Examensarbete

Characterization of advanced AlGaN HEMT structures

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Handledare
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During the last decade, AlGaN High Electron Mobility Transistors (HEMTs) have been intensively studied because their fundamental electrical properties make them attractive for highpower microwave device applications. Despite much progress, AlGaN HEMTs are far from fully understood and judged by the number of published papers the understanding of advanced structures is even poorer. This work is an exploration of the electrical and structural properties of advanced HEMT structure containing AlN exclusion layer and double heterojunctions. These small modifications had great impact on the electrical properties.

In this work, AlGaN HEMT structures grown on SiC substrates by a hot-wall MOCVD have been characterized for their properties using optical microscopy, scanning electron microscopy, transmission electron microscopy, capacitance/voltage, eddy-current resistivity, and by homebuilt epi-thickness mapping equipment.

A high electron mobility of 1700 [cm²/Vs] was achieved in an AlN exclusion-layer HEMT. A similar electron mobility of 1650 [cm²/Vs] was achieved in a combination of a double heterojunction and exclusion-layer structure. The samples had approximately the same electron mobility but with a great difference: the exclusion-layer version gave a sheet carrier density of 1.58*10¹³ [electrons/cm²] while the combination of double heterojunction and exclusion-layer gave 1.07*10¹³ [electrons/cm²]. A second 2DEG was observed in most structures, but not all, but was not stable with time.

The structures we grew during this work were also simulated using a one-dimensional Poisson-Schrödinger solver and the simulated electron densities were in fairly good agreement with the experimentally obtained. III-nitride materials, the CVD concept, and the one-dimensional solver are shortly explained.

HEMT, Hot-Wall MOCVD, GaN, AlGaN, AlN exclusionlayer, Double heterojunction, 1D Poisson-Schrödinger
ABSTRACT

During the last decade, AlGaN High Electron Mobility Transistors (HEMTs) have been intensively studied because their fundamental electrical properties make them attractive for highpower microwave device applications. Despite much progress, AlGaN HEMTs are far from fully understood and judged by the number of published papers the understanding of advanced structures is even poorer. This work is an exploration of the electrical and structural properties of advanced HEMT structure containing AlN exclusion layer and double heterojunctions. These small modifications had great impact on the electrical properties.

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Linköping, August 2007 – Anders Lundskog
The High Electron Mobility Transistor (HEMT) is a commonly used transistor for microwave and high power amplifiers around the world today. Typical application areas are space radio telescopes and cellular phones. Conventional HEMTs on today’s market use a Gallium-Arsenide (GaAs) substrate with an Aluminium-Gallium-Arsenide (AlGaAs) top layer; this old working horse has material limitations and scientists has pushed the GaAs material to its theoretical limit during the last 50 years. New techniques and materials are required to keep up the development of today’s technological society.

The research on group III nitride semiconductors consisting of Gallium-Nitride (GaN), Indium-Nitride (InN) and aluminium-nitride (AlN) started in 1960s. However, these semiconductors are a lot harder to grow than the regular Si and GaAs semiconductors and have not therefore not yet been able to compete with these. The group III-nitrides show some impressive material characteristics well suited for electronic applications. A broad range of GaN electronic-devices such as the bipolar junction transistor (BJT), heterojunction bipolar transistors (HBT) and the high electron mobility transistor (HEMT) have already been realized1.

Over the past fifteen years, group III-nitrides have been the focus of intense research. The group III-nitrides are classified as wide bandgap materials and become intrinsic at much higher temperatures than the regular Si, Ge and GaAs semiconductors2. This means that a GaN HEMT can operate at much higher temperatures with less cooling and does not need extra processing steps to maximize the heat extraction. GaN also has excellent electron transport properties with high electron saturate drift velocity. GaN also has a high breakdown field i.e. the ability of sustaining large electric fields which bodes for component downscaling3. Combining the features mentioned above gives a GaN based HEMT superior properties compared to GaAs one with power densities up to one order of magnitude higher.

The group III-nitrides have already established themselves as the next generation of opto-electronic materials. These wide bandgap materials enables construction of blue light emitting diodes which cannot be done with regular semiconductors such as Si, Ge or GaAs. This opens up a new possibility for manufacturing of large-scale full-colour displays and blue lasers. The blue laser has already been commercialised as the “blue ray” and has by now been implemented in the eagerly awaited Playstation3. However, opto-electronic components and devices are beyond the scope of this work.

Theoretical4 and experimental5 studies have shown that insertion of a thin AlN exclusion-layer between the GaN and AlGaN drastically changes the transport properties of the channel. Demonstrations in Ref. [6] showed that the electron mobility increased from 1308 to 2177 [cm²/Vs]. Another interesting mobility increasing modification of the AlGaN-HEMT is to introduce an AlGaN alloy into the GaN buffer layer. This version of the HEMT is known as the double heterojunction.

This Master’s thesis is a study of how the AlN exclusion-layer and double hetero-junction affect the electrical properties of an AlGaN/GaN heterostructure. It contains both experimental results measured in our laboratory as well as simulations of the structures. This work concludes my Master of Science study in Applied Physics and Electrical Engineering at Linköping University and I hope some of you find this work interesting.

1.1 HISTORICAL VIEW

The idea of world’s first High electron mobility transistor was presented in the late seventies by a man called Takashi Mimura working at Fujitsu laboratories, Japan. Mimura and his colleges had problems with the growth and manufacturing of the device but could in January 1980 obtain
the characteristics of the world's first HEMT transistor. The team published their results in March the same year as a transistor that could compete with the conventional GaAs MESFET in high frequency applications.\(^7\)

![Figure 1: One of Takashi Mimura's first sketches of the energy band diagram explaining the operation principle of a HEMT. Ref. [7]](image)

In 1985 the manufacturing knowledge had grown too such a level that the HEMT structure was announced as the device with the lowest noise characteristics in the world. The transistor quickly gained popularity and spread all over the world.\(^8\)

AlN nitride powder was first synthesized in the late 1920s by flowing ammonia over metallic Al at elevated temperature, and GaN powder was produced in a similar way some years later. Small crystals could be made from the powder but it was not until Maruska and Tietjen used hydride vapour epitaxy (HVPE) to produce GaN in the late 1960s that the material quality was improved.\(^9\) Asif Kahn demonstrated the first AlGaN HEMT in 1994.\(^3\)

It is also worth mentioning that 2DEG was of big academically interest. The 2-dimensional electron gases that appeared in GaAs MOSFET's (the MOSFET is very similar to the HEMT in both appearance and operation) lead to the discovery of the quantum hall effect by Klitzing in 1980. Klitzing got the Nobel price in 1985 for his discoveries and Laughlin, Stomer and Tsui later determined the properties of the quantum hall effect and where also rewarded with the Nobel price in 1998 for their work.\(^8\)
2 GROUP III-NITRIDES

2.1 INTRODUCTION

So why are the group III-nitrides attracting so much attention? To make a long story short, the nitrides have properties that make them very suitable for high-frequency power and optoelectronic device applications. This Chapter gives a brief introduction to the nitrides' physical properties.

The group III nitride materials of most interest as judged by the research focus of today are GaN, AlN and InN together with their ternary or even quaternary alloys. The research and understanding of these III-nitrides are still quite young and far from complete. For instance some physical properties of InN and AlN are not even determined yet, or at least determined with very poor accuracy. So the group III nitride devices are still just in the start pit and what we have seen and learned so far might just be the tip of the iceberg.\(^\text{10}\)

2.2 CRYSTAL STRUCTURE

There are three possible crystal structures that the group III-nitrides can crystallize in, wurtzite, zincblende and rocksalt. Under thermodynamically stable growth conditions, the binary group III-nitrides and its alloys will naturally crystallize into \textbf{hexagonal wurtzite structure}. The wurtzite crystal structure is also thermally stable i.e. no phase or decomposition change will occur once it is formed. The zincblende and rocksalt structures are on the other hand metastable, which means that atoms do not crystallize in a stable minimum energy state. This causes the crystal structure to depose into a more stable phase during cooling (growth techniques usually have high temperatures, see \textit{Chapter 3} for more details). However it is possible to stabilize zincblende in epitaxy layers, which of course, gives the nitrides different properties compared to the regular wurtzite. The majority of all AlGaN HEMTs are grown with wurtzite structure and therefore this crystal structure is the only structure that will be considered further on.

The wurtzite structure has a hexagonal unit cell and consists of two sub lattices, one lattice that consists of the metal (Ga, Al, In) and one of nitrogen. The two lattices are then brought together and will therefore form the wurtzite. The offset of the two lattices is 5/8c and can be seen in \textit{Figure 2}. Another way of saying this would be that the lattice consists of two altering atomic planes of Ga and N pairs in the (0001) direction stacked in an ABABAB sequence so that the atoms in the first and third layer are aligned directly on top of each other.\(^\text{11}\)

<table>
<thead>
<tr>
<th>Properties</th>
<th>GaN</th>
<th>AlN</th>
<th>InN</th>
</tr>
</thead>
<tbody>
<tr>
<td>a lattice constant (Å)</td>
<td>3.19</td>
<td>3.11</td>
<td>3.83</td>
</tr>
<tr>
<td>c lattice constant (Å)</td>
<td>5.19</td>
<td>4.98</td>
<td>5.69</td>
</tr>
</tbody>
</table>

\textit{Table 1: Lattice constants of group III-nitrides, taken from Ref. [10].}
2.3 TERNARY ALLOYS

Group III-nitrides consisting of GaN, InN and AlN all have unique properties. By mixing alloys of Al, In, and Ga their properties can be tailored. Ternary alloys use a notation with molar percentage \( x \). For example In\(_x\)Ga\(_{1-x}\)N, with \( x=0.7 \) means 70\% In and 30\% Ga incorporated in the lattice together with N.\(^{10}\)

Group III-nitrides and its ternary alloys have direct bandgaps i.e. band-to-band transitions can occur without phonon involvement. This makes the group III-nitrides with their alloys highly illuminant materials. SiC and silicon have indirect band gaps, this makes them low illuminant and not suited as an opto-electronic material\(^{13}\). The bandgap of a ternary alloy can be described with Vegard’s rule

\[
E_{Alloy}(x) = xE_A(x) + (1-x)E_B(x) - bx(1-x) \tag{1}
\]

where \( b \) is the bowing parameter of the alloy\(^{10}\). Often are the properties like stress, polarization and lattice constants linearly interpolated even though it is not fully correct\(^{14}\).

Combining Al and In would give the possibility to engineer the band-gap between 6.2 eV to 0.7 eV by simply changing the amount of Al or In in the alloy. This enables devices such as light emitting diodes (LED’s) and laser diodes (LD’s) working anywhere from the far infrared to deep ultraviolet spectral region.\(^{10}\)

2.4 DISLOCATIONS IN GROUP III – NITRIDES

Dislocations are very common in the group III-nitrides grown today (typically \( \sim 10^8 – 10^{11} \) cm\(^{-2}\) in GaN) and crystal quality must be substantially improved in order to achieve better HEMT performance. Dislocations work like scattering centers for carriers in HEMTs and affect the electron mobility drastically, this phenomenon especially comes clear under high current densities.\(^{2}\) It is not really fair to blame the all of the scattering of electrons only on the number of dislocations. To be a bit more specific impurity scattering by remote donors and due to interface charge, acoustic deformation potential scattering, piezoelectric scattering and polar-optical phonon scattering should be taken into count. However, the easiest way to get huge improvements in device performance would be to minimize the number of dislocations.\(^{15}\)

The most common dislocations in pure GaN are screw and edge dislocations. Screws in GaN have a tendency to form small empty pipes and are usually called nanopipes (compared to
SiC’s bigger micropipes). However, all types of dislocations affect the device performance in the end in a negative way and scientists all over the world are trying to find techniques to get rid of them. Figure 3 shows how the electron mobility can increase in the 2DEG (read Chapter 4 for more details) if the number of dislocations could be reduced.

