

POLARIZATION ENGINEERING, GROWTH AND TRANSPORT IN NEXT-GENERATION TRANSISTORS ON ALN PLATFORM

A Dissertation

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NEXT-GENERATION TRANSISTORS ON ALN PLATFORM

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Aluminum Nitride with a direct ultra-wide bandgap (UWBG) of 6.1 eV and a very high Debye temperature has traditionally been considered as a piezoelectric *insulator*. AlN, as an electronics platform, can lead to a revolution in power and RF electronics where it has a much higher breakdown field than GaN (15 MV/cm) and its ability to operate at higher temperatures. Recently, the AlN/GaN/AlN high electron mobility transistors (HEMTs) on the AlN platform have demonstrated output powers of ~ 2 W/mm at operating frequencies up to 94 GHz. Building on these transistors, this dissertation aims to push the capabilities of AlN HEMTs to new limits through innovative heterostructure design, polarization engineering, and theoretical transport studies.

The dissertation begins with the exploration of UWBG material AlGa_N as a potential electron channel on the AlN platform. With a systematic study of the properties of metal-polar AlN/AlGa_N/AlN heterostructure, we examine 2d electron gases (2DEGs) obtained by polarization-doping in some of the widest bandgap semiconductors to date. Next, the device applications of these AlN/AlGa_N/AlN 2DEGs, specifically in AlN HEMTs for mm-wave power amplifiers (PAs) are presented. The effect of increasing Al composition on the transistor characteristics of AlGa_N channel quantum well HEMTs is shown. Finally, the RF operation of UWBG channel AlN/Al_{0.25}Ga_{0.75}N/AlN HEMTs with a record high f_T/f_{max} of 67/166 GHz is demonstrated.

Next, the discussion shifts to the bulk single crystal N-polar AlN platform, and its advantages over the Al-polar AlN platform are examined. For the first time, the molecu-

lar beam homoepitaxy of high-quality N-polar AlN on the N-face of bulk AlN substrates is demonstrated. Building on this, various epitaxial structures hosting polarization-induced electron gases on the N-polar AlN platform are presented. Structures presented range from the undoped N-polar GaN/AlN 2DEGs, N-polar AlGaN/AlN 2DEGs, and N-polar graded AlGaN/AlN 3d electron gases.

Lastly, the discussion is moved to theoretical aspects of carrier transport where a novel analytical formulation for calculating ballistic transport properties of fermions and bosons in arbitrary dimensions and for generic dispersions is presented. This model is then applied to polar semiconductors to obtain the intrinsic limit of optical phonon scattering limited electronic currents.

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11. N-polar GaN/AlGaIn/AlN high electron mobility transistors on single-crystal bulk
AlN substrates
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Nomoto, Austin Hickman, Cheng Wang, Patrick Fay, Masato Toita, Debdeep

Jena, and Huili Grace Xing

Applied Physics Letters, 122(9), 092104 (2023).

10. Toward AlGa_N channel HEMTs on AlN: Polarization-induced 2DEGs in AlN/AlGa_N/AlN heterostructures

Jashan Singhal, Reet Chaudhuri, Austin Hickman, Vladimir Protasenko, Huili Grace Xing, and Debdeep Jena

APL Materials, 10(11), 111120 (2022).

9. Molecular beam homoepitaxy of N-polar AlN: Enabling role of aluminum-assisted surface cleaning

Zexuan Zhang, Yusuke Hayashi, Tetsuya Tohei, Akira Sakai, Vladimir Protasenko, **Jashan Singhal**, Hideto Miyake, Huili Grace Xing, Debdeep Jena, and YongJin Cho

Science Advances, 8(36), eabo6408 (2022).

8. Molecular beam homoepitaxy of N-polar AlN on bulk AlN substrates

Jashan Singhal, Jimmy Encomendero, Yongjin Cho, Len van Deurzen, Zexuan Zhang, Kazuki Nomoto, Masato Toita, Huili Grace Xing, and Debdeep Jena

AIP Advances, 12(9), 095314 (2022).

7. High-density polarization-induced 2D electron gases in N-polar pseudomorphic undoped GaN/Al_{0.85}Ga_{0.15}N heterostructures on single-crystal AlN substrates

Zexuan Zhang, Jimmy Encomendero, Eungkyun Kim, **Jashan Singhal**, YongJin Cho, Kazuki Nomoto, Masato Toita, Huili Grace Xing, and Debdeep Jena

Applied Physics Letters, 121(8), 082107 (2022).

6. In Situ Crystalline AlN Passivation for Reduced RF Dispersion in strained-channel AlN/GaN/AlN HEMTs

Reet Chaudhuri, Austin Hickman, **Jashan Singhal**, Joseph Casamento, Huili

Grace Xing, and Debdeep Jena

physica status solidi (a), 219 (4), 2100452 (2022).

5. Epitaxial Ferrimagnetic Mn₄N Thin Films on GaN by Molecular Beam Epitaxy
Zexuan Zhang, Yongjin Cho, Mingli Gong, Shao-Ting Ho, **Jashan Singhal**, Jimmy Encomendero, Xiang Li, Hyunjea Lee, Huili Grace Xing, and Debdeep Jena
IEEE Transactions on Magnetics, 58(2), 1-6 (2021).
4. Unified ballistic transport relation for anisotropic dispersions and generalized dimensions
Jashan Singhal and Debdeep Jena
Physical Review Research, 2 (4), 043413 (2020).
3. Magnetic properties of MBE grown Mn₄N on MgO, SiC, GaN and Al₂O₃ substrates
Zexuan Zhang, Yongjin Cho, **Jashan Singhal**, Xiang Li, Phillip Dang, Hyunjea Lee, Joseph Casamento, Yongjian Tang, Huili Grace Xing, and Debdeep Jena
AIP Advances, 10(1), 015238 (2020).
2. Materials Relevant to Realizing a Field-Effect Transistor Based on Spin-Orbit Torques
Phillip Dang, Zexuan Zhang, Joseph Casamento, Xiang Li, **Jashan Singhal**, Darrell G Schlom, Daniel C Ralph, Huili Grace Xing, and Debdeep Jena
IEEE Journal on Exploratory Solid-State Computational Devices and Circuits, 5(2), 158-165 (2019).
1. The new nitrides: Layered, ferroelectric, magnetic, metallic and superconducting nitrides to boost the GaN photonics and electronics eco-system
Debdeep Jena, Ryan Page, Joseph Casamento, Phillip Dang, **Jashan Singhal**, Zexuan Zhang, John Wright, Guru Khalsa, Yongjin Cho, and Huili Grace Xing
Japanese Journal of Applied Physics, 58(SC), SC0801 (2019).

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*I dedicate this dissertation to my parents
for their unwavering support and countless sacrifices.*

Pick a flower on Earth and you move the farthest star...

- Paul A. M. Dirac

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I not only use all the brains that I have, but all I can borrow.

- Woodrow Wilson

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... In what is following, you will read about a part of my technical experience here at Cornell. Of course, it is difficult to fit everything in one dissertation; and I apologize in advance in case I have left any details out. Nevertheless, I hope the following pages will give you a peek into my contribution to expanding the boundaries of human knowledge by a teeny microscopic amount.

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CHAPTER 1

INTRODUCTION

1.1 Evolution of the transistor channel material

The transistor, along with semiconductors in general, has been one of the greatest technological achievements of the human age. At its core, a transistor is an electrical switch with amplification capability. It converts static energy into signal energy, transforming it into a physical tool for logical transformations and communication. Transistors serve as the foundation of 'Power Electronics' when they are used for switching at high voltages, and also the basis of 'RF Electronics' when used to obtain gain at high speeds.

The first transistors from Bell Labs used the semiconductor **Ge** with an energy bandgap of **0.66 eV** [22]. The difficulties in purifying Germanium, and its temperature-sensitive electrical characteristics, prompted the hunt for alternative semiconductors which led to the discovery of Si based bipolar junction transistors [168, 192]. Following a breakthrough in developing the process of thermally grown silicon dioxide to passivate the surface of Silicon [55], the first Silicon MOSFET (metal-oxide-semiconductor field-effect transistor) was developed and became the most common type of transistor [10]. The bandgap of **Si** is **1.1 eV**. Today, much of the power electronics around us is Silicon-based. The two most popular Si-based power switching devices currently are the Insulated Gate Bipolar Transistor (IGBT) and the power MOSFET. Si-based MOSFETs are used for low voltage, low power, and high-frequency applications, dominating the power electronics market below 600 V [21, 165]. Si-based IGBT devices, on the other hand, are employed for high voltage, high power, and low-frequency applications, for applications between 600 V and 6.5 kV.

