{xy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 1$ V</td>
<td>top</td>
<td>-4.3100</td>
<td>6.384E-04</td>
<td>1.394E-05</td>
<td>6.244E-04</td>
<td>3.897E-06</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>top</td>
<td>-4.3460</td>
<td>1.300E-03</td>
<td>4.057E-04</td>
<td>8.664E-04</td>
<td>1.035E-04</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>top</td>
<td>-4.3460</td>
<td>1.835E-03</td>
<td>7.281E-04</td>
<td>1.110E-03</td>
<td>1.852E-04</td>
</tr>
<tr>
<td>$V_g = -1$ V</td>
<td>$V_d = 1$ V</td>
<td>top</td>
<td>1.1520</td>
<td>6.314E-04</td>
<td>8.164E-06</td>
<td>6.233E-04</td>
<td>2.780E-06</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>top</td>
<td>1.1065</td>
<td>9.478E-04</td>
<td>1.942E-04</td>
<td>7.484E-04</td>
<td>5.125E-05</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>top</td>
<td>1.1060</td>
<td>1.270E-03</td>
<td>3.861E-04</td>
<td>8.884E-04</td>
<td>9.860E-05</td>
</tr>
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<td>$V_d = 1$ V</td>
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<td>1.2300</td>
<td>6.250E-04</td>
<td>1.570E-06</td>
<td>6.234E-04</td>
<td>1.860E-06</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>top</td>
<td>1.1640</td>
<td>7.006E-04</td>
<td>4.537E-05</td>
<td>6.553E-04</td>
<td>1.590E-05</td>
</tr>
</tbody>
</table>

6.7. Thermal stress/strain contribution

When inverse piezoelectric effects were neglected by setting all voltage boundary conditions to 0 V (i.e. grounded) and removing the surface charge density representing the 2DEG inherent in an HEMT device, the result was to obtain the thermal stress/strain distribution.

Using the principles outlined in section 6.3, the locations with highest von Mises stress ($\sigma_v$) and volumetric strain ($\varepsilon_{\text{vol}}$) were identified in the thermal model (see Fig. 48 and Fig. 49). Individual stress and strain tensor components in the coupled model were quantified at these same locations (see Table 10 and Table 11). The critical locations of von Mises stress and volumetric strain were not identical, but were always located within the AlGaN layer of the device, and most often near the top of this layer near the contacts. The maximum stress and strain values in the thermal model itself are tabulated in Table 12.
Figures 46 and 47 show surface plots of the worst case scenarios of thermal stress and strain, respectively.

As mentioned earlier in Fig. 36 and Fig. 37 when discussing stress concentration buildup due to thermal effects, the predominant mode of maximum stress in the device is compression – opposite to the tensile piezoelectric stress also present in the coupled model; an exception to this compression trend was $\tau_{xy}$ whose maximum values were found to be positive in most cases (excepting cases of $V_g = 1$ V and $V_d = 14-19$ V).

Fig. 42 - Surface plot of von Mises stress in the piezoelectric model for the worst case scenario of $V_g = -3$ V and $V_d = 19$ V at the location of highest von Mises stress in the AlGaN layer (210.741 MPa), at the drain-side of the gate contact. Note high stress exclusively in the AlGaN layer.
Fig. 43 – Surface plot of volumetric strain in the piezoelectric model for the worst case scenario of $V_g = -3$ V and $V_d = 19$ V at the location of highest volumetric strain in the AlGaN layer ($6.664E-4$), at the drain-side of the gate contact. Note high strain exclusively in the AlGaN layer.

6.8. Direct piezoelectric effect

As was mentioned in the heading of Table 11, based on the strain results obtained, it became apparent that the direct piezoelectric effect was likely causing additional strain to occur in the electrically-conductive domains of the model (AlGaN, GaN, and substrate) because of electric potential (i.e. voltage) being produced due to thermal expansion. Figure 50 shows the electric potential values that were obtained in the thermal model. Although not as large as the inverse piezoelectric stress, the direct piezoelectric strain which induced additional stress in the device was important to consider.
6.9. Quantifying uncoupled contributions to coupled model

After uncoupled piezoelectric and thermal analyses were conducted and their individual stress/strain values were obtained at the locations of highest von Mises stress and volumetric strain in the coupled model, it became apparent how gate and drain voltage had such a great effect on how large or small their contribution to the coupled model would become (see Fig. 51 and Fig. 52 which illustrate this very well). Similar plots could easily be formulated for each stress/strain tensor component using information from Table 5 - Table 8 and Table 10 - Table 11.