![Graph showing electron mobility vs. density of dislocations](image)

**Figure 3:** Calculated dependence of the low-temperature mobility on the density of dislocations for a few values of ionized impurities concentration. Ref. [15]

Many dislocations in heterostructure are caused by the stress or strain that is built up from the differences in lattice and thermal expansion constants between epitaxial layers or substrates. A pseudomorphic epitaxial layer i.e. a non-relaxed epi-layer can be grown without misfit dislocations if the thickness of the layer is sufficiently small. However, if the layer on the other hand exceeds the critical thickness the layer will collapse and the result is a epitaxy layers built of small grains or with high values if dislocations instead of a continuous crystal. However, the stress or strain within pseudomorphic heterostructures gives rise to piezoelectric effects, which leads to the next section topic.

### 2.5 POLARIZATION FIELDS

Crystals without inversion symmetry become electrically polarized when they are elasticity strained and this phenomenon is called piezoelectricity. The strain on the solid pushes the atom out of their equilibrium position and the displacement of the atoms form a polarization field within the material. The cause of the strain in heterostructures is the misfit of lattice constants and thermal expansion coefficient like mentioned in the previous chapter. But strain can also be achieved by adding high amounts of impurities to the lattice. The polarization can be expressed with the following tensor-equation

\[
P_{ij}^P = e_{ijk} \varepsilon_{jk} \tag{2}
\]

where \(e_{ijk}\) are the piezoelectric coefficient tensor and \(\varepsilon_{jk}\) the strain tensor. The piezoelectric coefficient tensor contains material constants and specific values for the nitrides can be found in Ref. [14] while the strain tensor is dependent on how the solid is exposed to the strain. For a biaxial (Figure 4) strained wurtzite layer all terms cancels in the tensor-equation except one component in the (0001) direction, this leaves Equation 3

\[
P_{zz}^P = 2(e_{xx} - e_{zz} \frac{C_{xx}}{C_{zz}}) \frac{a - a_0}{a_0} \tag{3}
\]

where \(a_0\) and \(a\) are the lattice constants without and with strain respectively and \(C_{xx}\) are the stiffness constants of the wurtzite lattice, which can be found in Ref. [14].
However, even in the absence of strain the lower symmetry of the wurtzite causes another type of polarization named \textit{spontaneous polarization}. The spontaneous polarization is the result of the large difference in electronegativity between the group III metal and the nitrogen atom and this causes the III-N bond to be highly ionic. The lack of inversion symmetry in the wurtzite structure together with the highly ionic bond causes the spontaneous polarization fields\cite{17}. Group III-nitrides posses two different polarities and the polarity of the crystal are dependent on what types of bonds there is along the (0001) direction i.e. if the cation (Ga) or anion (N) sites of the crystal planes are facing towards the sample surface. If the bonds go from cation (Ga) to anion (N), the polarity is said to be of \textit{Ga polarity} and if the bonds go from the anion to cation, the polarity is said to be \textit{N polarity}\textsuperscript{14}.

The total polarization of the crystal is simply the sum of the spontaneous and pizoelectrical (\textit{Equation 3}). In cation-face samples the spontaneous polarization field point away from the surface towards the back layer and vice verse in anion-faced\textsuperscript{14}.

\begin{equation}
P_{z}^{total} = P_{z}^{sp} + P_{z}^{pc} \tag{4}
\end{equation}

The spontaneous polarization is larger than the pizoelectrical in AlGaN/GaN structures. But both spontaneous and pizoelectrical polarizations are very important to consider during the engineering of an AlGaN/GaN HEMT since it strongly affects the potential profile in the structure (see \textit{Chapter 4} for more details)\textsuperscript{17}.

\section*{2.6 THERMAL AND ELECTRICAL PROPERTIES}

The close packing with the strong bonding between atoms gives a robust, wide bandgap material with electrical and thermal properties superior to conventional Si and GaAs semiconductors. The table below compares some important electrical and thermal properties of some commonly used semiconductor materials.
<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal expansion coeff. [10^6/K]</th>
<th>T_M [°C]</th>
<th>E_G [eV]</th>
<th>( \sigma_T ) [W/cmK]</th>
<th>( \mu ) [cm^2/VS]</th>
<th>( E_C ) [10^6V/cm]</th>
<th>( V_{sat} ) [10^7cm/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>a:5.59</td>
<td>2500</td>
<td>3.43</td>
<td>1.3</td>
<td>1000</td>
<td>4</td>
<td>2.7</td>
</tr>
<tr>
<td>AlN</td>
<td>a:4.2</td>
<td>2275</td>
<td>6.2</td>
<td>3.2</td>
<td>1100</td>
<td>6-15*</td>
<td>1.8</td>
</tr>
<tr>
<td>InN</td>
<td>a:3.83</td>
<td>1925</td>
<td>0.7</td>
<td>0.8</td>
<td>2700</td>
<td>2</td>
<td>4.2</td>
</tr>
<tr>
<td>4H-SiC</td>
<td>a:3.08</td>
<td>2830</td>
<td>3.3</td>
<td>5</td>
<td>900</td>
<td>2.2</td>
<td>2.7</td>
</tr>
<tr>
<td>6H-SiC</td>
<td>a:4.2</td>
<td>2830</td>
<td>3.0</td>
<td>5</td>
<td>370</td>
<td>2.4</td>
<td>2.0</td>
</tr>
<tr>
<td>Diamond</td>
<td>1.5</td>
<td>~5000</td>
<td>5.45</td>
<td>1.5</td>
<td>1900</td>
<td>5.6</td>
<td>2.7</td>
</tr>
<tr>
<td>Si</td>
<td>2.56</td>
<td>1415</td>
<td>1.12</td>
<td>1.57</td>
<td>1350</td>
<td>0.3</td>
<td>1.0</td>
</tr>
<tr>
<td>GaAs</td>
<td>6.8</td>
<td>1238</td>
<td>1.43</td>
<td>0.54</td>
<td>8500</td>
<td>0.4</td>
<td>2.0</td>
</tr>
</tbody>
</table>

*Table 2: Thermal and electrical properties at 300K. Data collected from Ref [10].*

In this table \( \sigma_T \), \( E_G \), \( \mu \), \( E_C \) and \( V_{sat} \) are the thermal conductivity, energy band-gap, electron mobility, electric-breakdown field and saturation velocity for the charge carriers respectively.
3 CHEMICAL VAPOR DEPOSITION

3.1 INTRODUCTION

There are several epitaxial growth methods of group III-nitrides like Molecular beam epitaxy (MBE), Hydride vapour phase epitaxy (HVPE) and Chemical Vapour Deposition (CVD). The growth method used during this work was CVD.

CVD is an epitaxial crystal growing process first developed over forty years ago. In contrast to high pressure and high temperature crystal synthesis the CVD technique is generally, but not always, performed at reduced pressure and used to grow microns-thick coatings onto surfaces of a few square centimetres. Development of CVD technology led to growth of millimetres thick, self-supporting layers over larger areas (including group III-nitrides). CVD are most often used to grow high purity semiconductor structures and the technique is nowadays frequently used in the semiconductor-industry. The CVD technique is sometimes called Vapour Phase Epitaxy (VPE) and the name is related to which school you have been raised at. If the precursors contain metal-organic compounds the process usually called Metal Organic CVD (MOCVD).

3.2 PROCESS PRINCIPLE

There are many different CVD techniques like Low pressure-CVD (LPCVD), Atmospheric Pressure-CVD (APCVD) and Metal Organic-CVD (MOCVD) but they all build upon the same principle. The principle is to transport stable compounds with a carrier gas to a hot zone where compounds decompose thermally into atoms or larger molecules. After the decomposition particles will diffuse to the surface and nucleate at a substrate placed inside or near the hot zone and build epitaxial layers.

The growth process can be summarized in the following steps:

(1) Gas phase precursor transports into a hot zone by a carrier gas i.e. stable compounds that carry tracers of the materials that eventually will end up in the epitaxial layers moves into a hot zone together with a carrier gas.

(2) The heat in the hot zone causes the precursors to decompose and form the so-called reactants.

(3) Some of the reactants absorb on the surface of the sample but most of the gas (precursor and carrier –gas) passes the substrate.

(4) Surface diffusion starts i.e. the reactants moves around on the surface trying to find a low energy state where it can nucleate.

(5) Nucleation of the reactants on the surface or redesorption.

(6) Desorption of byproducts.

(7) Transport of byproducts away by carrier gas from the deposition zone.
The CVD growth process from gas mix to epitaxial layer is a complex system. Thermodynamics can be considered as a helping tool and several models have been developed in order to understand the ongoing reactions in the reactor. The laws of thermodynamics determine whether a reaction inside the reactor is possible or not. However, the use of thermodynamics implies that chemical equilibrium has been achieved; this may be true in a closed system but not in system where gases continuously flow in and out. Simulations with thermal dynamic models are powerful tools to investigate physical phenomenons of the CVD process. The number of parameters however are far too many that need to be taken into account to predict for example growth rates and therefore the susceptor is sometimes referred to as a black box even by the most experienced.

The driving force of the growth process is nature’s will to even out the chemical potential difference between the solid and gas phase. The chemical potential is related to the pressure of the reactive gases. It is also worth to mention that if the absorption of reactants are lower than the desorption, the process will etch (i.e. remove material from the substrate) instead of grow material.\(^{13}\)

### 3.3 The CVD Reactor

The susceptor can without doubt be called the heart of the CVD process. The design and positioning of the substrate are critical for growth rates and crystal quality of the grown material. The susceptor is the heating element of the reactor and the most common type of susceptor is the cold-wall. In a cold wall susceptor the heating supplied from one side (usually from beneath the substrate). A hot-wall susceptor reminds a lot about the cold-wall, but here, heat is supplied from all sides. The temperature homogeneity in a hot-wall susceptor is better than in a cold-wall, this means that it is easier to effectively control the precursor decomposition. The susceptor is usually made of graphite and the heating is usually performed by radio frequency induction by an RF coil (plasmas or optical source can also be used, but are relative unusual). The substrate is often rotating around its own axis to smooth out eventual gas concentration differences inside the susceptor, resulting in improved thickness and doping uniformity.\(^{18}\)

The CVD process used in this work is a horizontal hot-wall (Figure 6) MOCVD i.e. the precursors contain metal organic compounds.
3.4 PRECURSORS AND CARRIER GASES

The precursors for CVD can either be in solid, liquid or gas form (by heating or the use of a bubbler the precursors can transform to gas-phase). Liquid precursors are preferred over solid and gas since it is easier to stabilize a steady pressure.

In a MOCVD process common precursors of gallium, aluminium and indium are trimethylgallium (TMGa or (CH$_3$)$_3$Ga) and trimethylaluminum (TMAI or (CH$_3$)$_3$Al) and trimethylindium (TMI or (CH$_3$)$_3$I) respectively. Ammonia (NH$_3$) is most often used as a precursor for nitrogen and the gas-flow of the nitrogen precursor is usually several orders of magnitude larger than for the group III-metals.

The carrier gas task is to carry the precursors into the susceptor and balance the chemical reactions. Most often, purified argon or hydrogen is used. However, the combination of ammonia and trimethyl (Ga, Al, In) can form adduct and adduct-derived species. These gas-phase reactions can result in condensations near the reactor inlets, outlets and form wall-deposits and large particle formations. This can and will affect the epitaxial layers negatively if a large particle lands on the substrate or if a wall-deposition changes the gas-flows in the susceptor.

3.5 THE CHOICE OF SUBSTRATE

In theory would the best substrate selection for GaN epitaxy and device construction would be GaN itself. But, this is barely ever approached in practice since there are no large area, good quality, and low cost GaN wafers commercially available. Instead, it is very common to use heteroepitaxy to manufacture group III-nitride devices.