Since the 1970s, the superior electron mobilities in conventional III-V semiconductors such as GaAs compared to Si or Ge, led to the development of high electron mobility transistors (HEMTs) [135, 128] and heterojunction bipolar transistors (HBTs) [103] on Gallium Arsenide (GaAs). The bandgap of **GaAs** is **1.42 eV**. The discovery of two-dimensional electron gas (2DEG) at the AlGaAs/GaAs heterojunction [183] was instrumental in the development of HEMTs, which have since found applications in high frequency radio-frequency (RF) electronics, but not in power electronics applications that require high breakdown voltage, high electric field operation.

Ge, Si, and the "conventional" III-V semiconductors were the most common semiconductor materials in use up until the late 1980s. They have relatively narrow bandgaps of less than 2.3 eV. In the late 1980s and early 1990s, a series of pivotal material science breakthroughs in the nitride semiconductors family (GaN, InN, AlN etc.) were made by Isamu Akasaki, Hiroshi Amano, and Shuji Nakamura which allowed for the invention of the blue light emitting diode (LED). An explosion of optoelectronic innovations like white LEDs, lasers and ultra-energy-efficient displays soon followed. They were also awarded the 2014 Nobel Prize in Physics for their discoveries [195, 136]. While the wide bandgap (WBG) GaN was transforming the photonics industry and driving the material innovation in wide bandgap semiconductors, a WBG electronics revolution started brewing alongside silently.

SiC with a bandgap of **3.25 eV** and **GaN** with a bandgap of **3.4 eV** became the next frontiers of research to capitalize on the properties of WBG semiconductors for RF and power electronics. The first SiC MOSFETs were demonstrated in the late 1980s [165, 145], followed by power MOSFETs in 1994. SiC junction field effect transistors eventually reached the market in 2006 followed by MOSFETs in 2010 [163]. SiC has found commercial applications in power factor correction, railway traction, unin-

interrupted power supply, solar and wind energy, etc. This material gained significant momentum when the electric vehicle (EV) manufacturer Tesla decided to incorporate silicon carbide (SiC) chips in its Model 3 vehicle in 2018. It was considered a bold move when Tesla decided to dethrone Si IGBTs for SiC MOSFETs mainly to allow switching at higher voltages and reduction in component size, thus carving a niche for SiC in the EV industry.

With the improvements in the substrate technology and epitaxial growth techniques for GaN, thanks to the developments in GaN photonics, the first AlGaIn/GaN HEMT was demonstrated in 1993 [12] and RF properties began to be published 3 years later [95]. As is so often the case, military applications drove the early adoption stage of GaN technologies. GaN's thermal stability and electronic properties made it an attractive candidate for the military to use in radar, electronic warfare and communication devices. Due to their substantially higher electric breakdown field and electron sheet density, GaN-based transistors were immediately found to have a significant operating power advantage over GaAs-based transistors. GaN's entry into the military RF world led to the adoption of GaN HEMTs by industry [86, 129]. Power switching applications using GaN transistors are evolving more slowly, partly because they require normally-off (enhancement-mode) operation, while RF devices do not. Nonetheless, GaN power switching devices are commercially available today and have advantages such as fast switching with < 650 V voltage restrictions [86]. In fact, the 140 Watt charger of the 2021 Apple 16-inch Macbook Pro is a GaN charger. The GaN wall charger's rapid consumer adoption is probably the most public sign of GaN's rising prominence in the semiconductor power electronics industry.

One way to think about the history of power and high-temperature electronics is as a succession of increasing bandgaps in its semiconductors from 0.66 to 1.1 to 1.42 to

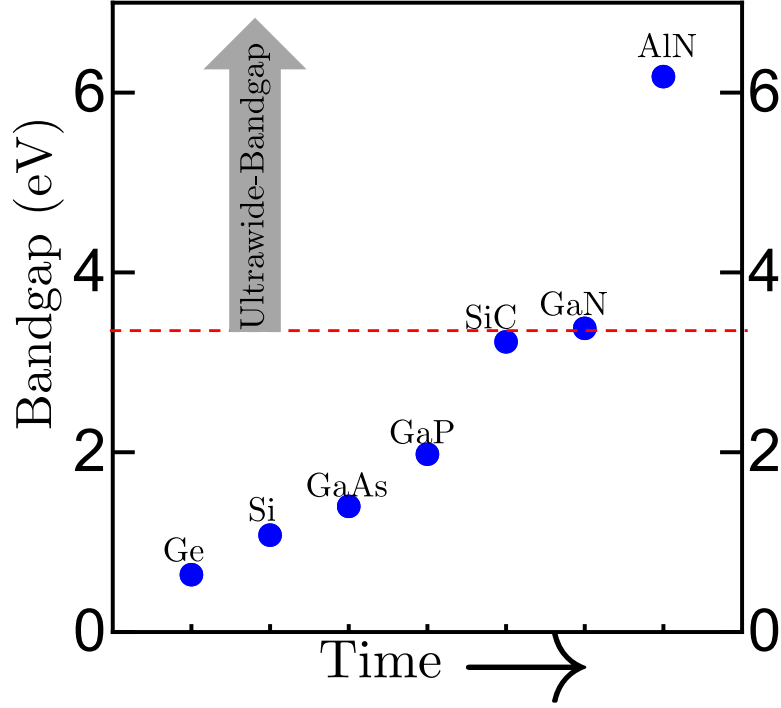


Figure 1.1: Evolution of the bandgap of the transistor channel material over the years.

2.0 to 3.25 to 3.4 eV as shown in Figure 1.1. Given the momentum and commercial success of WBG semiconductors, the following logical questions arise: "What is the next material system for RF and power electronics?" and "How can the trend toward larger bandgap semiconductors be maintained?". This dissertation aims to provide one approach to answer these questions. The answer lies in the development of ultrawide bandgap (UWBG) semiconductors which have energy bandgaps (> 3.4 eV), much wider than the conventional WBG semiconductors.

1.2 Ultrawide bandgap semiconductors

UWBG semiconductors represent an emerging new area of research covering a wide spectrum from materials, physics, devices, and applications. This new class of semi-

conductors has promising applications for future generations of RF and high-power electronics, as well as deep-UV optoelectronics, quantum electronics, and harsh-environment applications. UWBG semiconductor candidates primarily include diamond, Ga_2O_3 , and AlGaN .

1.2.1 Critical Electric Field

For next-generation electronics, the high critical electric field that an UWBG semiconductor can withstand is an important metric. It is well known that the maximum electric field at breakdown (also known as the critical electric field E_{cr}) increases with the semiconductor bandgap E_g . The relationship between E_g and E_{cr} is typically found to fit to a power-law $E_{cr} \propto E_g^\gamma$. This dependence is what has ultimately driven the adoption of WBG and, more recently, UWBG semiconductors in RF and power electronics.

Various power device figures of merit such as Baliga's figure of merit $BFOM = \epsilon_s \mu E_{cr}^3 / 4$ and the lateral device figure of merit $LFOM = n_s \mu E_{cr}^2$ for lateral devices like GaN HEMTs have very strong dependence on E_{cr} and hence a commensurately strong dependence on E_g . Here ϵ_s is the dielectric constant, μ is the electron mobility, and n_s is the carrier density. The relevant figure of merit for high-frequency high-power applications is the Johnson figure of merit $JFOM = E_{cr} v_{sat} / 2\pi$, where v_{sat} is the saturated carrier velocity. Since a wider bandgap material would have a larger E_{cr} , it will achieve a higher $JFOM$.

The underlying fundamental material parameter that appears in both RF and power device figures of merit is E_{cr} , the electric field at which avalanche breakdown occurs. More specifically, it is the parallel-plane maximum electric field when an avalanche breakdown occurs in a device without electric field crowding. So, the principal promise

of UWBG semiconductors lies in the high breakdown fields they can sustain. However the E_{cr} in AlN, Ga₂O₃, and diamond are yet to be accurately determined. In fact, in general it is difficult to directly measure the critical electric field in semiconductors. However, employing the physics of impact ionization and avalanche breakdown, E_{cr} can be indirectly estimated for a device (not for material!) using ionization integral. Ionization integral can be solved if we know the device structure (doping, epitaxial thickness) and impact ionization coefficients. Such measurements of impact ionization coefficients and the following estimation for E_{cr} have been done for 4H-SiC and GaN. Recently, a theoretical Monte Carlo simulation study showed that E_{cr} in WBG semiconductors not only depends on bandgap, but also depends on the entire band structure and scattering environment, underscoring the fact that the process (and physics) of impact ionization is quite complicated.