![Piezoelectric model: Maximum von Mises stress](image)

Fig. 44 – Piezoelectric stress increased linearly for negative gate voltages, and quadratically for positive gate voltage, as drain voltage was increased. More positive gate voltage decreased stress. Maximum stress was always located in the AlGaN layer near the contacts, and was always at the drain-side of the gate - except for the case of $V_{\text{g}} = 1$ V, $V_{\text{d}} = 1-2$ V (at gate-side of the source contact).
Fig. 45 – Piezoelectric strain increased linearly for negative gate voltages, and nearly linearly for positive gate voltage, as drain voltage was increased. More positive gate voltage decreased strain. Maximum locations were identical to those of stress (Fig. 44).

6.10. Comparison of results to those in literature

The coupled FE results of this thesis report show stress concentration in AlGaN most commonly at the drain-side of the gate, which is consistent with literature; critical values of coupled volumetric strain did not normally coincide with the location of highest von Mises stress. Chowdhury et al. [4] found that stress was the highest in the AlGaN layer at the drain side of the gate, and was high enough to cause pit-shaped defects and cracks. The tensile stress incurred in their experimental specimen would have had to exceed the point of yielding in order to produce this pitting, and cracking in some cases. The major contributor to the high stress at this point was the inverse piezoelectric effect.
A peak in stress was also experienced at the source side of the gate, and although strong enough to begin material pitting, was smaller in magnitude than that experienced on the drain side of the gate.

High stress concentration beside the drain-side edge of the gate, in the AlGaN layer, was also reported by Faqir et al. [2], which found “electric” stress at this location. Researchers del Alamo and Joh [9] found that when subjected to a critically-high gate voltage, their HEMT device exhibited electric current leakage defects, generated either within the AlGaN layer or near the gate’s lower edge. The authors of that study concluded the inverse piezoelectric effect was stressing the AlGaN layer and eventually produced electrical defects in the device. Sarua et al. [7] also found stress to be the highest in the AlGaN at the drain side of the gate contact. As the interrelated $V_{ds} (= V_d)$ and $P_{diss}$ were increased, their respective piezoelectric and thermal stresses incurred in the device both increased linearly in magnitude. Although these two types of stresses were

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>$\sigma_y$ (MPa)</th>
<th>$\sigma_x$ (MPa)</th>
<th>$\sigma_z$ (MPa)</th>
<th>$\tau_{xy}$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 1$ V</td>
<td>191.830</td>
<td>191.693</td>
<td>0.052</td>
<td>191.865</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>196.390</td>
<td>196.230</td>
<td>0.076</td>
<td>196.390</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>191.773</td>
<td>191.650</td>
<td>0.042</td>
<td>191.806</td>
</tr>
<tr>
<td>$V_g = -1$ V</td>
<td>$V_d = 1$ V</td>
<td>192.545</td>
<td>192.435</td>
<td>0.056</td>
<td>192.540</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>197.470</td>
<td>197.335</td>
<td>0.074</td>
<td>197.485</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>202.580</td>
<td>202.400</td>
<td>0.082</td>
<td>202.590</td>
</tr>
<tr>
<td>$V_g = -3$ V</td>
<td>$V_d = 1$ V</td>
<td>193.770</td>
<td>193.638</td>
<td>0.068</td>
<td>193.762</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>198.492</td>
<td>198.360</td>
<td>0.066</td>
<td>198.494</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>203.185</td>
<td>203.035</td>
<td>0.066</td>
<td>203.206</td>
</tr>
</tbody>
</table>

Table 7 – Effect of gate and drain voltage on stress in piezoelectric model at location (see Table 5) of maximum von Mises stress ($\sigma_v$) in coupled model. All other stress tensor components were zero.
Table 8 – Effect of gate and drain voltage on strain in piezoelectric model at location (see Table 6) of maximum volumetric strain ($\varepsilon_{\text{vol}}$) in coupled model. All other strain tensor components were zero.