It is very common that the lattice mismatch is the primarily criteria for the choice of the substrate. This does not really work out in reality for successful device manufacturing but at least gives an idea about what kind of substrates that can be used. The choice of substrate is often a balance of crystal structure, surface finish, composition, reactivity, chemical, thermal and electrical properties. All of the mentioned properties affect the epitaxy layers in some way and some common properties are summarized in (table 2). For device production process, there must be substrates available in sizes of 2 inches or larger at reasonable prices and there are not that many materials left that fit all these criteria’s. There are especially two substrates left of interest, the silicon carbide (SiC) and sapphire (Al$_2$O$_3$).
3.6 SAPPHIRE (AL\(_2\)O\(_3\)) AS SUBSTRATE

Until 1985 GaN was deposited directly on sapphire substrates; this lead to a surface morphology as presented in Figure 7 with rough surfaces and crack formations. This was a huge problem and this is one of the reasons why the research on group III-nitrides is so far behind common semiconductors like Si and GaAs.

![Figure 7 GaN grown on a Sapphire substrate without a nucleation layer. Ref. [19]](image)

In 1986 Amano and his co-workers introduced a two-step growth process by inserting an AlN seed-layer between the substrate and the epitaxial layers grown at low temperature (~600 °C). This drastically improved the surface morphology as well as the electrical and optical properties. The insertion of the seed layer can be considered as the starting point of all modern research on group III-nitrides.\(^{19}\)

Sapphire is the most extensively used substrate for growth of group III-nitrides and there is large area, good quality commercially wafers available at low cost. Sapphire has a large lattice mismatch (15%) to GaN and therefore has sapphire/GaN heterostructures generally relative high amounts of dislocation densities compared to SiC/GaN. The thermal coefficient mismatch of sapphire/GaN is smaller in the SiC/GaN case but still sufficiently large. Because of the poor thermal conductivity constant of sapphire (0.35W/cmK\(^{20}\)), SiC is the best choice of for microwave power devices. Many groups have though demonstrated HEMT devices grown on sapphire but they usually have poor performance compared to HEMT structures grown on SiC substrates.\(^{21}\)

3.7 SILICON CARBIDE (SiC) AS SUBSTRATE

SiC has some properties that are well suited for group III-nitride epitaxy. For example SiC is possible to manufacture in large quantities and there are large good quality wafers commercially available. SiC also has decently low lattice and thermal expansion coefficient mismatch with GaN (3.5 and 30% respectively). However, the mismatches are still sufficiently high to cause large densities of defects in the subsequent epilayers. Group III-nitrides grown on SiC are therefore usually under biaxial strain at room temperature and high amounts of dislocations caused by stress are very common. Even today’s state of the art SiC wafers are far from free of dislocations; these dislocations may propagate into the subsequent epilayers and cause extra dislocations that degrade device performance.\(^{2}\)

Growing GaN directly on SiC is problematic due to the poor wetting between these materials. This problem can be avoided with an AlN or Al\(_{1-x}\)Ga\(_x\)N seed or nucleation layer just like in the sapphire case\(^{19}\). The AlN layer increases the wetting resistance between the GaN and
the substrate and allows growth. The nucleation layer in the SiC case also decreases the number of dislocations because of the improved lattice match between GaN and AlN.

Pure SiC is insulating, but by inserting a controlled amount of impurities it is possible to alter the crystal's conducting properties. From an electrical device design prospective the availability of conductive substrates is an advantage since contacts can be applied on the backside and thereby allow simplification of the device structure. SiC is available with all kinds of impurity levels, from low-doped semi insulating to highly doped n++ and p++ substrates. The thermal conductivity is higher for SiC than for sapphire, which makes SiC better suited for high power devices such as the HEMT. SiC is rather expensive compared to sapphire.
4 THE HIGH ELECTRON MOBILITY TRANSISTOR

4.1 INTRODUCTION

This Chapter is a brief introduction to the function and physics behind AlGaN and AlGaAs HEMT.

4.2 THE HEMT DEVICE AND THE OPERATION PRINCIPLE

A transistor is a component for controlling and amplifying currents which is the fundamental building block for all modern electronics. Modern transistors are normally divided into two categories: the bipolar junction transistor (BJT) and the field effect transistor (FET). The HEMT, is one type of FET with excellent high frequency characteristics. A HEMT device has three contacts called drain, source and gate and the operation principle is as follows: Upon appliance of a source-drain voltage the current that passes through the device can be controlled by the gate voltage; this means in practice that the device can behave like a switch. The current that passes through the device is also amplified. An AlGaN HEMT usually works in depletion mode i.e. current flows through the device even without an external gate-voltage. The voltage gate voltage necessary to stop the current flow between the source and drain is defined as the pinch-off voltage \( V_p \).

The HEMT device consists of epi layers grown on top of each other with three contacts attached to the surface. The AlGaAs HEMT structure appearance is very similar to a GaAs MESFET. The only difference is the top layer, a MESFET has an n+ doped GaAs and a HEMT has an n+ doped AlGaAs layer (Figure 8). The operation principle of a MESFET is more or less identically to a HEMT with the use of a Schottky gate contact to deplete a channel. The appearance and the function of an AlGaN HEMT is on the other hand very similar to an AlGaAs HEMT. The AlGaN HEMT is also shown in Figure 8 and consists of a thin layer (\(~25\)nm) of \( Al_{0.25}Ga_{0.75}N \) grown upon a semi insulating GaN buffer-layer (\(~2\) \( \mu \)m). The high resistive or semi-insulating GaN layer is needed to avoid parallel conduction and thereby decreasing leakage currents of the device. However, the AlGaN HEMT does not require an n+ doped top layer unlike the AlGaAs to operate (see Chapter 4.3 for more details).

The operation principle of the HEMT device from a physical point of view is demonstrated in Figure 1, which demonstrates the behaviour of the conduction and valence bands of an AlGaAs HEMT at different gate-voltages. The figure to the far left in Figure 1 is the bandstructure under zero bias (no gate voltage) and the figure to the far right in Figure 1 shows the structure biased with a gate voltage that exceeds the pinch off voltage, the picture in the middle have a gate voltage in between the other ones. When the gate voltage is zero there is a potential well or valley present at the AlGaN/GaN hetero interface. This valley is absent when the voltage exceeds the pinch off voltage and this energy valley is the reason why the device can
either conduct or throttle a current. Inside this valley a **two-dimensional electron gas** will be formed, which leads to the next topic:

### 4.3 THE TWO DIMENSIONAL ELECTRON GAS

The 2DEG is usually a couple of nanometers thick. It is in this thin layer all electrons are gathered to minimize their energy. This thin channel is also known as a conducting channel where electrons travel from source to drain. The phenomenon of electrons gathering up in the channel originates from the bandstructure-bending in the junctions of a heterostructure.

When two or more semiconductors with different bandgaps are grown on top of each other a heterostructure is formed. Inside a heterostructure will the energybands bend because the Fermilevel, \( E_F \), must be continuous over the entire heterostructure since the semiconductor materials are in contact.\(^{16}\) Figure 9 shows the conduction band of AlGaAs/GaAs junction and as mentioned in Chapter 4.2, an energy valley or potential well forms at the heterointerface\(^1\). The low energy valley is the place with the lowest potential energy in the entire heterostructure. Since the well is very thin, electrons prefer to move sideways in two dimensions instead of up and down because otherwise they would have to move out of the well into a less preferable energy state.\(^{16}\)

The physics behind the formation of the 2DEG described above is correct for an AlGaAs-GaAs heterojunction. The description is almost correct for an AlGaN/GaN heterojunction, but, the AlGaN-GaN heterojunction requires some special attention due to its polarization fields described in Chapter 2.5. The potential profile and amount of charges induced at the interface in an AlGaN/GaN interface are strongly dependent of the polarization fields that GaN and AlGaN materials pose.\(^{14}\)

GaN is a strongly polar material, that is, it possesses a spontaneous polarization that leads to sheet charge accumulation on the end faces of the crystal. These sheet charges are, of course, equal in magnitude and opposite in sign to maintain overall charge neutrality. AlGaN also has a spontaneous polarization, similar to GaN but of different magnitude (in fact, a function of the aluminium content of the ternary). As a result, there is a discontinuity of the spontaneous polarization vector at the AlGaN/GaN heterointerface. Basic electrostatics states that such a discontinuity results in an interface charge proportional to the polarization difference. Furthermore, the strain resulting from growing lattice-mismatched AlGaN on GaN induces a piezoelectric charge, which supplies additional electrons to the HEMT channel.\(^{14}\)

Most of the electrons in the 2DEG originate from the n+ doped AlGaAs layer in the AlGaAs HEMT. However, the AlGaN HEMT does not require an n+ doped top layer since group III-nitrides are polar materials. In fact, the polarization fields are so strong that it alone can provide high amount of electrons to the junction.\(^{23}\)
4.4 THE ADVANTAGE OF GROUP III-NITRIDES FOR MICROWAVE POWER TECHNOLOGY

One simple but not always fair way to compare how good a certain semiconductor is suited for high frequency components is comparing their figures of merit. There are usually three figures of merit that is used Johnson’s, Keye’s and Baligas.

Johnson’s figure of merit (JFM) estimates the ultimate high frequency capability by reflecting the trade off between power and speed.

\[ JFM = \frac{E_c^2 \cdot v_{sat}^2}{4\pi^2} \]  \hspace{1cm} (5)

Keye’s figure of merit describes the attainable of a given material for integrated circuits and includes the thermal limitation. In the equation below are \( \varepsilon \) the semiconductor permittivity, \( \lambda \) the thermal conductivity and \( c \) the speed of light.

\[ KFM = \sigma_T \cdot \sqrt{\frac{c \cdot v_{sat}}{4\pi \cdot \varepsilon}} \]  \hspace{1cm} (6)

Baliga’s figure of merit describes how good a semiconductor can deal with minimizing conduction losses as a transistor.

\[ BFM = \varepsilon \cdot \mu \cdot E_c^3 \]  \hspace{1cm} (7)

In generally high values for the figures of merits are good, but these figures of merits do not give a completely fair picture of the suitability as a semiconductor device. For example does not JFM include the thermal conductivity and KFM should only be used on a homoeptaxy structures (which certainly not is the case for AlGaN HEMT’s). Therefore especially the KFM should be considered as unjust.
### Table 3: Si-normalized figures of merit for some common semiconductors. Ref. [17]

<table>
<thead>
<tr>
<th>Material</th>
<th>Si</th>
<th>GaAs</th>
<th>4H SiC</th>
<th>6H-SiC</th>
<th>GaN</th>
<th>Diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>JFM</td>
<td>1</td>
<td>7.1</td>
<td>180</td>
<td>260</td>
<td>760</td>
<td>2540</td>
</tr>
<tr>
<td>KFM</td>
<td>1</td>
<td>0.45</td>
<td>4.61</td>
<td>4.68</td>
<td>1.6</td>
<td>32.1</td>
</tr>
<tr>
<td>BFM</td>
<td>1</td>
<td>15.6</td>
<td>130</td>
<td>110</td>
<td>650</td>
<td>4110</td>
</tr>
</tbody>
</table>

Table 3 clearly shows that SiC, Diamond and GaN are superior the commonly used Si and GaAs. Diamond appears to be the best semiconductor choice but diamond fails in real life because of processing challenges and the lack of commercial wafers available.\(^{17}\) SiC and its polytypes look on the other hand promising judged from these figure of merits and the research on the material is huge all over the world including at Linköping University.

One unique attribute of the AlGaN/GaN heterostructure is the possibility of building very high channel charges due to its polarization properties. This total channel charge can be one order of magnitude larger for AlGaN compared to AlGaAs\(^24\) and higher channel charge increases the device’s current handling capability. Together with the higher breakdown voltage (which bodes for component downscaling)\(^3\) it is clear why the AlGaN HEMT-structure is well suited for high power applications.