The physical mechanisms responsible for breakdown in UWBG materials will likely involve new physics. Since the bandgaps of most UWBG materials are larger than the electron affinity, breakdown processes such as the initiation of the avalanche process by impact ionization need carriers in the conduction band to have a kinetic energy greater than the electron affinity. This means that the carrier briefly exists in vacuum states before producing impact ionization. This type of physics is novel and specific to UWBG semiconductors, and it has exciting implications for device design and operation. While the critical electric fields in WBG SiC and GaN have been measured to reach beyond ≈ 4 MV/cm, rather than making any concrete quantitative claims about the E_{cr} in UWBG semiconductors based on any power-law estimate, we can qualitatively say that due to such an extreme bandgap, UWBG materials will have high impact ionization threshold energy, small impact ionization coefficients and hence a much higher E_{cr} compared to WBG semiconductors.

Table 1.1: Energy bandgaps and electron effective masses of various UWBG semiconductors

UWBG material	Diamond	Ga ₂ O ₃	AlN
Bandgap (eV)	5.5	4.9	6.2
m^*/m_0	0.57	0.28	0.4

1.2.2 Bandstructures, Effective Masses and Mobilities

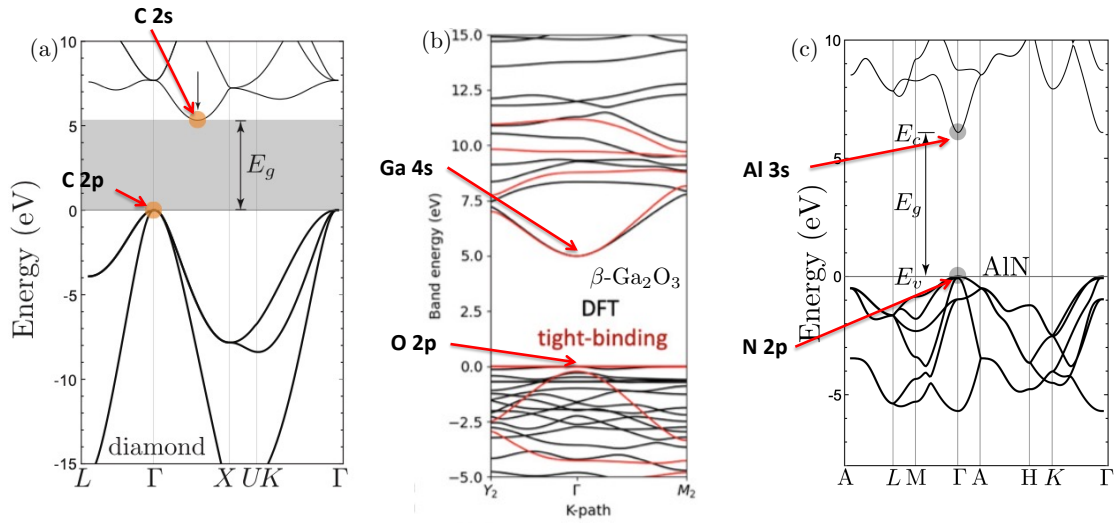


Figure 1.2: Tight binding bandstructures of UWBG semiconductors (a) diamond, (b) Ga₂O₃ and (c) AlN. As indicated by the red arrows, the conduction band minimum is primarily formed from the s orbitals from group III cations and the valence band maximum is formed from the p orbitals from group V or VI anions. Figure reproduced from the CSW presentation [81] with permission.

UWBG semiconductors (Diamond, AlN, Ga₂O₃) are all composed of *light* atoms such as C, Al, N, Ga and O from the top of the periodic table. As a general rule of thumb, bandgaps decrease as we move down the periodic table mainly because the bond lengths increase as we go down a group. For example, in the group-IV FCC elemental crystals, the indirect bandgaps decrease from diamond (5.5 eV) to Si (1.1 eV) to Ge (0.6

eV).

The bandstructures of the three candidate UWBG semiconductors are shown in Figure 1.2. They have a relatively low curvature in their conduction band minima, leading to large conduction band edge effective masses m^* compared to narrow bandgap materials. This is a direct manifestation of the quantum mechanical theory of solids. If the bandgap is small, then the conduction band and valence band are close to each other at $k = 0$ and they will repel each other and separate quickly for non-zero k values resulting in a small effective mass. If the two bands are energetically apart i.e. they have a larger bandgap, they essentially don't couple as well and have effective mass closer to free electron effective mass. We know that electron mobility μ is inversely proportional to m^* , so UWBG materials have lower μ than narrower gap semiconductors.

To summarize, small effective masses are typically connected to small energy bandgaps which are found in semiconductors that have heavy elements from the lower part of the periodic table such as InSb or InAs. Because of the small effective masses, the mobilities are high as well, but the semiconductors typically have small breakdown fields because of the small energy gaps. Furthermore, due to the heavy atoms, the optical phonon energy is quite low (~ 20 meV), as is the thermal conductivity and capacity to dissipate large amounts of heat. On the other hand, in UWBG semiconductors with light atoms from the top of the periodic table, the optical phonon energies are large (~ 100 meV), but the bandgaps and the effective masses are also large. This leads to poor electron mobility in UWBG semiconductors. Thus, this trade-off between bandgap and mobility needs to be taken into consideration when designing UWBG channel based transistors.

Why is low-field mobility important? For power devices, mobility determines the device's on-resistance, which directly correlates to power dissipation and consequently

total system power efficiency. Mobility is an important parameter for RF devices as well because, for the same bias conditions in devices with similar dimensions, higher mobility devices yield higher transit velocity ergo lower transit delays. Although velocity in low-mobility devices can be greatly increased by physically shrinking the device dimensions with minimal performance compromise, having higher mobility in general presents an inherent advantage.

1.2.3 Diamond versus Ga₂O₃ versus AlGaN for next-generation electronics

The trio of emerging UWBG materials: diamond, Ga₂O₃, and AlGaN, have experimentally demonstrated reasonable performance in unipolar field-effect transistors and/or UV light-emitting devices. They are the "new kids on the block," taking photonics and electronics to uncharted territories. However, each one of them comes with its own relative merits and demerits, which must be taken into account for expanding the palette of applications. This section highlights some of these virtues and drawbacks of this trio with regard to power and RF electronics.

Diamond possesses exceptional material features. Apart from having an UWBG, it has high electron and hole mobility (1060 cm²/(V.s) for electron and 2000 cm²/(V.s) for hole) and the highest known thermal conductivity (2290-3450 Wm⁻¹K⁻¹) of any material. However, it suffers from limited size and poor quality of substrates, and ineffective doping, particularly for n-type doping. The range of dopants that fit into the diamond lattice is highly limited because of the small lattice constant, and the best substitutional donor (phosphorus) has a high activation energy of 0.57 eV.

β -Ga₂O₃ is currently the subject of intensive research activity due to the availability of affordable semi-insulating native substrates and good controllability of n-type conduction ($n_s = 10^{15}$ - 10^{19} /cm³) through Si or Sn doping. However, it has a poor thermal conductivity (11 Wm⁻¹K⁻¹ (|| a) and 27 Wm⁻¹K⁻¹ (|| b)) which limits device operation due to inefficient heat removal. Additionally, p-type doping has not been demonstrated in Ga₂O₃ and therefore it cannot be used for bipolar devices. These two challenges stem from its low-symmetric, monoclinic crystal structure and localized oxygen orbitals, leading to a flat valence band (thus, heavier hole effective mass) and phonon band folding.