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>$\varepsilon_{\text{vol}}$</th>
<th>$\varepsilon_x$</th>
<th>$\varepsilon_y$</th>
<th>$\gamma_{xy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 1$ V</td>
<td>$6.167E-04$</td>
<td>$-3.365E-07$</td>
<td>$6.170E-04$</td>
<td>$4.430E-08$</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>$6.182E-04$</td>
<td>$-1.945E-07$</td>
<td>$6.183E-04$</td>
<td>$2.480E-08$</td>
</tr>
<tr>
<td>$V_g = 0$ V</td>
<td>$V_d = 1$ V</td>
<td>$6.183E-04$</td>
<td>$-3.178E-07$</td>
<td>$6.186E-04$</td>
<td>$5.230E-08$</td>
</tr>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 10$ V</td>
<td>$6.258E-04$</td>
<td>$-1.945E-07$</td>
<td>$6.260E-04$</td>
<td>$2.772E-08$</td>
</tr>
</tbody>
</table>

Table 9 – Maximum piezoelectric von Mises stress and volumetric strain values, and respective locations in the device. Most of these maximum values occurred at the drain-side of the gate contact; exceptions were the two cases of $V_g = 1$ V, $V_d = 1, 2$ V where the maximum values occurred at the gate-side of the source contact.

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>$y_{nv}$</th>
<th>$x_{av}$</th>
<th>$\sigma_v$</th>
<th>$y_{v,\text{vol}}$</th>
<th>$x_{v,\text{vol}}$</th>
<th>$\varepsilon_{\text{vol}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 1$ V</td>
<td>top</td>
<td>-3.740</td>
<td>192.235</td>
<td>top</td>
<td>-3.739</td>
<td>$6.181E-04$</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>middle</td>
<td>1.256</td>
<td>195.227</td>
<td>top</td>
<td>1.259</td>
<td>$6.360E-04$</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>top</td>
<td>1.260</td>
<td>207.004</td>
<td>top</td>
<td>1.259</td>
<td>$6.565E-04$</td>
</tr>
<tr>
<td>$V_g = -1$ V</td>
<td>$V_d = 1$ V</td>
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<td>193.135</td>
<td>top</td>
<td>1.260</td>
<td>$6.205E-04$</td>
</tr>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 10$ V</td>
<td>top</td>
<td>1.260</td>
<td>201.002</td>
<td>top</td>
<td>1.259</td>
<td>$6.409E-04$</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>top</td>
<td>1.260</td>
<td>208.880</td>
<td>top</td>
<td>1.259</td>
<td>$6.614E-04$</td>
</tr>
<tr>
<td>$V_g = -3$ V</td>
<td>$V_d = 1$ V</td>
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<td>$6.254E-04$</td>
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<td>202.868</td>
<td>top</td>
<td>1.259</td>
<td>$6.459E-04$</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>top</td>
<td>1.260</td>
<td>210.741</td>
<td>top</td>
<td>1.259</td>
<td>$6.664E-04$</td>
</tr>
</tbody>
</table>
found to be on the same order of magnitude (i.e. piezoelectric: 250 MPa for $V_{ds} = 40$ V; thermal: -330 MPa for $P_{diss} = 20$ W/mm), the piezoelectric stress was tensile whereas the thermal stress was compressive. Thus it was concluded that the thermal stress had the effect of decreasing the overall stress in the device because of its opposite sign. The results of this thesis report showed that although the compressive thermal stress did in many cases decrease the magnitude of a given stress tensor component, the coupled von Mises stress failure criterion had higher values in the coupled model than in the uncoupled piezoelectric model in every single case considered.

Fig. 46 – Surface plot of von Mises stress in the thermal model for the worst case scenario of $V_g = 1$ V and $V_d = 19$ V at the location of highest von Mises stress in the AlGaN layer (670.25 MPa), at the source-side of the gate contact. Note mismatch in stress between layers consisting of different materials.
Fig. 47 – Surface plot of volumetric strain in the thermal model for the worst case scenario of $V_g = 1$ V and $V_d = 19$ V at the location of highest volumetric strain in the AlGaN layer (1.220E-3), just to the left of the gate-side of the source contact. Note mismatch in strain between layers consisting of different materials.

Although von Mises theory is widely accepted as a viable failure criterion, some question its applicability to crystalline structures such as GaN and AlGaN. However, studies in literature have suggested and shown accuracy of analytical modeling of similar materials using von Mises (or Tresca)-type failure criterion [68, 69].