#### 4.5 THE AlN EXCLUSION LAYER

The exclusion-layer AlGaN-HEMT is a regular AlGaIn-GaN HEMT with a very thin layer (~ 1-3 nm) of AlN between the AlGaN and GaN layers. The idea behind this version of a HEMT structure is to minimize a scattering phenomenon called *alloy scattering*.\(^{25}\) The principle of the exclusion-layer AlGaN-HEMT and the alloy-scattering phenomenon is illustrated through the following scenario: In a regular AlGaIn-HEMT the 2DEG is located at the junction between GaN and AlGaN, but there is not a defined border where the 2DEG starts or ends i.e. some of the 2DEG is located inside the AlGaN and some inside the GaN. The lattice of AlGaN consists of Al and Ga atoms randomly distributed in a wurtzite lattice and when an electron travels through such a lattice some of the electrons will be scattered because of the atomic disorder, this is known as alloy scattering. AlN has a bandgap of 6.2 eV and this thin layer works as a barrier that prevents electrons from entering the AlGaN i.e. the AlN layer “pushes” all electrons of the 2DEG into the GaN layer.\(^{26}\)

The transport properties of the 2DEG in an AlGaN-HEMT were investigated in detailed by M. Miyoshi in 2005. Miyoshi and his co-workers modelled the electron mobility of the 2DEG through various kinds of scattering processes such as polar-optical phonons, acoustic phonons, piezoelectric fields, alloy disorder, interface roughness and dislocations. They lay down that the mobility of exclusion-layer AlGaN HEMT had similar transport properties as a regular AlGaN HEMT if alloy scattering was neglected.\(^{25}\)

L. Shen\(^{27}\) and his co-workers first suggested the insertion of a thin AlN-epilayer in 2001 and they achieved electron mobility and a sheet charge density of 1522 [Vs/cm²] and 1.22*10\(^{13}\) [carriers/cm\(^2\)] respectively as compared to a regular structure with 1200 [Vs/cm²] and 1.1*10\(^{13}\) [carriers/cm\(^2\)] respectively. A bit more modern numbers (2004) can be found in Ref. [28] was the electron mobility was increased from 1308 to 2177 cm\(^2/\)Vs and sheet carrier density from 1.1*10\(^{13}\) to 1.21*10\(^{13}\) with and without the exclusion-layer.
4.6 THE DOUBLE HETEROJUNCTION

The double heterostructure is shown in Figure 11 and the GaN buffer layer in this heterostructure is substantially smaller (~50 nm) than in a regular AlGaN HEMT structure (~2 µm). The double heterojunction has two semi-insulating buffer layers consisting of a thin GaN layer and a thick (~2 µm) AlGaN with low aluminium content. Otherwise the layer thickness and doping levels are the same.

![Double heterojunction HEMT structure](image)

A double heterojunction HEMT on the other hand has two heterointerfaces (Al_{0.25}Ga_{0.75}N/GaN and GaN/Al_{0.07}Ga_{0.93}N) relatively close to each other where positive and negative polarization charges will emerge. The emerged heterointerfaces cause an increased electric field in the channel layer that leads to a confinement of the electron density or in other words, a narrower 2DEG. The confinement of the electron density leads to an enhanced 2DEG mobility as a result of the enhanced screening effects.

![Comparison of electron mobility](image)

In a regular AlGaN HEMT all positive polarization charges will emerge at one heterointerface (Al_{0.25}Ga_{0.75}N/GaN). A double heterojunction HEMT on the other hand has two heterointerfaces (Al_{0.25}Ga_{0.75}N/GaN and GaN/Al_{0.07}Ga_{0.93}N) relatively close to each other where positive and negative polarization charges will emerge. The emerged heterointerfaces cause an increased electric field in the channel layer that leads to a confinement of the electron density or in other words, a narrower 2DEG. The confinement of the electron density leads to an enhanced 2DEG mobility as a result of the enhanced screening effects.

Drastically improvements of the mobility at especially low temperatures (Figure 12 a) have been achieved experimentally by introducing a double heterojunction. Double heterojunction are also thought to improve interface roughness between grown layers. This is thought to be one of the reasons for the tremendously increased mobility at lower temperatures. The double heterojunction seems to lower the sheet charge density of the heterostructure.

![Comparison of electron mobility and band structure](image)

Figure 12: a) Measured electron mobility versus temperature for a standard AlGaN-HEMT (SH) and a double heterojunction HEMT (DH).

b) Simulated valence bands and electron densities for a SH and DH. Notice that the narrow electron density of the DH compared to the SH. Ref. [29]
All of the content in this Chapter is in some way directly coupled to the characterization techniques used during this work, therefore the Chapter should not be seen as a general overview of semiconductor characterization but as a brief overview of the techniques used during this work.

5.1 CAPACITANCE-VOLTAGE (C-V)

Capacitance-voltage profiles are widely used as a diagnostic tool of semiconductors. It is a non-destructive, quick, and accurate method and the C-V curve can in many cases be directly associated with the impurity profile of the semiconductor device. The C-V technique relies on the principle that the width of the depleted space-charge region in a semiconductor depends on the applied voltage. Figure 13 shows a typical setup for a C-V measurement. However, it is also very common that the Ohmic contact is placed on the backside of the semiconductor but this requires a conductive substrate. All samples in this work were grown on semi-insulating substrates and therefore the configuration used was as in the picture below.

![Figure 13: Typical C-V setup. The Schottky and Ohmic contacts are usually of the same material but with different areas. The depth of depleted space charge region W depends on the applied negative voltage.](image)

Consider the Schottky barrier in Figure 13 and assume that the semiconductor has a non-uniform donor-impurity distribution \( N_d \). When a dc bias, \( V \), is applied to the metal Schottky contact the applied bias will produce a depleted space charge region of width \( W \) inside the semiconductor (Figure 13). The charges that actually move away and cause the depleted space charge region in response to the applied voltage are the mobile carriers and not the lattice dopants. This means that the C-V profiling technique determines the carrier density (\#donors - \#acceptors) and not the doping density (\#donors). What is actually measured is an apparent or effective carrier density. Under the assumption that the depletion approximation is valid i.e. the mobile carriers densities (both p and n) are zero in the depleted space-charge region and that all donors are fully ionized at the measured temperature it is then possible to derive the following expression of the apparent carrier concentration \( N_e \)
\[ N_d = -\frac{C^3}{q\varepsilon_s\varepsilon_0 A^2} = \frac{2}{q\varepsilon_s\varepsilon_0 A^2} \frac{dC}{dV} = \frac{2}{q\varepsilon_s\varepsilon_0 A^2} \frac{d\left(\frac{1}{C^2}\right)}{dV} \quad (8) \]

where \( A, q, \varepsilon_s, \varepsilon_0 \) are the area of the Schottky barrier, the elementary charge, relative dielectric constant and permittivity respectively.

\[
C = \frac{\varepsilon_s \varepsilon_0 A}{W} \Leftrightarrow W = \frac{\varepsilon_s \varepsilon_0 A}{C} \quad (9)
\]

and Equations 8 and 9 are the key equations for doping profiling.\(^{30}\) The assumption of that the semiconductor behaves like parallel capacitor may seem reasonable if the contacts are placed on different sides of the semiconductor. However, this is not the case in Figure 13 but the assumption still gives good and accurate results. The reason why this assumption still is valid is thought to be the large area of the Ohmic contact compared to the Schottky contact.

The sheet carrier density is defined as all effective carriers within a semiconductor or heterostructure. This can easily be obtained by insertion and integration of Equation 9 and 8:

\[
n_s = \int_0^\infty N_w(w)dw = \int_0^\infty N_d(C)dV \quad (10)
\]

The sheet carrier density is usually in units of [electron/cm\(^2\)].

By plotting the sheet carrier density versus the applied bias it is possible to determine the AlGaN layer thickness of a GaN HEMT. Making the same assumption of that the heterostructure behaves as a parallel capacitor it is possible to derive Equation 11:\(^{31}\):

\[
W_{\text{AlGaN}} = \varepsilon_s \varepsilon_0 A \frac{dV}{dn_s} \quad (11)
\]

The AlGaN thickness accuracy calculated can be as low as 10%. This is a very impressive result for such a simple model of a complex system. Although to gain such good results a precise area measurement of the Schottky contact is critical. This does not only apply to the thickness calculation since the area appears as \( A^2 \) in Equation 7. Often are mercury droplets used as a
temporary Schottky contacts. The mercury droplet is a liquid at room temperature and can therefore easily be applied and taken off the surface. Room-temperature mercury has a high viscosity and therefore the area can be decently controlled. The mercury contact appears not to damage the wafer nor leave any residues on the surface. For better area control or permanent contacts, a metal such as gold or nickel can be evaporated onto the surface.  

By measurement technical reasons, is usually a sinusoidal ac voltage with amplitudes of 10-20 mV and frequencies of 10 kHz to 1 MHz added to the dc voltage.

![Figure 15: A typical Sheet carrier density versus bias curve for a GaN HEMT.](image)

From the sheet carrier density versus bias is it possible to determine the pinch off voltage $V_p$ and the AlGaN thickness of the wafer and the curve is characterized by the sudden stop of sheet carrier density at $V_p$. The pinch off voltage is the bias voltage necessary to deplete the 2DEG.

The inverse slope of the curve is directly proportional with the AlGaN thickness.

5.2 RESISTIVITY MEASUREMENTS

The resistivity $\rho$ depends on the free electron and hole densities $n$ and $p$ (in cm$^{-3}$), and the electron and hole motilities $\mu_n$ and $\mu_p$ according to the relationship:

$$\rho = \frac{1}{q(n\mu_n + p\mu_p)} \quad (12)$$

For extrinsic materials in which the majority carrier density is much higher than the minor carrier density, it is generally sufficient to know the majority carrier density and mobility. If we assume that the hole density is small compared to the electron density the resistivity can approximately be calculated by Equation 13.

$$\rho = \frac{1}{qn\mu_n} \quad (13)$$

Thin layers, are often characterized by their sheet resistance $R_\square$ expressed in units of Ohms/Square. The beauty of this particular unit is that the squares size is independent of the size of the square (when the square size increase the distance electrons have to travel also increase, but on the other hand, will also the area increase so more electrons can conduct current). When
this term is used, the current is passing along the sheet and not through it. For materials with non-uniform doping the sheet resistance is defined by Equation 14. A common and practical approximation for non-uniform doped materials is to assume that the electron mobility is uniform through the entire wafer. This is certainly not the case when dealing with 2DEGs but the approximation is generally accepted. Equation 14 becomes 15 under this approximation where \( n_\text{s} \) are the sheet carrier density.

\[
R_s = \frac{1}{\int_0^n n(x)q\mu_n(x)dx}, \quad R_s \approx \frac{1}{n_\text{s}q\mu_n} \quad (14), \quad (15)
\]

In case of a HEMT structure the sheet resistance is referred to as the resistance of 2DEG parallel to the surface or in other words, the resistance electrons “feel” when they travel from source to drain.

Resistivity measurements can be done in many ways and the most commonly used are the four-point probe. Other techniques are eddy-current techniques or Hall measurements. The technique used in this work was a contact-less eddy current method and the concept is shown in Figure 16.