AlGa_N alloys has a direct band gap spanning a wide range (3.4 to 6.0 eV) and a high electron mobility (room-temperature mobility up to 300 cm²/(V.s) for AlN), which can be exploited for various electronic and optoelectronic requiring heterostructure and band gap engineering. Moreover, AlN has a high thermal conductivity of 340 Wm⁻¹K⁻¹, making it an attractive platform for high-power RF electronics. Even though large-area AlN single crystal substrates with negligible bowing and low dislocation densities aren't as readily available in the market, AlN substrates for epitaxy have made much progress, with commercial suppliers like HexaTech and Crystal IS being the key players. Such substrates are expensive and limited in diameter to up to 2 inches. Prototype AlN substrates with 3-4 inches diameter are under development. Obtaining controlled doping in AlGa_N using external dopants such as Si and Mg for n-type and p-type has its own challenges. The doping efficiencies decrease with Al content as the dopant ionization energy increases, and compensating defects form more easily with increasing x in Al _{x} Ga_{1- x} N. Moreover, the electron mobility in AlGa_N gets suppressed by alloy-disorder scattering.

Since the discovery of semiconductors, controlled shallow donor and acceptor dop-

ing has been the single critical step that transforms a semiconductor material from scientific curiosity to technological relevance. However, as seen from the above discussion, there are some challenges to dope UWBG semiconductors which are inextricably linked to fundamental material properties. In general, most dopant ionization energies increase with bandgap making it difficult to achieve the free carrier concentrations in UWBG semiconductors at room temperature necessary for many devices. Also, the extreme bandgaps of UWBG materials can make them prone to the self-trapping of carriers. Moreover, as mentioned previously, dopants tend to undergo compensation via impurities and defects easily in UWBG semiconductors as the formation energies of compensating defects decrease with increasing bandgap.

What distinguishes AlGa_N (AlN) in the trio of UWBG materials is that it possesses spontaneous and piezoelectric polarization which give it the unique property of polarization-induced doping for forming conductive channels. Polarization engineering strategies that exploit broken crystal symmetries can help in getting both n-type and p-type doping in AlGa_N without any chemical doping! Both diamond and Ga₂O₃ do not have the luxury of polarization doping where it is forbidden by symmetry. This makes AlGa_N a more promising candidate for next-generation transistor technology. Selected material properties of UWBG semiconductors relevant for high voltage power devices and for high power high-frequency electronics are summarized in Figure 1.3 for comparison.

These UWBG semiconductors are currently at the level of maturity that SiC was in the 1990s or GaN in the early 2000s, and several aspects of doping, defects, interfaces and heterostructure formation must be understood before they are ready for the consumer market. In this dissertation, we hedge our bets on AlGa_N (and by extension AlN) as the next big semiconductor technology. In the next section, we focus on how

Properties	Diamond	Ga ₂ O ₃	Al(Ga)N
Large Bandgap	Good	Good	Good
Doping: n-type	Not known	Good	Good
Doping: p-type	Good	Not known	Acceptable
High electron mobility	Acceptable	Acceptable	Acceptable
High hole mobility	Acceptable	Not known	Possible
Heterostructures	Not known	Good	Good
Polarization	Not known	Not known	Good
nFETs	Not known	Good	Good
pFETs	Good	Not known	Acceptable
CMOS	Not known	Not known	Acceptable
BJT	Possible	Not known	Possible
IGBT	Possible	Not known	Possible
High thermal conductivity	Good	Not known	Good
Large area epitaxy	Not known	Good	Good
Semiconductor in market	Not known	Not known	Good

Good
Acceptable
Possible
Not known

Figure 1.3: Selected properties of UWBG semiconductors relevant for power and RF electronics. "Good/ Acceptable / Possible / Not Known" are relative to the levels desirable for device technologies. Figure reproduced from the CSW presentation [81] with permission.

polarization-induced doping in AlGa_N can be exploited along with its high critical field and high thermal conductivity of AlN to provide an unmatched combination of physical properties for the next generation of transistors for power switching and radio-frequency applications.

1.3 AlGa_N (AlN) based next-generation transistor technology

Single crystal AlN with a direct bandgap of 6.1 eV and high Debye temperature provide technological opportunities to realize deep UV optoelectronics, extreme RF, and power

devices in addition to being an ideal host for quantum interaction. The inclusion of AlN in the existing transistor technology can lead to a revolution in power and RF electronics due to its high expected breakdown field (greater than 15 MV/cm), high thermal conductivity, and the possibility of high-temperature operation. Next, we argue how AlN-based HEMT technology can outperform with respect to the reigning semiconductor technologies in various different application spaces:

1.3.1 AlN-based Radio Frequency and Microwave Electronics

Radar and communication systems are widely used in military and commercial applications alike. The performance of these systems is determined by the signal-to-noise (S/N) ratio at the receiver and the transmitter's RF output power. In many application platforms, where the RF aperture is often limited in size, increasing the RF output power of the transmitter power amplifier (PA) is the only viable approach for improving system performance (e.g., extending radar or communication system range). The RF output power is directly proportional to the output power density of the PA transistor (i.e., transistor output power divided by transistor periphery width).

Over the past few decades, GaN-based HEMTs have established themselves in high-power, high-frequency applications - thanks to its wide bandgap (3.4 eV), high electron velocities (1.4×10^7 cm/s), and ability to form heterostructures exhibiting high carrier mobilities [130]. The operating output power densities achieved in today's state-of-the-art GaN-based RF transmitters are thermally limited to values substantially below theoretical electronic limits. While theoretically it is possible to achieve a further order-of-magnitude increase in P_{out} in the current GaN RF technology, this cannot be practically realized in sustained operation today due to excessive waste heat in the transistor

channel layer. GaN HEMT's inefficient DC-to-RF conversion generates waste heat that raises channel temperatures and has a rapid negative impact on transistor lifetime and performance. While GaN transistors can operate at high power in pulsed mode ($P_{out} = 40 \text{ W/mm}$), using these devices in PAs with real-world waveforms would result in unacceptably high channel temperatures and shorter lifetimes.

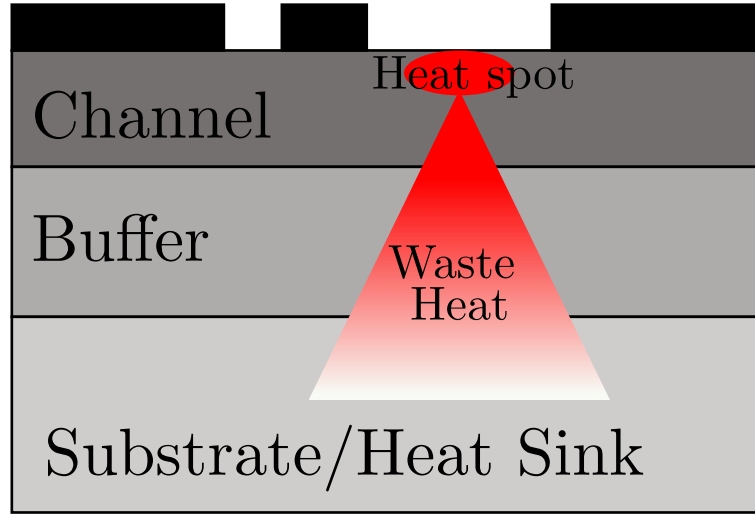


Figure 1.4: Cross-section of a typical HEMT device. In the absence of a top heat-conducting layer, the heat primarily conducts through the buffer, into the substrate and to the heat sink at the bottom.

The solution to this problem lies in efficient heat removal away from the high-power transistors without degrading the RF performance. Heat spreading is the means by which the waste energy produced by the transistor is conducted away from the transistor channel “hot spots” as shown in Figure 1.4. This is typically achieved by either increasing the gate pitch in a multi-finger transistor or by thermal via holes. While these approaches help in heat spreading, they come with an additional expense such as an increase in parasitic resistance and capacitance which degrades transistor gain and efficiency. Therefore, a more fundamental transistor heterostructure level design modification needs to be made to tackle this challenge of efficient heat removal without sacrificing RF performance.