Some key differences between the modeled device for this thesis report and the device analyzed by Sarua et al. [7] include different dimensions and substrate material. However, many key similarities make results of this thesis comparable to theirs, including:

- HEMT grown by MOCVD process on substrate
- 25% Al-content in AlGaN layer
- Same likely failure location (drain-side of gate – in AlGaN layer)
- Piezoelectric stress often linearly dependent with $V_{ds}$ between 0 and 20 V.
- Piezoelectric and thermal stresses having same order of magnitude, but opposite in sign to one another. A possible reason for more compressive thermal stresses in the device modeled for this thesis report was the different substrate; $\text{Al}_2\text{O}_3$ has a much lower thermal conductivity than that of SiC, which decreased its ability to dissipate heat away from the active device area.

**Thermal model: Maximum von Mises stress**

![Graph showing the effect of gate and drain voltage on von Mises stress](image)

Fig. 48 – The effect of gate and drain voltage had a great effect on the maximum von Mises stress experienced in the thermal model, which was found in the AlGaN layer near the contacts. The location of maximum von Mises stress was always at the source-side of the gate contact.
Fig. 49 – The effect of gate and drain voltage had a great effect on the maximum volumetric strain experienced in the thermal model, which was found in the AlGaN layer near the contacts. Locations of highest volumetric strain were as follows: Case 1 ($V_g = 1 \, \text{V}; \, V_g = -1 \, \text{and} \, V_d = 2 - 19 \, \text{V}$): just to the left of gate-side edge of source; Case 2 ($V_g = -1 \, \text{and} \, V_d = 1 \, \text{V}; \, V_g = -3 \, \text{and} \, V_d = 1 - 18 \, \text{V}$): at the gate-side edge of the drain; Case 3 ($V_g = -3 \, \text{and} \, V_d = 19 \, \text{V}$): at the gate-side edge of the source. Volumetric strain increased as drain voltage was increased for $V_g = 1, -1 \, \text{V}$; it also increased in magnitude with increased drain voltage for $V_g = -3 \, \text{V}$, but went in the negative direction (i.e. compressive strain).

6.11. Discussion of variation in results

In order to validate any experiment or study, understanding the variation in the results or quantifying the amount of expected error is essential. Thus, experiments are normally repeated using multiple test samples. All results are then averaged, and the standard deviation among the results is calculated and displayed on the graphs to represent the possible variations and errors. As tests are repeated, the natural variations
in materials properties, test conditions, operator performance, and testing device errors and variations (among other factors) all combine to create natural variability observed in the results. However, the research method of finite element by itself is a deterministic approach, meaning that it will only provide one value for stress, strain, or any other parameter measured at a given point. To determine the variability in FE results or to evaluate the effect of possible variations of input parameters (e.g. material properties and geometry taken from literature) on the solution, one can use Monte-Carlo simulation. Monte-Carlo simulation typically involves varying the input parameters according to a predefined probability distribution, and then assessing its effect on the response of the solution, such as stress and strain. This process of varying input parameters involves repetitively running the FE model to obtain a variation in results, which is then used to create a parameter-to-solution response distribution. Doing such a simulation is

Table 10 – Effect of gate and drain voltage on stress in thermal model at location (see Table 5) of maximum von Mises stress ($\sigma_v$) in coupled model. All other stress tensor components were zero.