![Figure 16: Schematic eddy current experimental arrangement.](image)

Eddy current measurements are done by the following principle: An oscillating voltage \( V \) in the radio frequency region will cause a current flow through the wire that is wrapped around a ferrite core. The current causes an oscillating magnetic field in the ferrite that passes over the gap through the semiconductor wafer and back into the ferrite core. The oscillating magnetic field induces eddy currents in the semiconductor that leads to joule heating of the material. The absorbed power can be described in mathematical terms and can be rewritten as:

\[
R_s = \frac{KV_{\text{rms}}}{n^2I} \quad (16)
\]

where \( K, V', n \) and \( I \) are ferrite core constant, root mean square voltage \( \langle V_{\text{rms}} \rangle = \frac{V_{\text{pp}}}{\sqrt{2}} \) applied over the ferrite core, number of turns around the ferrite core and the current feed through the wire, respectively.
5.3 THICKNESS MAPPING

The thickness mapping technique was invented by Paul D. T. Huibers in 1997 and is based upon the interference pattern created when two rays of light act together (interference patterns). By studying the reflected light and the interference pattern from a heterostructure it is possible to determine the layer thickness very precisely. The method is contact–free, non-destructive, and the technique only requires a standard white light diode and a spectrophotometer. The method is not only used as a semiconductor characterization technique, it is also eligible in for example measuring soap-bubble thickness.

In Figure 17 constructive interference between the two rays L2 and L2 will occur when the light from one ray has travelled an integral multiple of the wavelength with respect to the other ray with the assumption that both rays got the same wavelength. Destructive interference occurs when the path difference is a half integral multiple of the wavelength. However, different wavelengths give different constructive and destructive interference conditions and this is the key to the entire technique. By illuminating the sample with white light i.e. a mixture of all kinds of wavelengths and measuring the reflected intensity for all wavelengths separately with a spectrophotometer, provides enough information to calculate the layer thickness. The reflectance or absorbance intensities of the reflected light from the sample plotted versus the wavelength can look something like in the figure below.

![Figure 17: Schematic diagram of the reflected light through a thin film. It is a fundamental property of optics that light passing through an interface between materials of different refractive indices will be divided into transmitted and reflected components.](image)

![Figure 18: Typical absorption spectrum from two films with different thickness. D denotes the thickness of the film.](image)
Once the reflection or absorbance spectrum is measured, the layer thickness can be calculated with Equation 17 where \( N_{\text{cyc}} \) is the number of constructive or destructive interference points between \( \lambda_1 \) and \( \lambda_2 \) (\( \lambda_1 < \lambda_2 \)). Note that the refractive index \( n \) is wavelength dependent.

### 5.4 PHOTOLUMINESCENCE (PL)

Photoluminescence (PL) is an old, non-destructive characterization technique for estimating alloy compositions in direct bandgap materials. With the PL technique, it is also possible to estimate the defect and impurity densities. However, PL has a drawback, the sample has to be cooled down to liquid helium temperature (where \(^4\text{He} \) becomes super-fluent, and hence conduct heat extremely well and becomes totally transparent, this is known as the lambda point). The requirement of liquid helium makes the method fairly expensive and time consuming.

In a conventional PL experiment on a semiconductor is the sample excited photon energies above the bandgap of the semiconductor (\( E_{\text{exc}} > E_G \)). The excitation of the electron will promote an electron from the valence band to conduction band and leave a hole. The excited electron in the valence band will eventually de-excite and recombine with the hole. The excess energy can be used to emit a photon with the same energy as the semiconductor bandgap, \( E_G \). The emitted photon is collected and the intensity is recorded as a function of the emitted photon energy to produce a PL spectrum. The PL spectrum usually has discrete peaks and the position of the peaks corresponds to the bandgap. The radiative process of the electron is simplified in many matters in the model described above, but the model gives a good hint about how PL measurements are made.

![Figure 19: Typical PL spectrum with distinct peaks at certain energies.](image)

Compositions of ternary alloys can be determined if the bowing factor in Equation 1 is known.
This Chapter describes briefly how self consistent Poisson-Schrödinger problems are formed and solved. All equations descriptions are written in a one-dimensional perspective.

6.1 FORMULATION OF THE PROBLEM

The problem is formulated through two equations, Poisson’s and the time-independent Schrödinger and these equations are connected through the potential energy $\phi$ of the system. For a given material the mentioned equations are given by Equation 18 and 19 respectively where $x$ is the spatial coordinate.

$$\frac{d^2 \phi(x)}{d^2 x} = -\frac{q(N_D(x) - n(x))}{\varepsilon_0 \varepsilon_s} \quad (18)$$

$$H\phi(x) = E\phi(x) \Leftrightarrow \left[ \frac{-\hbar^2}{2} \frac{d}{dx} \left( \frac{1}{m^*(x)} \frac{d}{dx} \right) + V(x) \right] \phi(x) = E\phi(x) \quad (19)$$

Where $\varepsilon_0$, $\varepsilon_s$, $m^*$, $N_D$, $n$, $H$, $V$, $\phi$, $E$ are the permittivity, dielectric constant, effective mass, ionized donor concentration, electron density distribution, the Hamiltonian, potential energy, wave function and energy respectively. The ionized donor concentration is often given as a parameter independent of the temperature. The potential energy in Schrödinger’s equation can be written as:

$$V(x) = -q\phi(x) + \Delta E_c(x) \quad (20)$$

Where $\Delta E_c$ are a pseudo potential added to account for effects such as screening. However, the potential energy in Equation 20 do not contain any terms that involve the electron-electron interactions which means that the electron-electron interactions in this model are completely neglected. Neglecting the electron interactions are of course far from correct but the model seems to deliver some real physics in practice. The wave function $\phi(x)$ in Equation 19 is related to the electron density in Equation 20 by the following expression:

$$n(x) = \sum_{k=1}^{m} |\phi_k(x)|^2 n_k \quad (21)$$

Where $m$ is the number of bound states and $n_k$ is the probability for electron occupation for each state. The electron occupation of each state can be expressed with a Fermi-Dirac distribution:

$$n_k = \frac{m^*}{\pi \hbar^2} \int_{E_k}^{\infty} \frac{1}{1 + e^{(E-E_f)/kT}} dE \quad (22)$$

Where $E_k$ is the eigenenergy of state $m$ and $E_f$ the Fermi-energy. Another approximation was introduced into Equation 22 through Fermi-energy in fact should be replaced by the chemical potential. Equations 18-22 are enough to solve the problem and obtain for example electron densities or band diagrams.
6.2 SOLVING THE PROBLEM (PSEUDO-CODE)

In order to numerically solve the equations in Chapter 6.1 all equations must be discretized into a mesh. The discretization and design of the solver is only itself a science and more information can be found in for example Ref. [34]. The solving principle is an iteration process and it is demonstrated in the following pseudo-code:

1. Start with a trial potential \( \phi(x) \) and solve the Schrödinger equation (Equation 19) for the wave functions \( \phi_i(x) \) and their corresponding eigenenergies \( E_k \).
2. Calculate \( n(x) \) from the obtained wave functions with Equation 21 and 22.
3. Calculate \( \phi_{i+1}(x) \) using Poisson’s equation (Equation 18) by using \( n(x) \) obtained from the previous step and the given donor density \( N_d(x) \).
4. A new potential \( V_i(x) \) is obtained from the newly found value for \( \phi_{i+1}(x) \) with Equation 20.
5. Iterate in this manner until a certain error criteria is satisfied i.e.

\[
|\phi_i(x) - \phi_{i-1}(x)| \leq \varepsilon \quad \forall x
\]
7 EXPERIMENTAL DETAILS

7.1 THE SUBSTRATE AND SAMPLE PREPARATION

Eight different HEMT structures were grown in a hot-wall MOCVD reactor on a commercial two-inch 4H-SiC substrate cut in eight pieces. The substrate was of semi-insulating type with impurities levels \( \sim 10^{15} \text{ cm}^{-3} \) and a resistivity larger than \( \sim 10^5 \) [ohm*cm]. The epitaxial layers were grown on the silicon-face of the substrate. The 4H-SiC wafer were manufactured and sold by CREE research Inc. but the cutting was performed in our laboratory with a metal blade.

All samples were cleaned before growth with the following steps:

1. Boiling acetone in an ultrasonic bath for 60 min (remove wax and dust)
2. Ethanol bath at 80\(^\circ\)C for 5 min (remove acetone, dust and additional wax)
3. H\(_2\)O rinsing
4. Diluted ammonia and hydrogen peroxide in an ultrasonic bath for 5 min at 80\(^\circ\)C (NH\(_3\), H\(_2\)O\(_2\), H\(_2\)O) (remove organic compounds)
5. H\(_2\)O rinsing
6. Diluted hydrochloric acid and hydrogen peroxide for 5 min at 80\(^\circ\)C (HCl, H\(_2\)O\(_2\), H\(_2\)O) (remove metals)
7. H\(_2\)O rinsing
8. Diluted hydrofluoric acid dip (HF, H\(_2\)O) (remove SiO\(_2\))
9. H\(_2\)O rinsing and nitrogen drying

Boiling the sample for one hour in acetone removes wax-residues that might be left from the cutting of the wafer. Normally boiling tri and acetone are used for \( \sim 5 \) minutes in separate steps. This was also done, but it came clear with optical microscope that the procedure did not remove all wax. Boiling the sample in acetone for one hour on the other hand gave a pleasant result.

All substrates were etched with a hydrogen and nitrogen mixture before the growth started in order to remove additional SiO\(_2\) from the surface. The etching procedure was performed at 1200\(^\circ\)C in 50 mbar with a hydrogen and nitrogen flow of 15 l/min and 3 l/min respectively.

7.2 GROWTH DETAILS

Figure 21 shows the structures we tried to grow during this work and the gas-flows for each individual layer is summarized in Table 4. The values in Table 4 are the same for the corresponding layers in different structures. Purified hydrogen and nitrogen with a continuous flow of 15 and 3 l/min respectively was used as a carrier gas.

No rotation was used during the growth or hydrogen etching because the satellite in the susceptor was built for a full size two-inch wafer. If a one eight segment of a full size wafer is placed on a satellite built for two-inch wafer and rotation is used, there is a chance that the segment starts to move and spoil the run.
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₀.₂₅Ga₀.₇₅N</td>
<td>1000</td>
<td>50</td>
<td>2 min 10 sec</td>
<td>100</td>
<td>30</td>
<td>4000</td>
</tr>
<tr>
<td>AlN exclusion-layer</td>
<td>1000</td>
<td>50</td>
<td>10-40* sec</td>
<td>95-100**</td>
<td>0</td>
<td>4000</td>
</tr>
<tr>
<td>GaN</td>
<td>1000</td>
<td>50</td>
<td>70 min</td>
<td>0</td>
<td>100</td>
<td>4000</td>
</tr>
<tr>
<td>Al₀.₀₇Ga₀.₉₃N</td>
<td>1000</td>
<td>50</td>
<td>70 min</td>
<td>57</td>
<td>100</td>
<td>4000</td>
</tr>
<tr>
<td>AlN nucleation-layer</td>
<td>1100</td>
<td>50</td>
<td>40 min</td>
<td>70</td>
<td>0</td>
<td>2000</td>
</tr>
</tbody>
</table>

Table 4: CVD growth parameters for the structures. *10, 20, 30 and 40 seconds of growth were tried. See Chapter 8.2 for more details. ** 100 ml/min on the structure d and e in Figure 21.

7.3 CHARACTERIZATION DETAILS

Thickness mapping, C-V, optical microscope and resistivity characterization was performed as soon as the sample left the growth chamber and these results are presented in the Chapter 8 if nothing else is specifically told. Contact-less methods i.e. all techniques named above except C-V, were always measured before other methods in order to minimize surface contaminants. None of the samples was cleaned with any chemicals after the growth.

The C-V measurement was performed with a mercury droplet with a diameter of 1 mm at 10kHz without any kind of preparation. No special treatments were performed after the C-V measurements even though it may reduce the reproducibility of the measurement. The resistivity measurements were performed with a commercial contact-less eddy current method build by Eichhorn-Hausmann and the equipment was calibrated with a calibration silicon-wafer ($R_0 = 398.6$ ohms/square) manufactured by Okmetic. All samples were cooled to 2.2 K (below the lambda point for $^4$He) and a 244 nm second harmonic line of $Ar^+$ laser for optical excitation was used.