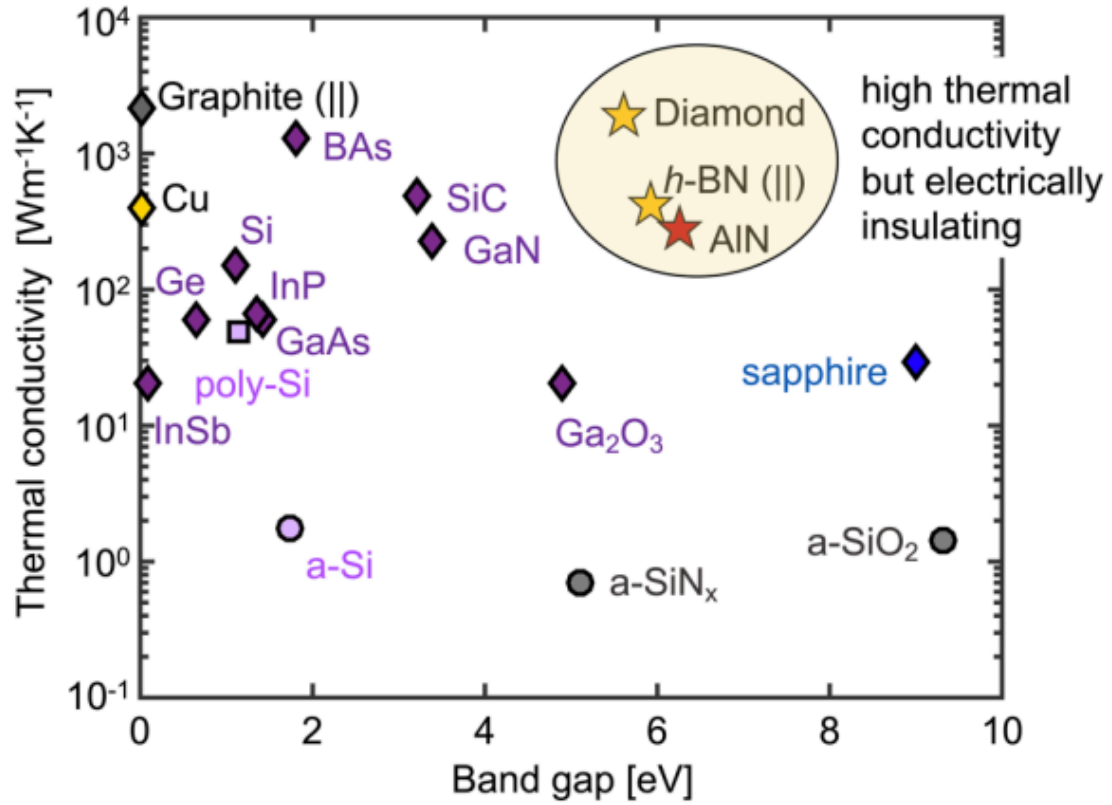


Figure 1.5: The thermal conductivity times energy bandgap (which is proportional to the electrical resistivity) of AlN is among the highest among all known materials. Figure reproduced from [208].

Just like how GaN provided a 5X improvement in RF power output (P_{out}) compared to the previous generation transistor technology, GaAs, it is time for another material paradigm shift in RF transistors. Figure 1.5 shows the experimentally measured thermal conductivities of several important semiconductor and dielectric materials used in transistor technologies [208]. Materials that have the highest thermal conductivity and energy bandgap product are most desirable for current and future RF and mm-wave technologies. High thermal conductivity allows efficient heat removal, and a large bandgap allows high electrical resistivity of the substrate, which is essential to minimize RF and mm-wave loss by absorption of electromagnetic waves by mobile carriers. Therefore,

if a material with high thermal conductivity such as AlN replaces the buffer layer in the transistor heterostructure, it could act as an efficient heat-conducting pathway for heat removal at high power levels. Thus, we envision a nitride HEMT structure with an AlN buffer layer that would be superior to the conventional RF GaN HEMT technology because of better thermal management.

Leveraging the high thermal conductivity of the AlN buffer layer will help spread waste heat effectively, and reduce transistor thermal resistance to maintain reasonably low channel temperatures, thereby increasing the net output power of the HEMT. The intrinsic power output of a RF HEMT is proportional to the product of the maximum usable voltage across the output of the device times the maximum allowed current through the device, and both voltage and current are determined by material properties. The maximum voltage is determined by the critical electric field for the material in the given device geometry and doping concentration, and the maximum current is determined by the carrier sheet density and the saturation velocity of the electrons. Using AlGaIn as a channel material instead of GaN, which has a higher critical electric field due to the wider bandgap, enables an increase in intrinsic output power due to the higher drain voltages that can be sustained in a HEMT-based amplifier. This translates directly to a superior Johnson's figure of merit in AlGaIn HEMTs, which can be up to four times higher than current GaN HEMTs, making them attractive for high-power RF applications [39]. Therefore, a key research opportunity is to realize thermally managed UWBG-channel RF transistors that generate higher output powers and power densities than the incumbent GaN technology.

1.3.2 High Power Electronics

High-power electronics feed all applications that require power switching—standing off high voltages when the switch is off while conducting high currents with low resistance when the switch is on. SiC vertical devices are currently chosen for higher voltages (breakdown voltages $V_{BR} \geq 1200$ V) because very thick drift layers (tens of μm or more) can be produced homoepitaxially and controllably doped at low concentration (in the 10^{14} cm^{-3} range). While, one may argue that, given its higher critical electric field, AlN can replace SiC vertical devices once the doping challenges in AlN are solved in the future, here we focus on more immediate applications where AlN can be utilized in power electronics.

Today, for lower voltages (breakdown voltages $V_{BR} < 650$ V), GaN devices are increasingly preferred. Contrary to SiC devices, these are lateral HEMTs; hence they can be viewed as close relatives of RF GaN devices. This is because of the high 2DEG mobility in GaN HEMTs ($\mu \sim 1500 \text{ cm}^2/(\text{V.s})$) compared to SiC MOSFETs where the mobility is two orders of magnitude lower $\mu \sim 15 \text{ cm}^2/(\text{V.s})$. The lateral geometry of GaN HEMTs makes electric-field management challenging and limits the achievable device breakdown voltage. How do we achieve higher breakdown voltages? For metal-polar AlGaIn/GaN HEMTs, this could be achieved by replacing the AlGaIn barrier with AlN and the buffer layer with AlN including just a thin strained GaN channel for hosting the 2DEG. This would lead to the majority of the heterostructure being AlN, thus a very high theoretical breakdown voltage. Moreover, such an AlN/GaN/AlN heterostructure would be very efficient due to extremely low on-resistance (R_{on}) enabled by a 2DEG with a large electron concentration ($n_s = 3 - 4 \times 10^{13}/\text{cm}^2$) at the AlN/GaN interface, thus maximizing the $BFOM = V_{BR}^2/R_{on}$. Furthermore, since the AlN barrier is unstrained when grown on AlN, it can be grown thicker for more 2DEG charge by

maximizing the polarization discontinuity, or thinner for E-Mode operation.

The performance of such an AlN/GaN/AlN HEMT can be further boosted by replacing the GaN channel with the UWBG AlGaIn channel. What is interesting about this AlN/AlGaIn/AlN heterostructure is that the whole material stack, consisting of a conductive AlGaIn quantum well active region embedded in an insulating AlN matrix, has a very high bandgap, thus potentially enabling access to the highest breakdown electric fields and operating temperatures, beyond the reach of GaN HEMTs [125, 124].