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>$\sigma_v$ (MPa)</th>
<th>$\sigma_x$</th>
<th>$\sigma_y$</th>
<th>$\sigma_z$</th>
<th>$\tau_{xy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_g = 1$ V</td>
<td>$V_d = 1$ V</td>
<td>2.846</td>
<td>-4.102</td>
<td>-4.959</td>
<td>-4.340</td>
<td>1.583</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>267.400</td>
<td>-205.200</td>
<td>-145.860</td>
<td>-162.050</td>
<td>151.200</td>
</tr>
<tr>
<td>$V_g = -1$ V</td>
<td>$V_d = 1$ V</td>
<td>3.876</td>
<td>-1.997</td>
<td>-2.789</td>
<td>-2.462</td>
<td>2.200</td>
</tr>
<tr>
<td></td>
<td>$V_d = 10$ V</td>
<td>124.200</td>
<td>-83.760</td>
<td>-76.502</td>
<td>-74.418</td>
<td>70.966</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>262.280</td>
<td>-198.180</td>
<td>-146.370</td>
<td>-159.410</td>
<td>148.550</td>
</tr>
<tr>
<td>$V_g = -3$ V</td>
<td>$V_d = 1$ V</td>
<td>1.321</td>
<td>-0.801</td>
<td>-0.866</td>
<td>-0.773</td>
<td>0.758</td>
</tr>
<tr>
<td></td>
<td>$V_d = 19$ V</td>
<td>55.328</td>
<td>-32.280</td>
<td>-38.692</td>
<td>-34.655</td>
<td>31.958</td>
</tr>
</tbody>
</table>
Table 11 – Effect of gate and drain voltage on strain in thermal model at location (see Table 5) of maximum volumetric strain (ε_v) in coupled model. All other strain tensor components were zero. Values for thermal expansion in a- and c-lattice directions of AlGaN at the same points are also provided for comparison to ε_x and ε_y, respectively; the assumed reasons for their difference include: 1) direct piezoelectric effect causing additional strain in the material, and 2) mismatch of thermal expansion coefficients and structural properties near interface of AlGaN and contacts where high strain is present.

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>ε_v</th>
<th>ε_x</th>
<th>α_0(T - T_0)</th>
<th>ε_y</th>
<th>α_0(T - T_0)</th>
<th>γ_xy</th>
</tr>
</thead>
<tbody>
<tr>
<td>V_g = 1 V</td>
<td>V_d = 1 V</td>
<td>2.167E-05</td>
<td>1.427E-05</td>
<td>7.271E-06</td>
<td>7.400E-06</td>
<td>6.666E-06</td>
<td>3.853E-06</td>
</tr>
<tr>
<td>V_g = 1 V</td>
<td>V_d = 10 V</td>
<td>6.547E-04</td>
<td>4.060E-04</td>
<td>2.332E-04</td>
<td>2.487E-04</td>
<td>2.155E-04</td>
<td>1.035E-04</td>
</tr>
<tr>
<td>V_g = -1 V</td>
<td>V_d = 1 V</td>
<td>1.315E-05</td>
<td>8.484E-06</td>
<td>4.567E-06</td>
<td>4.666E-06</td>
<td>4.186E-06</td>
<td>2.736E-06</td>
</tr>
<tr>
<td>V_g = -1 V</td>
<td>V_d = 10 V</td>
<td>3.221E-04</td>
<td>1.997E-04</td>
<td>1.145E-04</td>
<td>1.224E-04</td>
<td>1.056E-04</td>
<td>5.123E-05</td>
</tr>
<tr>
<td>V_g = -3 V</td>
<td>V_d = 1 V</td>
<td>2.978E-06</td>
<td>1.925E-06</td>
<td>1.228E-06</td>
<td>1.053E-06</td>
<td>1.126E-06</td>
<td>1.725E-06</td>
</tr>
<tr>
<td>V_g = -3 V</td>
<td>V_d = 10 V</td>
<td>-5.624E-06</td>
<td>2.960E-06</td>
<td>2.498E-05</td>
<td>-8.582E-06</td>
<td>2.292E-05</td>
<td>7.686E-05</td>
</tr>
<tr>
<td>V_g = -3 V</td>
<td>V_d = 19 V</td>
<td>-6.830E-06</td>
<td>1.097E-05</td>
<td>5.957E-05</td>
<td>-1.756E-05</td>
<td>5.479E-05</td>
<td>1.756E-04</td>
</tr>
</tbody>
</table>

Table 12 – Maximum thermal von Mises stress and volumetric strain values, and respective locations in the device