We characterized three spots on each sample and these are from now on denoted as spot 1, 2 and 3. If nothing is specifically told, is the result presented in Chapter 8 taken from an area which is thought to characterize the entire sample. Appendix B presents the results from each spot.

![Figure 20: Sketch characterization spots (1 in the figure corresponds to spot 1 etc.)](image)

7.4 SIMULATION DETAILS

We used a 1D Poisson-Schrödinger solver written by Greg Snider at Notre Dame University. The solver is generally accepted and has been used in published articles like Ref [6][27]. The solver includes both pizoelectric and spontaneous polarization contributions.

To reassemble the Schottky barrier from the mercury probe, a surface bias was attached to the top AlGaN surface. According to the affinity rule, the barrier height of metal–semiconductor contact is given by:
\[ q\phi_b = q\phi_m - \chi \quad (23) \]

where \( q\phi_b \) is the work function of the metal and \( \chi \) the electron affinity for the semiconductor. The Schottky barrier height is approximately 0.87-0.93 eV for AlGa\(_x\)N with \( x=0.25-0.28 \). These values of the Schottky barrier height were calculated through linear extrapolation of GaNs and AlNs electron affinity of 4.2 and 2.05 eV respectively\(^{35}\) together with mercury's work function of 4.53 eV\(^{36}\).

The donor density was set to \( 10^{16} \) electrons/cm\(^3\) in the top AlGaN layer the donor density of the rest of the structure was set to \( 10^{10} \) electrons/cm\(^3\). The low number of \( 10^{10} \) electrons/cm\(^3\) might be confusing since donor densities usually are a lot higher in regular epilayers, but the real epilayers also consists of p-type donors like carbon and oxygen. This means that some p and n dopants will cancel and the total effective donor density will drop with several orders of magnitude. The high number of donors in the AlGaN layer was introduced to reassemble surface states.

The AlN nucleation layer was biased with –3.5 V since otherwise the solver calculates the electron densities at deep levels incorrectly. The “error” was caused by a huge band bending in the GaN buffer-layer –2 um away from the AlN nucleation layer. Adding a negative bias to the nucleation layer “tricked” the simulation and forced the band bending to occur closer to the nucleation layer. Setting the bias to – 3.5 V seemed to be in good agreement with the measured quantities.

The temperature was set to 300K and all material parameters, apart from the bandgap, were standard parameters prewritten in the program. The bandgap parameters were set to 3.45 and 6.13 eV for GaN and AlN respectively with a bending parameter of 1.3 eV\(^{37}\).

<table>
<thead>
<tr>
<th>Layer</th>
<th>Alu-content [%]</th>
<th>Donor density [cm(^{-3})]</th>
<th>Thickness [nm]</th>
<th>Bias [V]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top AlGaN (Barrier)</td>
<td>28 - 25</td>
<td>( 10^{16} )</td>
<td>25</td>
<td>0.87 - 0.92(^*)</td>
</tr>
<tr>
<td>AlN exclusion</td>
<td>100</td>
<td>( 10^{10} )</td>
<td>1 - 3</td>
<td>0</td>
</tr>
<tr>
<td>GaN buffer</td>
<td>0</td>
<td>( 10^{10} )</td>
<td>50 – 2500</td>
<td>0</td>
</tr>
<tr>
<td>AlGaN double heterojunction</td>
<td>7</td>
<td>( 10^{10} )</td>
<td>2.5</td>
<td>0</td>
</tr>
<tr>
<td>AlN nucleation</td>
<td>100</td>
<td>( 10^{10} )</td>
<td>80</td>
<td>-3.5</td>
</tr>
</tbody>
</table>

Table 5: Simulation parameters for all layers. *) biased at the surface
8.1 INTRODUCTION

This Chapter contains the characterization results and discussions of the grown structures. The outlay of the Chapter is the following: A brief presentation of the grown structures, characterization results from all samples combined with simulation results without discussions, and the simulated band diagrams and ends with the discussion.

Complete thickness maps and electrical characterization results for all samples and Areas can be found in Appendix A and Appendix B respectively.

8.2 GROWN HEMT STRUCTURES

Figure 21 shows the heterostructures we grew during this work. The AlN exclusion-layer in structure b) was grown in four different performances with growth times of 10, 20, 30 and 40 seconds respectively. The other samples were only grown once.

![Diagram of HEMT structures](image)

Figure 21: Grown structures. Using Al$_{x}$Ga$_{1-x}$N notation described in Chapter 2.3.

a) Standard AlGaN-HEMT structure (single heterojunction (SH)). b) SH-HEMT with an AlN-exclusion-layer. c) SH-HEMT with an Al$_{0.05}$Ga$_{0.95}$N buffer layer. d) Double heterojunction AlGaN-HEM (DH). e) DH AlGaN-HEMT with an AlN-exclusion-layer.

8.3 SH AlGaN-HEMT - RESULTS

The surface morphology of the SH AlGaN-HEMT looked smooth without any visible crack formations in the optical microscope. The optical microscope showed that the sample had some minor crystal defects and particles spread over the surface but nothing extraordinary.

We believe that spot 2 is characteristic for this sample and the following result was taken from that area. We observed small variations in sheet resistance across the wafer with typical values around 320 [ohms/square] the day the sample was unloaded, however, these values changed considerably under three months and the sheet resistance increased to ~600 [ohms/square]. The degradation process was also found to be continuous i.e. the degradation did
not go off during one night; this was observed over the whole sample. PL measurements gave higher aluminium content than expected, 29.5% compared to the aimed value of 25.0%.

*Figure 22* was obtained through C-V measurements and the curve contains two distinct peaks located at 24.5 and 25.3 nm. The corresponding simulated curve did not contain two peaks. We obtained a sheet carrier density of $1.47 \times 10^{13}$ [electrons/cm$^2$], which leads to an electron mobility of 1299 [cm$^2$/Vs] through *Equation 15*. The simulation gave a sheet carrier density of $1.44 \times 10^{13}$ [electrons/cm$^2$].

![Figure 22: Measured and simulated carrier concentrations. Note: the simulated curve was translated on the Depletion-axis to fit the curve.](image)

The same measurement was performed three months later and the resulting curve was translated approximately 3 nm away from the surface. Furthermore, the curve did not have two peaks three months after the growth. We obtained a sheet carrier density of $1.33 \times 10^{13}$ [electrons/cm$^2$] and a sheet resistance of 640 [ohms/square], which gives an electron mobility of 730 [cm$^2$/Vs]. The simulated curve fitted well with the measured.

### 8.4 SH AlGaN -HEMT WITH AN ALN EXCLUSION-LAYER – RESULTS

As stated earlier, four different samples with 10, 20, 30 and 40 seconds of AlN exclusion-layer growth were investigated. The surface morphology varied a lot for these samples and the samples with 10 and 40 seconds of growth cracked, which could be observed in optical microscope (*Figure 23*). We could not observe any cracks on the samples with 20 and 30 seconds of growth with the optical microscope. It become clear at higher magnifications (using SEM) the sample with 30 seconds of growth had small crack formations on the surface. The sample with 20 seconds of growth was never examined with SEM.
The samples with 10 and 40 seconds of growth had one corner (close to spot 2), which appeared to be crack-free in the optical microscope. Again, SEM-magnification showed that this area also had small cracks formations (Figure 24) that remind about the small cracks observed in the sample with 30 seconds of growth. The small cracks were distinct and focused around small areas of a couple of \( \mu \text{m}^2 \). Nearby areas a couple of micrometers away from the small cracks appeared free from cracks.
The sheet resistances on areas with large grains like in Figure 23 were very high ($R_\text{c} > 1000$ [ohms/square]) and areas that seemed crack-free in the optical microscope usually had lower sheet resistances. The sheet resistances for all of the structures described in this Chapter, except the sample with 20 seconds of growth, was highly area dependent at a local level i.e. moving the sample a couple of millimetres in one direction gave huge differences in $R_\text{c}$ ($\sim 1-200$ [ohms/square]). This made it hard to determine the exact sheet resistance of an area so the $R_\text{c}$ -values was calculated through averages. The sample with 20 seconds of growth was sent for device fabrication approximately one week after the growth and therefore we could not determine if the sample degraded or not. However, during the week we had it, the sample did not show any degrading behaviour. All other samples degraded seriously, two months later all areas on these samples had a $R_\text{c}$ value over 500 [ohms/square]. As in the SH-case the aluminium content was higher for the barrier AlGaN layer than expected. We believe that spot 2, 1, 1 and 2 are characteristic for the samples with 10, 20, 30 and 40 seconds of growth respectively and we obtained aluminium contents of 28.9, 30.0 and 29.5 % in the AlGaN barrier layer for 10, 30 and 40 seconds of the AlN exclusion layer growth respectively.

The sheet carrier density seemed to increase with the growth time of the exclusion-layer, zero seconds of growth gave i.e. a SH AlGaN-HEMT gave a sheet carrier density of $1.45 \times 10^{13}$ [electrons/cm$^2$] and 10, 20, 30 and 40 seconds of growth gave $1.42, 1.54, 1.66$ and $1.82 \times 10^{13}$ [electrons/cm$^2$] respectively. An increasing behaviour was also observed in the pinch of voltage. The minimum sheet resistance was 234 [ohm/square] and was obtained on the sample with 20 seconds of exclusion-layer growth. Figure 25 shows how the mobility changed with the growth time.

![Electron mobility versus growthtime](image)

**Figure 25: Electron mobility versus growth time.**

*Figure 26 and Figure 27 was obtained through C-V measurements and just like in the SH case, the carrier concentration versus depleation-curves show two distinct peaks located $\sim 1 – 2$ nm away from each other on all samples. On the other hand the double peaks did not disappear after three months as in the SH case but the peaks individual separation from each other increased. The curves measured three months after the growth had translated 3-5 nm away from the surface compared to the curve measured directly after the growth. Because of the heavy degradation of the 10 seconds of growth sample it was only possible to measure the 30 seconds of growth sample to 720 [ohms/square], which gave an electron mobility of 550 [cm$^2$/Vs]. None of the simulated carrier concentrations had two peaks. We obtained a sheet carrier density of 1.17 and $1.58 \times 10^{13}$ [electrons/cm$^2$] for 10 and 30 seconds of growth respectively after three months. The*
simulation gave a sheet carrier density of 1.65, 1.82 and 1.98 * 10¹³ [electrons/cm²] for the 1, 2 and 3 nm exclusion-layers respectively; all of these values are a bit higher than what we measured quantities.

The samples with 10 and 40 seconds of exclusion-layer growth were also examined with cross-section TEM (Figure 28 and Figure 29). Figure 28 was taken from an area with crack formations like Figure 23 and Figure 29 was taken from an area that seemed crack free in the optical microscope. The cross-sectional TEM-pictures showed that the sample with 10 seconds of growth had something that looks like vertical features stretching from the AlN nucleation layer to the surface. The sample with 40 seconds of growth (Figure 29) also had similar features in the GaN layer but these did not have the same vertical appearance. From Figure 29 the AlN nucleation layer thickness can be calculated to ~200 nm, however if this is the true value is doubtful since Figure 28 show three individual layers (or four interfaces) from the same region. The layer thickness of ~200 nm is a lot higher than the expected value of 80 nm. The thin bright line in Figure 29 is probably the top AlGaN layer with a calculated thickness through the image of approximately ~30 nm. The black line in Figure 28 and Figure 29 is a metal coating applied during sample preparation.
Figure 27: Measured and simulated carrier concentrations. Note: the simulated curve was translated on the Depletion-axis to fit 30 seconds growth curve. The peaks in 30 seconds of growth stretch to $3.8-4.0 \times 10^{20}$ electrons/cm$^3$.