1.3.3 Realization of AlN-based HEMTs

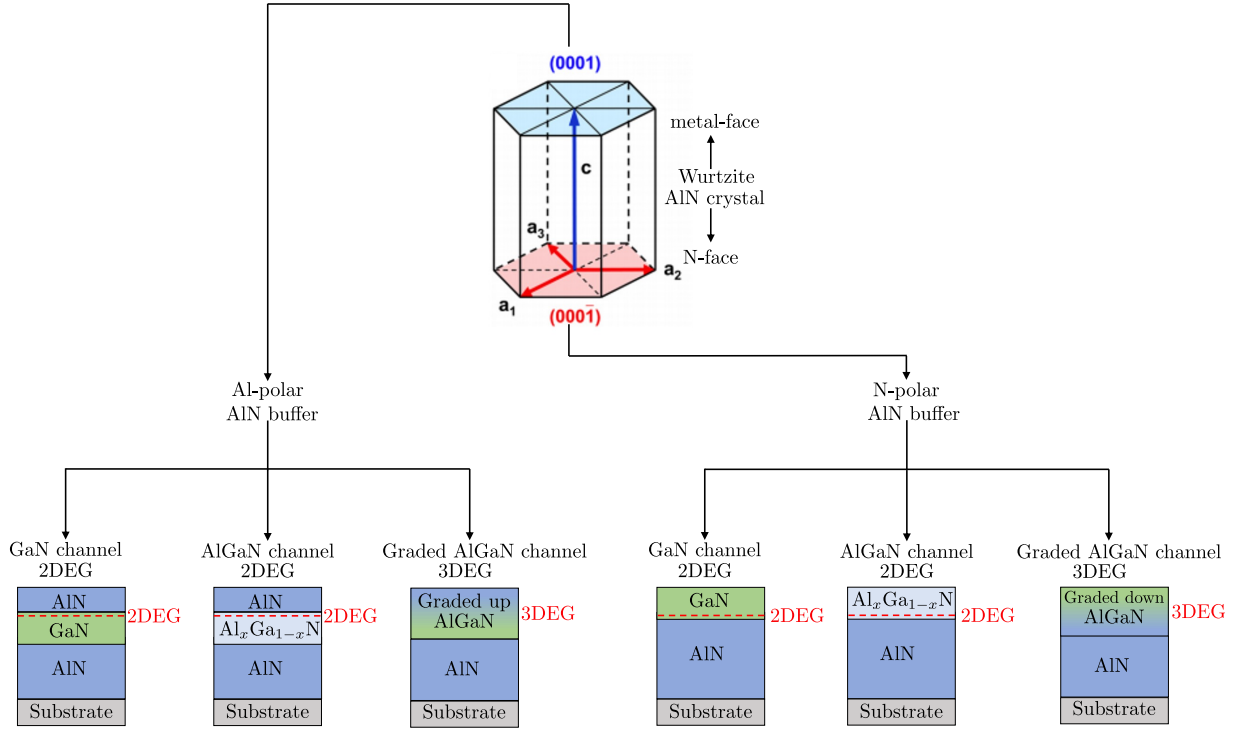


Figure 1.6: Various heterostructure realizations of next-generation of AlN-based transistor technology.

AlN is traditionally considered a piezoelectric *insulator*, but in 2014 Li *et al.* [116]

demonstrated the first high-performance AlN-based transistors with high gain and high speed. This result on Al-polar AlN demonstrated the viability of using AlN as the barrier layer as well as the buffer layer and paved way for the current state of the art AlN based quantum well (QW) HEMTs with regrown contacts capable of current drives greater than $I_d^{max} \sim 3$ A/mm, $f_T/f_{max} = 140/240$ GHz and high mm-wave output powers of > 3 W/mm at 10 GHz [69] and 2 W/mm at 94 GHz [70].

AlN is a wurtzite III-Nitride as shown in Figure 1.6, so it is non-centrosymmetric, and it lacks inversion symmetry along the c-axis. As a result of this, the Al-face and the N-face have significantly different chemical, electrical, and optical properties. The polar orientation (metal-polar or N-polar) determines the direction of spontaneous polarization in the crystal which in turn controls the type of charge induced at the surfaces or interfaces. Most of the work on AlN-based HEMTs so far has focused on the metal-polar AlN/GaN/AlN double heterostructures without exploiting either the N-polar AlN buffer or the wider bandgap AlGaN as the electron channel. The various possible heterostructure realizations of AlN-buffer based transistor technologies are listed in Figure 1.6. This also includes the polarization graded AlGaN channels which host 3-dimensional electron gases (3DEGs) to engineer the charge/velocity profiles for advantages such as superior gain linearity in RF applications.

1.4 Layout of this Dissertation

As detailed in the previous section, the ultrawide-bandgap semiconductor AlN is a newly emerging platform for mm-wave integrated circuits (MMICs) and for high-power electronics. The workhorse device on this platform has been the metal-polar AlN/GaN/AlN HEMT till now. Building on these, this dissertation aims to push the capabilities of AlN

HEMTs to new limits through innovative heterostructure design, polarization engineering, and theoretical transport studies.

Chapter 2 introduces polarization-induced 2DEGs in the UWBG AlGa_N channel on the AlN buffer platform. With a systematic study of structural, electrical, and optical properties of metal-polar AlN/AlGa_N/AlN heterostructures, we examine 2DEGs obtained by polarization-doping in some of the widest bandgap semiconductors to date.

Chapter 3 presents the device applications of these AlN/AlGa_N/AlN 2DEGs, specifically in AlN HEMTs for mm-wave power amplifiers (PAs). The key challenges in AlGa_N channel transistor development, notably the difficulties in making ohmic contacts to AlGa_N are highlighted, as well as the approaches taken to overcome those. The effect of increasing Al composition on the transistor characteristics of AlGa_N channel QWHEMTs is shown. Finally, the RF operation of UWBG channel AlN/Al_{0.25}Ga_{0.75}N/AlN HEMTs with a record high f_T/f_{max} of 67/166 GHz is demonstrated.

In **Chapter 4** the discussion moves to N-polar AlN, by literally flipping the AlN crystal on its head. The potential performance advantages of moving away from AlN-on-SiC and instead using single-crystal AlN substrates are discussed. Then, the molecular beam homoepitaxy of high quality N-polar AlN on the N-face of bulk AlN substrates is demonstrated. A brief discussion on the structural, chemical and optical characterization of N-polar AlN follows. These results lay the groundwork for next-generation electronics and photonics on the N-polar AlN platform.

Enabled by the demonstration of excellent quality of N-polar AlN growth on single crystal AlN substrates, various epitaxial structures hosting polarization-induced electron gases on the N-polar AlN platform are presented in **Chapter 5**. Structures presented

range from the undoped N-polar GaN/AlN 2DEGs, N-polar AlGaIn/AlN 2DEGs and N-polar graded AlGaIn/AlN 3DEGs. HEMT devices showing the very first transistor operation on the undoped N-polar GaN/AlN heterostructures, are also shown.

Chapter 6 moves the discussion to the theoretical aspects of carrier transport. It begins with the presentation of a novel analytical formulation for calculating ballistic transport properties of fermions and bosons in arbitrary dimensions and for generic dispersions. This generalized transport model is then applied to semiconductors with strong polar Fröhlich interaction such as GaN, AlN, h-BN etc. to obtain the phonon-limited electron velocity saturation in solids with dimensions $d = 1, 2$ and 3 , having either a parabolic or ‘massless’ conical energy bandstructures. Thus, the intrinsic limit of optical phonon scattering limited electronic currents in such polar semiconductors is presented.

CHAPTER 2

**TOWARDS ALGAN CHANNEL HEMTS ON ALN: POLARIZATION
ENGINEERING OF 2DEGS IN THE ALGAN CHANNEL**

2.1 Introduction and background

As discussed in the introductory chapter, AlGa_N, a ternary alloy of GaN and AlN, displays a broad spectrum of bandgaps from 3.4 eV (GaN) to 6.2 eV (AlN) and has various device applications ranging from optoelectronics to RF amplification and power switching. Recently, AlGa_N channel HEMTs based on metal-polar Al_yGa_{1-y}N/Al_xGa_{1-x}N heterostructures with $x < y \leq 1.0$ are being explored for potential advantages over the conventional AlGa_N/GaN HEMTs [89, 14]. Two material properties are the primary contributors to the expected improvement in performance for Al-rich transistors relative to GaN transistors, for both power switching and RF applications. These are the breakdown properties implicit in E_{cr} and the transport properties. For electrical transport, the relevant properties are the low-field mobility and the saturation velocity for power and RF devices, respectively. Next, we discuss some key material properties of AlGa_N alloys that are important for the design of AlGa_N channel HEMTs:

- **Critical Electric Field:** Operating AlGa_N at a high electric field is needed to differentiate it from state-of-the-art technologies. As discussed in the previous chapter, critical electric field, which dictates maximum field strength, is generally accepted to be related to bandgap by $E_{cr} \propto E_g^\gamma$, although there is uncertainty regarding the value of the exponent γ . For AlGa_N alloys spanning from GaN up to AlN, E_{cr} is estimated to be about 5 to 15 MV/cm. Despite multiple reports of devices with extremely high aluminum content, the experimental breakdown

voltage remains low in comparison to theoretical projections. Khachariya *et al.* [94] recently reported a record high mesa breakdown field of ~ 11.5 MV/cm in an $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}/\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ HEMT, underscoring the promise of AlGaN channel for extreme electronics at high voltages and high temperatures. Unlike vertical devices (p-n junctions) which have approached their material's predicted breakdown fields [153, 141, 3], lateral devices such as HEMTs are limited by non-uniformities in their electric fields due to device layout constraints and gate tunneling currents.