<table>
<thead>
<tr>
<th>Gate voltage</th>
<th>Drain voltage</th>
<th>y_m (μm)</th>
<th>x_m (μm)</th>
<th>σ_v (MPa)</th>
<th>y_v (μm)</th>
<th>x_v (μm)</th>
<th>ε_v</th>
</tr>
</thead>
<tbody>
<tr>
<td>V_g = 1 V</td>
<td>V_d = 1 V</td>
<td>-1.2588</td>
<td>12.715</td>
<td>2.137E-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V_g = 1 V</td>
<td>V_d = 10 V</td>
<td>-1.2588</td>
<td>368.510</td>
<td>6.547E-04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V_g = 1 V</td>
<td>V_d = 19 V</td>
<td>-1.2588</td>
<td>670.250</td>
<td>1.220E-03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V_g = -1 V</td>
<td>V_d = 1 V</td>
<td>-1.2588</td>
<td>7.985</td>
<td>-1.503E-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V_g = -1 V</td>
<td>V_d = 10 V</td>
<td>-1.2588</td>
<td>188.950</td>
<td>3.296E-04</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>V_g = -1 V</td>
<td>V_d = 19 V</td>
<td>-1.2588</td>
<td>369.020</td>
<td>6.511E-04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V_g = -3 V</td>
<td>V_d = 1 V</td>
<td>-1.2588</td>
<td>2.152</td>
<td>-4.06E-06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V_g = -3 V</td>
<td>V_d = 10 V</td>
<td>-1.2588</td>
<td>43.155</td>
<td>-8.046E-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V_g = -3 V</td>
<td>V_d = 19 V</td>
<td>-1.2588</td>
<td>101.000</td>
<td>-1.851E-04</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
suggested as future work in addition to this thesis, as it is beyond the scope previously defined for this study.

Monte-Carlo simulation is especially valuable when an unexpected trend in results occurs. Such a case can be seen in Fig. 49, where increasingly negative gate voltage decreased the rate of increase in the thermal volumetric strain with respect to drain voltage, to the point where this rate turned negative for the case of $V_g = -3 \, \text{V}$.

Fig. 50 – Quantities of electric potential produced in the device (both positive and negative) because of the direct piezoelectric effect which creates electric potential as a result of thermal strain in the device (Note: Labels on x-axis signify only the thermal distribution associated with said gate and drain voltage values, since no external voltage levels were applied for this thermal model). The values shown in this chart were maximums for the entire device; the values which were closer to critical locations of von Mises stress and volumetric strain were considerably smaller (maximum: $-20e^{-7} \, \text{V}$ for $V_g = 1 \, \text{V}$ and $V_d = 19 \, \text{V}$ case); electric potential values among the entire AlGaN domain could get as large as 0.12 V.
Fig. 51 – Change in drain and gate voltages altered the contribution of each uncoupled physics group (i.e. piezoelectric and thermal) to the overall von Mises stress in the coupled model. Piezoelectric contribution decreased with increased gate voltage, and decreased as drain voltage was increased; the exact opposite was the case for the thermal contribution. High drain voltages in the thermal model resulted in higher maximum von Mises stresses than what was experienced in the coupled model; the assumed reason for this was that the tensile piezoelectric stress was counteracting the predominantly compressive thermal stress.

Although Monte-Carlo simulation could potentially show how model input parameters are creating this trend, there are also other possible reasons. Table 11 shows that for $V_g = -3$ V, all thermal strain components calculated at the location of highest volumetric strain in the coupled model were positive, except for $\varepsilon_y$ which was positive for a drain voltage of 1 V, but then progressively became negative and increased in magnitude with increased drain voltage. One other interesting observation is apparent in
Fig. 52 which shows the fraction of contribution of thermal and piezoelectric volumetric strain to the resultant value in the coupled model. For most $V_g - V_d$ cases shown in that figure, the fractions of the two uncoupled physics add up close to the coupled value; one notable exception was the case of $V_g = -3$ V, which showed an overall decrease of 20% in piezoelectric contribution as drain voltage was increased to 19 V, but no accompanying increase in thermal contribution. Thus the question arises of where the other portion of the coupled volumetric strain contribution is originating from for this case; the author of

![Uncoupled contributions to coupled volumetric strain: Ratio of uncoupled-to-coupled maximum values](image)

Fig. 52 – Change in drain and gate voltages altered the contribution of each uncoupled physics group (i.e. piezoelectric and thermal) to the overall volumetric strain in the coupled model. Following a similar trend to maximum von Mises stress, the piezoelectric contribution decreased with increased gate voltage, and decreased as drain voltage was increased. The thermal contribution trend was opposite to that of piezoelectric contribution, with negligible contribution for the case of $V_g = -3$ V.
this thesis report has reason to believe the direct piezoelectric effect is the main cause, stemming from the negative thermal $\varepsilon_y$ values observed only for the case of $V_g = -3$ V.