Figure 28: Cross-section TEM image from the sample with 10 seconds exclusion-layer growth.
8.5 SH ALGAN-HEMT WITH AN AL\textsubscript{0.07}Ga\textsubscript{0.93}N BUFFER LAYER – RESULTS

The surface morphology of the SH with an Al\textsubscript{0.07}Ga\textsubscript{0.93}N buffer layer was smooth without any visible cracks in optical microscope and we obtained a sheet resistance of 882 [ohms/square] (spot 3). The sample did not show any degrading behaviour during two and a half months and we obtained a sheet carrier density of approximately 1.00*10\textsuperscript{13} [electrons/cm\textsuperscript{2}], which gives an electron mobility of 696 [cm\textsuperscript{2}/Vs]. This is the lowest value that we obtained through all structures during these work. No PL measurement was performed on this sample.

The apparent carrier concentration versus depletion curve did not contain two distinct peaks like the SH and exclusion-layer structures. The same C-V measurement was performed two and a half month later and the carrier concentration versus depletion curvature was more or less the same. We obtained a sheet carrier density of 0.90*10\textsuperscript{13} [electrons/cm\textsuperscript{2}], which gives an electron mobility of 780 [cm\textsuperscript{2}/Vs] two and a half months after the growth.
The simulation gave a sheet carrier density of 0.75*10^{13} electrons/cm\(^2\) with 9 \% aluminium in the buffer layer. This value is a bit lower than the measured the fit in Figure 30 is far from good.

8.6 DH AlGaN-HEMT WITH AND WITHOUT AN ALN EXCLUSION-LAYER – RESULTS

We grew two samples with double heterojunctions, one with 20 seconds of AlN exclusion-layer growth and one without the exclusion-layer (Figure 21 d and e). The surface morphology of these samples was smooth and no visible grains or crack could be observed in an optical microscope. The samples sheet resistance was studied for five to six weeks and the samples did show some minor degrading behaviour (~350 -> 380 with exclusion-layer and ~540 -> 750 [ohms/square]). The sample without the exclusion-layer had 25.0 \% aluminium in the top layer and 9.0 \% aluminium in the buffer-layer. The sample with the exclusion-layer had similar aluminium content with 25.9 \% in the top AlGaN layer 8.1 \% in the buffer-layer. Surprisingly, the aluminium content is ~5 \% lower in top AlGaN layer for these samples compared to the SH-junction HEMTs (including 10-40 sec of exclusion-layer growth) even despite the fact that we did not change any growth parameters between these runs.

The double heterojunction without the AlN exclusion-layer had an electron mobility (spot 3) of 1290 [cm\(^2\)/Vs]; this value is almost identical to the value we obtained in the SH of 1299 [cm\(^2\)/Vs]. However, it is worth noting that the sheet carrier density of the SH (1.45*10^{13} [electrons/cm\(^2\)]) is approximately 54\% higher than the DH (0.92 *10^{13} [electrons/cm\(^2\)]). The sheet resistance is on the other hand approximately 56\% lower for the SH (321 [ohms/square]) compared to the DH (517 [ohms/square]). The parts approximately cancel in Equation 15 when the mobility is calculated.

The insertion of the AlN exclusion-layer changed the electrical properties of the structure notably and we obtained an electron mobility of 1648 [cm\(^2\)/Vs] through Equation 15 (spot 2, n\(_s\) = 1.07*10^{13} [electrons/cm\(^2\)] and \(R\(_c\) = 348 [ohms/square]). The electron mobility is almost as high.
as the SH with 20 seconds of exclusion-layer growth which had an electron mobility of 1702 [cm²/Vs]. The same phenomena of decreased sheet carrier density and increased sheet resistance in the SH-DH comparison was found here, but the magnitude of deviation is only ~35% compared to the ~55% for the SH.

![Figure 31: Measured and simulated DH structures with and without exclusion-layer. Note that the simulated curves are translated on the depletion axis.](image)

The carrier concentration versus depletion curve for the sample with the exclusion-layer contained two distinct peaks located approximately 2 nm away from each other (Figure 31), just like the SH and SH’s with exclusion-layers. The DH without exclusion-layer, did not contain two peaks. Neither of the simulated curves contained two peaks which otherwise had a fairly good fit to the measured curves in the 25-35 nm region. Figure 32 shows that the fit between the simulated curve and the measured once are very bad in the 35 nm-2 µm region. All free electrons seem to gather up close to the AlGaN/GaN junction in the simulation but it does not correspond to the experimental data. The DH reduced the number of free electrons in the buffer-layer with approximately half an order of magnitude when compared to a SH.

The same C-V measurement was performed approximately one and a half month after the growth the apparent carrier density versus depletion curves are shown in Figure 33. The double peak in the DH with an exclusion-layer were gone and the maximum carrier density increased to 1.43×10²⁰ [electrons/cm³], the curve was also translated on the depletion axis with ~3 nm away from the surface. The DH sample without exclusion-layer curve was also translated on the depletion axis with ~1.5 nm but otherwise the curve seemed unchanged. We obtained an electron mobility of 1800 and 1150 [cm²/Vs] (n = 0.90 and 0.75×10¹³ [electrons/cm³]) for the samples with and without exclusion-layer respectively. The simulated corresponding values are 1.41 and 1.01×10¹³ [electrons/cm³].
Figure 32: Carrier concentrations at deeper levels for the DH and SH. Note: the Apparent carrier concentration axis is also logarithmic.

Figure 33: Measured apparent carrier concentrations for the DH structures directly after the growth and approximately one and a half months later.
The double heterostructure with exclusion-layer was also wet-etched in a low percentage solution of hydrofluoric acid (HF) and purified water five weeks after the growth with intention of removing oxides of the surface. We etched the samples for 30, 60, 90, 180 and 210 seconds (referring to the total etching time) and measured the same spot after each etching step with C-V. Some of the resulting carrier concentrations are presented in Figure 34.

![Figure 34: Apparent carrier concentrations versus depletion curves for a DH structure with exclusion-layer at different etching steps and moments. Note: the 30 and 90 seconds etching curves were removed but they lay around 28-29 nm.](image)

From Figure 34 shows that HF etching seems to translate the curves towards lower levels on the depletion axis. The translation on the depletion axis was found to be area dependent and this is most likely the reason 60 second of etching curve ended up behind the “0 seconds of etching – 5 five weeks after growth” curve. We stopped etching the sample after 210 seconds when the curve finally passed the curve directly after growth. Note that the double peak that we observed directly after the growth could not be seen after the etching. The etching procedure did not seem to affect the sheet carrier density.

8.7 BAND DIAGRAMS

The following bandstructures were calculated with one-dimensional solver described in Chapter 6. We used 25% aluminium content in the top AlGaN layer in all of the underlying figures. The Fermi level is set to 0 eV for all structures.
Figure 35: Comparison of a single heterojunction HEMT with exclusion-layer HEMTS with thickness of 1 and 3 nm. The picture shows the bands from the surface to the substrate.

Figure 36: Close-up of Figure 30 which show the bands at the AlGaN/GaN or AlGaN/AlN/GaN - junction. The depth of the energy well is \(-0.33\), \(-0.37\) and \(-0.44\) eV for the SH, SH with 1 nm exclusion-layer and 3 nm exclusion-layer respectively.
Figure 35 shows that the bandgap for Al$_{0.28}$Ga$_{0.72}$N (0-25 nm) equals 3.98 eV which correlates well with Equation 1 if $b = 1.3$ eV. The bandgap at the GaN level equals 3.4 eV and the AlN area gives a bandgap of 6.2 eV just as it should. Figure 36 shows that depth of the energy well is increasing with the thickness of the AlN.

![Figure 35: Diagram showing bandgap for Al$_{0.28}$Ga$_{0.72}$N and AlN areas.](image)

Figure 37 shows the bands for the double heterojunction (both with and without the exclusion-layer) is continuously increasing in the GaN buffer layer (25-75 nm) till the Al$_{0.07}$Ga$_{0.93}$N layer is reached at 1.8 eV. Note that the potential well bottom is under the Fermi level in all figures.

8.8 DISCUSSION

Appendix A (Chapter 10) shows that all samples grown during this work had a large epilayer thickness gradient across the sample with a typical wafer minimum and maximum thickness of ~2 and 3 µm. The thickness gradient is most likely caused by a hot spot somewhere in the susceptor and rotating the sample during the growth would most probably reduce the gradient. The epilayer-thickness differences leads to high amounts of stress bundled into the material at thick areas compared to the thin since the induced stress is thickness dependent (Chapter 2.4). The bundled stress affects the electrical properties of the structure by increasing dislocation densities and piezoelectrical contributions, therefore it is hard to make any general conclusions about the structures we grew.

However, it is possible to observe patterns through the structures we grew; like increasing sheet carrier density with increasing growth time of the exclusion-layer. This is reasonable since the exclusion-layer most probably do not contain pure AlN. The exclusion-layer most probably consists of a ternary alloy of Al$_{x}$Ga$_{1-x}$N (where $x < 1$) because of Ga traces left in susceptor after
GaN growth. Increased growth time of the exclusion-layer should therefore increase the Al-content (more Ga tracers pumped out of the susceptor), which results in a deeper potential well (since AlN got a wider bandgap than GaN) and stronger polarization effects (AlN spontaneous polarization along the [0001] direction is 0.081 [C/m²] compared to GaN’s 0.029 [C/m²]). Demonstrations in Ref. [21] also showed that the interface between AlN and GaN grown under similar circumstances is not well defined i.e. the Al and Ga content at the interface is not legible. Increased sheet carrier density by increased AlN thickness also is in accordance with the simulation even though we simulated the structures with perfect AlN junctions with x=1. AlN screening of the AlGaN is probably causing the increasing carrier density in the simulation case. This effect should not be neglected in the experimental case either, since it probably contributes to the increased number of electrons in the experimental case as well. The sheet resistance on the other hand does not seem to decrease with the exclusion-layer growth time and we obtained a minimum sheet resistance for the sample with 20 seconds of exclusion-layer growth. The growth time of 20 seconds seems like a good trade-off between sheet resistance and sheet carrier density for maximum mobility. The growth time of 20 seconds probably is not optimal from an electron mobility prospective and further investigation about the growth times around 20 seconds should be made.

Figure 31 for example, shows that the AlN exclusion-layer effectively suppresses the carriers out of the AlGaN layer in agreement to the literature Ref. [21]. The exclusion-layer curve in Figure 31 does not bend downwards at the lowest depletion level like the curve without the exclusion-layer and this phenomenon can be observed through all samples. There is also a possibility that the Schottky barrier caused by the mercury droplet applied during the C-V measurement depletes to parts of the 2DEG, this however was confirmed not to be the case when we ran a C-V measurement in the positive direction since we obtained a higher maximum apparent carrier density without any downward bending.

The DH structure did not deliver the electron mobility enhancement we expected29 (the result can not be compared to 100% since the structure in the literature had a higher aluminium content in the buffer layer) with an electron mobility of ~ 1300 [cm²/Vs], almost identical to the regular SH. But the differences in sheet carrier density and sheet resistance make the structure an interesting option to the regular HEMT. The same goes for the DH with the exclusion-layer when compared to the SH with 20 seconds of exclusion-layer growth. There are great differences in sheet carrier density and sheet resistance between the structures, which make both structures of high interest. However, it should not be forgotten that the aluminium content of the top AlGaN layer in the DH’s are approximately ~ 3-5 % lower than SH and therefore the sample should not be comparable to 100%. Why the aluminium content dropped for the DH’s even though we used higher trimethyl aluminium flow (5 ml/min) is uncertain but it seems like we do not have vast reproducibility in our equipment.