- **Low Field Mobility:** For the AlGaN alloys, the low-field electron mobility is a strong function of alloy composition. Electron mobility calculations for 2DEGs in the AlGaN channel are done here using the dominant scattering mechanisms at room temperature and above - alloy scattering and optical phonon scattering [204]. Figure 2.1(a) shows the calculated alloy-scattering limited and optical phonon scattering limited mobilities for $n_s = 10^{13}/\text{cm}^2$. The alloy-scattering limited mobility (temperature independent) degrades as the AlGaN alloy composition increases, but again recovers at higher AlN compositions with reduced alloy disorder. Note that, however, the portion of the plot for high Al fraction (above about 85% Al) is experimentally inaccessible due to insufficient band offset with the AlN barrier to produce a 2DEG. The optical-phonon limited mobility illustrates a severe degradation as the channel temperature rises from 300 K to 700 K. Figure 2.1(b) shows the total 2DEG mobility calculated at operating temperatures of 300K, 500K, and 700K. The 2DEG mobility, which strongly affects current density, drops more strongly for the GaN 2DEG and only drops moderately for high Al-content AlGaN over the 300-700 K temperature range. This suggests that the performance degradation at higher temperatures for AlGaN channel HEMTs may not be as severe as GaN HEMTs. Such a possibility might suggest that Al-

GaN could surpass SiC as the high-temperature electronics material of choice in power-switching applications. Furthermore, while the thermal conductivity of SiC decreases considerably at elevated temperatures, it doesn't drop as much for AlGaN.

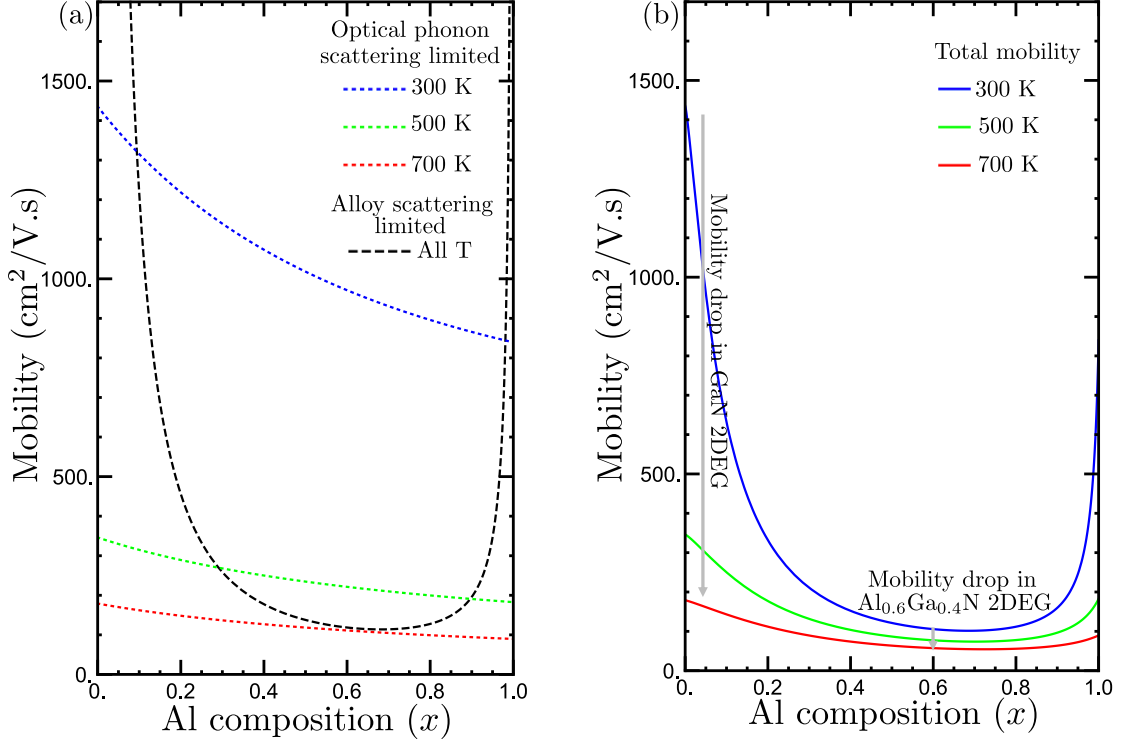


Figure 2.1: 2DEG mobility calculated as a function of Al mole fraction in Al-GaN channel ($n_s = 10^{13}/\text{cm}^2$) (a) alloy scattering limited and optical phonon limited mobility components; and (b) temperature-dependent total mobility at 300 K, 500 K and 700K.

- **Saturation velocity (high field transport):** At a high electric field, the carrier velocity saturates; is no longer proportional to the electric field (the proportionality constant being the mobility) but rather saturates. Monte-Carlo calculations of electron saturation velocity v_{sat} in AlGaIn have indicated that in comparison to mobility, it is only a weak function of alloy composition [53]. Because of its higher breakdown field and comparably high v_{sat} for Al-rich AlGaIn relative to

GaN, UWBG AlGaN is expected to have a high Johnson figure of merit $JFOM$. For example, in an applied electric field range of 100 – 600 kV/cm, the predicted saturation velocity in GaN channels is about 1.9×10^7 to 3×10^7 cm/s, while for AlGaN channels ranging from $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ to $\text{Al}_{0.8}\text{Ga}_{0.2}\text{N}$, v_{sat} is about 0.75×10^7 to 1.7×10^7 cm/s. An experimental value of 3.8×10^6 cm/s for an $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}/\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$ HEMT was lower than predicted [98], and is about 35% of the typical experimentally-reported values for v_{sat} of GaN. Similarly, an approximate v_{sat} of 5×10^6 cm/s was reported for a $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ HEMT [210]. Although the experimental AlGaN v_{sat} has not yet achieved parity with GaN, it is expected that it can be improved with more advanced field management. It may seem that AlGaN should have similar transport characteristics as GaN in the high-field regime due to the similar expected v_{sat} . However, since the mobility in AlGaN is much lower ($< 10\times$) than GaN, the electrons may not experience sufficiently high fields to be able to transit at saturated velocity. In other words, the electric field at which velocity saturation occurs would increase. Therefore the gate length of AlGaN channel HEMTs must be scaled to the point where the critical field for velocity saturation is achieved which might present a device fabrication challenge.

- **Thermal conductivity:** The thermal conductivity is crucial because materials with low thermal conductivity can have a limited operating temperature range. This leads to limitations in current density, switching power ability, or RF power output, making materials with low thermal conductivity unsuitable for next-generation electronics. AlGaN alloys display a bathtub-like curve for thermal conductivity (κ) as a function of Al composition x given by $\kappa \propto 1/x(1-x)$, indicating reduced thermal conductivity for ternary $\text{Al}_x\text{Ga}_{1-x}\text{N}$ compared to binary (GaN, AlN) alloys [117]. However, the thermal conductivity limitation can be

mitigated to some extent through the use of thin AlGa_N layers along over high thermal conductivity AlN buffer layers.

Aluminum nitride (AlN) is an emerging platform for mm-wave integrated circuits (MMICs) [71] due to its ultrawide and direct bandgap (6 eV), high thermal conductivity (~ 340 W/mK) and high piezoelectricity. AlN/GaN/AlN HEMTs [116, 152, 68, 149, 34] on this platform, which consist of *thin* and *strained* GaN quantum wells (QWs) hosting 2D electron gases (2DEGs) surrounded by AlN buffer and barrier layers, provide enhanced thermal management and improved breakdown compared to conventional GaN HEMTs. In this work, we wish to combine the benefits offered by the AlN platform with the merits of an AlGa_N channel to realize AlN/AlGa_N/AlN double heterostructures and study the physics of polarization-induced charges in them. The study of the crystal and electrical transport properties of such structures is needed to determine their potential for applications in RF and power electronics.