It should be noted here that in contrast to the case of volumetric strain, the plot in Fig. 51 shows the von Mises stress does not, on the other hand, show such a clear-cut sum-of-parts composition of piezoelectric and thermal uncoupled contribution; this is greatly because of the more complex analytical equation behind von Mises stress when compared to that of volumetric strain, which is basically a sum-of-parts formulation of the three diagonal strain tensor values. Table 13 illustrates how simply summing uncoupled strain values for the case of $V_g = -3$ V did not show a direct correlation to the coupled strain calculated in the FE model. The sum-of-parts calculation for $\varepsilon_y$ showed a decreasing trend with higher $V_d$ due to the thermal contribution; however, the coupled model result conversely showed an increasing trend. The sum-of-parts result for $\varepsilon_{vol}$ did not show a definitive trend, but the coupled result did show an increasing trend. The information in Table 13 as well as the previous discussion of Fig. 52 illustrate the great effect that coupling of physics present can have in an HEMT simulation, which more accurately typifies the stress/strain behavior of the device in real life than if one were to

Table 13 – Comparing sum-of-parts strain values to actual coupled strain values at location of highest volumetric strain for $V_g = -3$ V.

<table>
<thead>
<tr>
<th>$\varepsilon_{vol}$ $[V_g = -3\ \text{V}]$</th>
<th>Piezo</th>
<th>Thermal $\varepsilon_{vol}$</th>
<th>Uncoupled sum $\varepsilon_{vol}$</th>
<th>Coupled $\varepsilon_{vol}$</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>$\varepsilon_{v}$ $[V_g = -3\ \text{V}]$</th>
<th>Piezo</th>
<th>Thermal $\varepsilon_{v}$</th>
<th>Uncoupled sum $\varepsilon_{v}$</th>
<th>Coupled $\varepsilon_{v}$</th>
</tr>
</thead>
</table>
assume a simple sum-of-parts calculation of uncoupled physics components. As Fig. 52 showed, coupling became more crucial as gate voltage became more negative.

6.12. Conclusion

The thermo-piezo-structural stress and strain distributions have been obtained using FE modeling of an HEMT device using geometry and material properties specified in literature. The contribution and interaction of individual stress mechanisms including piezoelectric effects and thermal expansion caused by device self-heating have been quantified. Critical stress/strain values and their respective locations in the device have been identified as likely failure locations, and have been compared to results in literature.

Based on simulation results, the main failure mechanism was found to be the combined effect of tensile inverse piezoelectric stress and compressive thermal stress; mismatch between layers was also a factor which helped produce stress concentration near interfaces. To mitigate the likelihood of failure due to these mechanisms, it is recommended to utilize substrate materials with high thermal conductivity to assist in mitigating thermal buildup, and also set reasonable gate and drain voltage levels when running these HEMT devices under active conditions to create power dissipation values which are not thermally excessive for the device to handle effectively.

In addition to the Monte-Carlo simulation described in the previous section, suggestions for future work using the information gained from this thesis include (in no particular order):

- Apply the mechanical approach used by the author of this thesis to other HEMT devices reported on in literature or others produced currently by semiconductor device manufacturers
• Vary drain and gate voltages in an even wider range to explore effect on piezoelectric and thermal stress/strain distribution; also optimize these voltage levels to minimize stress/strain buildup

• Extend gate and drain voltages to critical values to obtain: threshold voltage (i.e. point of 2DEG formation) and current saturation (i.e. point of maximum power output of device)

• Incorporate quantum physics differential equations in FE software to induce actual electron flow in 2DEG at AlGaN/GaN interface, and compare stress/strain results to those produced in this report

• Incorporate residual stress based on experimental studies in literature. Martinez-Criado et al. [70] report tensile residual stresses in AlGaN and compressive residual stresses in GaN; these values can vary depending on multiple parameters including the method of crystalline growth during fabrication and Al-content in AlGaN. The compressive stress in GaN is induced by both lattice and thermal expansion mismatches with the underlying substrate, and can affect the surface charge density at the 2DEG location.

• Explore the effect of doping of the piezoelectric materials on stress/strain

• Explore the effect of using different substrate materials on stress/strain

• Conduct a transient (i.e. time-dependent) study to predict long-term reliability of the HEMT device reported on in this thesis report, which would include effects of current frequency and pulsed transistor operation
REFERENCES


[38] Kordoš, P., 2011, *personal e-mail correspondence*.