The double peaks we observed in the apparent carrier concentration versus depleation curves are also hard to say anything about, but apparently the double peaks are not caused by the exclusion-layer since the phenomenon could be observed in a SH without exclusion-layer. The double peaks indicate that we have two 2DEGs with approximately the same amounts of electrons. Published literature like Ref. [25] showed one peak in a SH junction with an exclusion-layer and Ref. [27][29] shows one peak in regular SH structures. None of the calculated band structures got two potential wells. At the first glimpse, the double peak phenomenon looks like malfunctioning measuring equipment. However, this cannot be the case since we calibrated the measurement apparatus with another SH AlGaN-HEMT without exclusion-layer grown in our laboratory before and after the measurement. The calibration wafer did not show any signs of a second 2DEG. Another interesting property of the double peak is the fading over time at some samples (SH without exclusion-layer and DH with exclusion-layer). Five weeks after the growth the second peak was gone in the DH with exclusion-layer, and the curve was also found translated towards deeper levels of the depletion axis (Figure 34). We believe a surface oxide
caused the majority of translation on the depletion axis since AlGaN is oxide-reactive. Furthermore, the position of the apparent carrier density versus depletion curve was area dependent, which means it is hard to know for certain if the HF-etching removed the oxide or if the measurement was performed at another contiguous area. However, it is most likely a combination of both mentioned types. It is also reasonable to believe that we might have “missed” the double peak because of a large step size on the depletion axis, so we tested with a smaller voltage step size of 0.01V compared to the ordinary 0.1V (increases resolution on the depletion axis) and we confirmed that structure did not contain two peaks 5-6 week’s after growth. We can from the etching procedure with most certainty conclude that the material diffused or degraded in some manner during five weeks. What exactly caused the double peaks is uncertain but we should remember that the structure has a lot of stress bundled into the lattice unevenly across the wafer, if the stress caused by different epilayer thickness or not, could be determined by re-growth of the samples with rotation.

Overall the simulated carrier densities close to the 2DEG seem to be in good agreement with the experimental. However, in all structures we simulated the same trend can be observed: the experimental curves got a narrower and sharper 2DEG i.e. the simulation has a widespread 2DEG. In Figure 38 (edited Figure 31) this phenomenon of a widespread 2DEG is extra clear.

![Figure 38](image.png)

*Figure 38: The simulated curves are widespread compared to the experimental. This trend applies to all structures.*

The widespread 2DEG means that the band diagrams in Chapter 8.7 are incorrect. The potential well where the 2DEG form in Chapter 8.7 should be a bit narrower and thereby move electrons away from the widespread region in Figure 38 (possibly towards deeper regions where the simulation miss electrons like in Figure 32?). Therefore some numbers presented in Appendix B should be considered as unjust. What caused the “error” has not been investigated. The calculated band diagrams seem to be in good agreement of previous published articles.

We can only speculate about why two of our samples cracked up like mad (SH with 10 and 40 seconds of exclusion-layer-growth). The mean aluminium content of the top AlGaN layer for
the 10 and 40 seconds of growth are lower than the samples with 30 seconds of growth and the SH. This is unexpected since a higher aluminium content increases the lattice mismatch between the Al$_x$Ga$_{1-x}$N and GaN. A thin AlN-layer (10 seconds of growth) grown on top of GaN should in relative terms embrace less stress than a thick AlN (20 seconds and 30 seconds of growth) layer grown on top of GaN. Less stress in the material should decrease the desire of the material to collapse and form grains, therefore samples with thin layers should be more stable compared to samples with thick layers. This is not what we observed in our laboratory since the sample with 10 seconds of growth cracked up but 20 and 30 seconds of growth did not. Figure 28 showed that areas with large crack formations have high amounts of vertical features starting close to AlN nucleation layer and this might be the reason why the top layer cracked and formed large grains. What exactly caused these features is unknown.
9 CONCLUSIONS AND FUTURE WORK

We present an experimental and simulation study of a thin AlN exclusion-layers in undoped SH and DH AlGaN-HEMT structures. It is difficult to draw any general conclusions about the samples we grew in view of the fact that the samples were grown without rotation, but some results were however achieved.

The insertion of an AlN exclusion-layer improved the electron mobility in both SH and DH structures and the optimum growth time of the exclusion-layer was found to be 20 seconds. We observed a maximum electron mobility of 1700 \(\text{cm}^2/\text{Vs}\) in a SH structure with an exclusion-layer, compared to 1300 \(\text{cm}^2/\text{Vs}\) in a regular SH without an exclusion-layer. We achieved a similar electron mobility of 1650 \(\text{cm}^2/\text{Vs}\) for the DH with exclusion-layer, compared to \(~1300 \text{ cm}^2/\text{Vs}\) in a regular DH without exclusion-layer. Even though the samples had approximately the same mobility, had the samples great differences. The SH with exclusion-layer had \(\sim 45\%\) higher sheet carrier density and \(\sim 50\%\) lower sheet resistance compared to the corresponding DH. Device manufacturing and device comparison could be very interesting for these structures.

The sample with highest electron mobility (20 seconds of growth) was sent for device manufacturing. Unfortunately, we did not get any results back before the printing of this work but it would be very interesting to see device characteristics.

Some samples cracked and formed a grain pattern on the surface. TEM investigations showed that areas on samples with large grain formation observable on the surface had high amounts of vertical features in the GaN layer. Furthermore all samples did show degrading behaviour (the sheet resistance changed over time), which were especially clear in samples with high aluminium content in the top AlGaN-layer. The connection between the features, cracking, and degradation can be furthered investigated.

We observed something which looked like a second 2DEG with a mutual distance of \(\sim 1-4\) in all samples with an AlN exclusion-layer and in one sample without an AlN exclusion-layer and we also observed a fading over time of the second 2DEG and in some samples the second 2DEG disappeared completely. The reason for the appearance of the second 2DEG was never stated and we recommend re-growth of the samples with rotation as a further analysis. Rotating the sample during growth would smooth out the thickness gradient of the epi-layers and decrease the bundled stress in the material at thick areas. An examination like this could maybe answer if the thickness differences cause the second 2DEG or not.

The calculated apparent carrier concentrations from the simulation were in fairly good agreement with the experimentally obtained close to the 2DEG (referring to when no second electron gas is present) even though the calculated 2DEG shape was widespread compared to the experimental one. The widespread 2DEG is the result of the inaccuracy in the calculated band diagrams. What exactly caused this “error” needs further investigations.
This Chapter contains complete thickness maps for all grown samples. The pictures are presented in a scale of 1:1.25. All samples were placed in the way during the growth (referring to the susceptor).

Figure 39: To the left – Standard AlGaN HEMT; to the right – AlGaN HEMT with 10 sec of AlN exclusion-layer growth.

Figure 40: To the left – AlGaN HEMT with 20 sec of AlN exclusion-layer growth; to the right – AlGaN HEMT with 30 sec of AlN exclusion-layer growth.
Figure 41: To the left – AlGaN-HEMT with 40 sec of AlN exclusion-layer growth; to the right – AlGaN HEMT with AlGaN buffer layer.

Figure 42: To the left – Double heterojunction AlGaN-HEMT without AlN exclusion-layer growth; Double heterojunction AlGaN-HEMT with 20 sec AlN exclusion-layer growth.
This Chapter summarizes the resistivity, C-V and PL characterization data for all areas shown in Figure 20 for each sample. The tables also contain simulation data results. A field marked with “—” means that no data could be obtained from the specific area. A field marked with “/” means that no measurement was performed.

### Standard AlGaN HEMT

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Simulated</th>
<th>Spot 1</th>
<th>Spot 2</th>
<th>Spot 3</th>
<th>Mean</th>
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</thead>
<tbody>
<tr>
<td>Al-content of the top AlGaN layer [%]</td>
<td>28.0</td>
<td>29.6</td>
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<td>AlGaN thickness [nm]</td>
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<td>7.0</td>
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<td>Sheet carrier density [$10^{13}$/cm$^2$]</td>
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<td>Electron mobility [cm$^2$/Vs]</td>
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### AlN exclusion-layer, 10 seconds of growth

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<th>Parameter</th>
<th>Simulated (1nm excl)</th>
<th>Spot 1</th>
<th>Spot 2</th>
<th>Spot 3</th>
<th>Mean</th>
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<td>Al-content of the top AlGaN layer [%]</td>
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<td>27.1</td>
<td>28.4</td>
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<td>28.13</td>
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<td>AlGaN thickness [nm]</td>
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<td>25.1</td>
<td>28.1</td>
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<td>-</td>
</tr>
<tr>
<td>Pinch off voltage [V]</td>
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<td>7.6</td>
<td>8.0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sheet resistance [Ohms/Square]</td>
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<td>1935</td>
<td>265</td>
<td>348</td>
<td>849</td>
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<tr>
<td>Sheet carrier density [$10^{13}$/cm$^2$]</td>
<td>1.65</td>
<td>1.51</td>
<td>1.42</td>
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<tr>
<td>Electron mobility [cm$^2$/Vs]</td>
<td></td>
<td>210</td>
<td>1630</td>
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### AlN exclusion-layer, 20 seconds of growth

<table>
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<tr>
<th>Parameter</th>
<th>Simulated (2nm excl)</th>
<th>Spot 1</th>
<th>Spot 2</th>
<th>Spot 3</th>
<th>Mean</th>
</tr>
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<tbody>
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<td>Al-content of the top AlGaN layer [%]</td>
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<td>/</td>
<td>/</td>
<td>/</td>
<td>-</td>
</tr>
<tr>
<td>AlGaN thickness [nm]</td>
<td>25.0</td>
<td>25.2</td>
<td>22.9</td>
<td>24.0</td>
<td>24.0</td>
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<tr>
<td>Pinch off voltage [V]</td>
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<td>7.8</td>
<td>7.3</td>
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<td>Sheet carrier density [$10^{13}$/cm$^2$]</td>
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<td>1702</td>
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### AlN exclusion-layer, 30 seconds of growth

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<th>Spot 2</th>
<th>Spot 3</th>
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<tr>
<td>Al-content of the top AlGaN layer [%]</td>
<td>28.0</td>
<td>-</td>
<td>30.0</td>
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<tr>
<td>AlGaN thickness [nm]</td>
<td>25.0</td>
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<td>25.4</td>
<td>22.8</td>
<td>24.2</td>
</tr>
<tr>
<td>Pinch off voltage [V]</td>
<td>-</td>
<td>8.1</td>
<td>8.4</td>
<td>8.2</td>
<td>8.2</td>
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<tr>
<td>Sheet resistance [Ohms/Square]</td>
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<td></td>
<td>1195</td>
<td>1249</td>
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<td>1157</td>
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<tr>
<td><strong>AlN exclusion-layer, 40 seconds of growth</strong></td>
<td></td>
<td>Simulated</td>
<td>Spot 1</td>
<td>Spot 2</td>
<td>Spot 3</td>
</tr>
<tr>
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<td>---</td>
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<table>
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<th>Simulated (Al_{0.09}Ga_{0.91}N buffer layer)</th>
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<th>Spot 2</th>
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<td>25.0</td>
<td>/</td>
<td>/</td>
<td>/</td>
<td>/</td>
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<tr>
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<td>23.2</td>
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<td></td>
</tr>
<tr>
<td><strong>Pinch off voltage [V]</strong></td>
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<td>4.9</td>
<td>5.4</td>
<td>4.9</td>
<td>5.1</td>
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<td><strong>Sheet carrier density [10^{13}/cm^2]</strong></td>
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<td>0.96</td>
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<th>Spot 2</th>
<th>Spot 3</th>
<th>Mean</th>
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<td>/</td>
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<tr>
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<table>
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<th>Simulated (2nm excl)</th>
<th>Spot 1</th>
<th>Spot 2</th>
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<tr>
<td><strong>Al-content of the top AlGaN layer [%]</strong></td>
<td>25.0</td>
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</tr>
<tr>
<td><strong>Al-content of the AlGaN buffer layer [%]</strong></td>
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<tr>
<td><strong>Pinch off voltage [V]</strong></td>
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<td>5.5</td>
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