2.2 The AlN/AlGa_N/AlN heterostructure

Attaining an ultra-wide bandgap device structure while still having a highly conductive AlGa_N channel constitutes a heterostructure design trade-off. For metal-polar AlN/AlGa_N/AlN double heterostructures grown along the polar c-axis, the discontinuous electrical polarization $\vec{P}(z)$ across the AlN/AlGa_N top interface gives rise to a polarization sheet charge $q\sigma_\pi = -\Delta\vec{P}(z) \cdot \hat{z}$ at that interface. Here, $\Delta\vec{P}(z)$ is the polarization discontinuity at the heterojunction interface, q is the absolute value of the electron charge, and $\hat{z}$ is the unit vector along the growth direction which in this case is the positive c-axis. AlGa_N grown over AlN is under a compressive strain and thus has a piezoelectric component of polarization opposing the spontaneous one. Because

the top AlN has a higher polarization than $\text{Al}_x\text{Ga}_{1-x}\text{N}$ (where x is the Al mole fraction), the net unbalanced bound polarization charge $q\sigma_\pi(x)$ at the AlN/AlGa N interface is positive and decreases with x . [5, 204] This positive bound charge creates a high electric field and energy-band bending such that a mobile 2DEG forms at the AlN/AlGa N heterointerface. Similarly, a 2D hole gas (2DHG) should be formed at the bottom AlGa N /AlN interface due to the negative bound charge $-q\sigma_\pi(x)$ present there. Because of its polarization-generated nature, the 2DEG density should electrostatically depend on the thicknesses of the layers, the composition (x) of the AlGa N channel, and not on temperature. Furthermore, the conduction band offset $\Delta E_C(x)$ between AlN and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ which confines the 2DEG also decreases with x . [204]

Consequently, for fixed thicknesses of AlN barrier layer t_b and AlGa N channel layer t_{QW} , the 2DEG density should decrease with increasing Al composition x of the AlGa N channel. This tunability offered by the Al composition for the polarization control of the 2DEG density is of extreme importance in the design space of AlGa N channel polar heterostructures for transistor applications. However, the surface potential $q\phi_B$ (position of the conduction band with respect to the Fermi energy) complicates this simple picture and also influences the 2DEG density. The surface Fermi level is not pinned in AlN, and the processing of HEMT structures controls $q\phi_B$ and thus the 2DEG density. The pinning of the Fermi level decreases as the energy bandgap of the semiconductor increases. The strength of Fermi-level pinning is very weak for AlN [104]. This is due to the fact that as the bandgap widens, a fixed number of surface state electron energy eigenvalues resulting from dangling bonds (of the order of $10^{15}/\text{cm}^2$) spread over a larger band gap energy window.

So, the 2DEG density in such AlN/AlGa N /AlN heterostructures is a function of x , t_b , t_{QW} , and $q\phi_B$. These densities can be calculated numerically through a 1D

Schrodinger-Poisson solver or using simplified analytical equations proposed for similar AlN/GaN/AlN heterostructures by Bader [16]. Bader's model has been modified for AlGaIn channel and the analytically calculated 2DEG densities in the AlN/AlGaIn/AlN heterostructure are shown in Figure 2.2 for three cases:

1. Al content x in the channel and the thickness of the AlGaIn QW channel t_{QW} are varied while keeping the AlN barrier thickness constant at $t_b = 15$ nm and $q\phi_B = 2.2$ eV. Fig.2.2(a) shows that for a given t_{QW} , there exists a maximum x in the AlGaIn channel beyond which a polarization-induced 2DEG is not generated. Alternatively, as t_{QW} increases there is a larger range of x in the QW channel that can produce a 2DEG.
2. Al content x in the channel and the thickness of the AlN barrier t_b are varied while keeping the AlGaIn channel thickness constant at $t_{QW} = 24$ nm and $q\phi_B = 2.2$ eV. Fig.2.2(b) shows that for a given x , there exists a critical thickness t_b of the AlN barrier below which no 2DEG is formed. This critical thickness of the AlN barrier increases as x increases.
3. Al content x in the channel and the surface barrier height $q\phi_B$ are varied while keeping $t_{QW} = 24$ nm and $t_b = 15$ nm. For fixed thicknesses of the barrier and QW, the 2DEG density decreases as x increases if $q\phi_B$ is kept constant.

This calculation assumes the whole heterostructure is pseudomorphic to the AlN buffer layer, ignoring the limitations of growing thick, lattice-mismatched layers. The expected tunability of 2DEG density with the various heterostructure design parameters is shown and hence, if realized, these structures are very valuable from a scientific and device standpoint where high density of 2D electrons in the AlGaIn channel are desired. Abid *et al.* [2] and Maeda *et al.* [123] have recently demonstrated the epitaxial growth and promising HEMT device performance of AlN/Al_{0.5}Ga_{0.5}N/AlN double

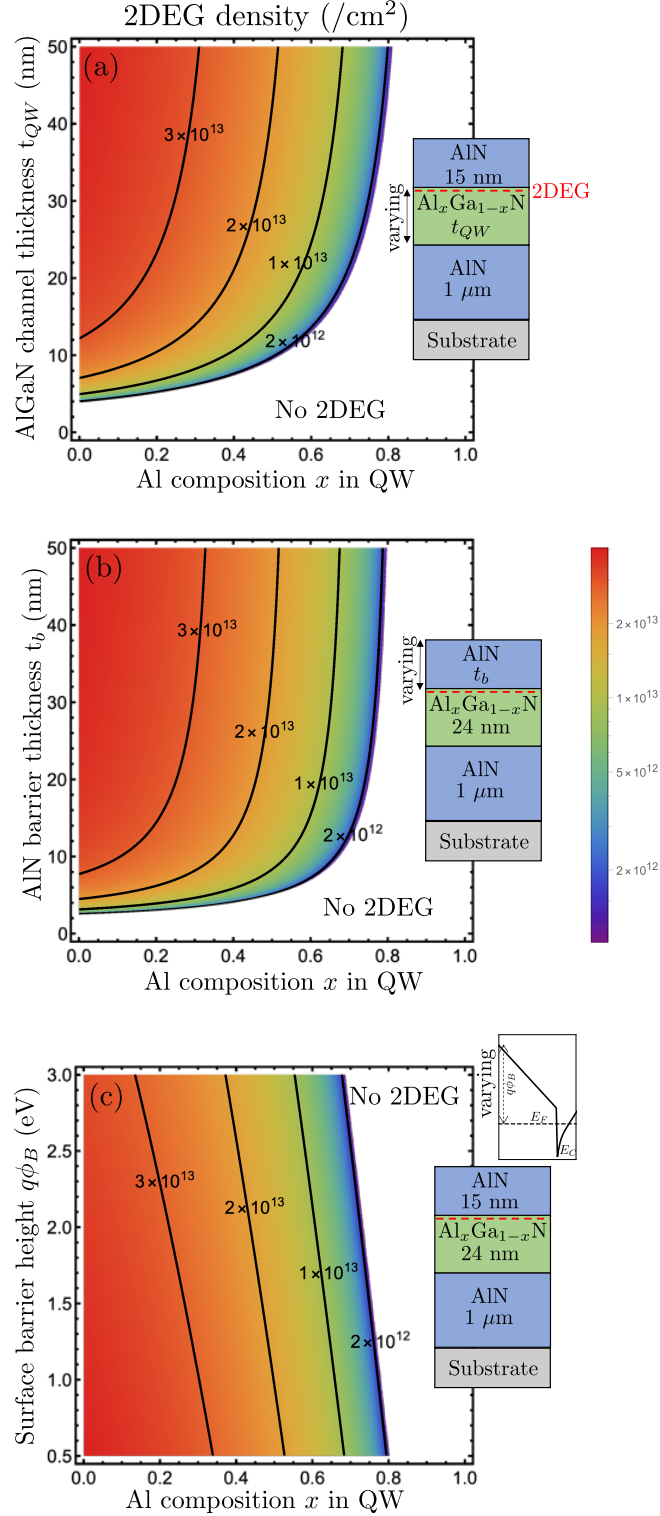


Figure 2.2: (a), (b) and (c) show the dependence of 2DEG densities in AlN/AlGaN/AlN heterostructures as a function of various heterostructure design parameters.

heterostructures by MOCVD and pulsed sputtering deposition respectively. The compositional dependence of 2DEG properties in such AlGaN channel HEMT heterostructures has not been examined yet.

2.3 Experimental Results

In this section, we report a systematic study of the structural, optical, and electronic transport properties of AlN/AlGaN/AlN double heterostructures grown using molecular-beam-epitaxy (MBE) with the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel composition ranging from $x = 0$ to $x = 0.74$. Photoluminescence spectra show that the bandgap of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel increases with x . Charge control observed in these heterostructures by AlGaN composition tuning agrees well with the polarization model, with 2DEG densities varying from $\sim 3.7 \times 10^{13}/\text{cm}^2$ in GaN channel to no measurable 2DEG in an $\text{Al}_{0.74}\text{Ga}_{0.26}\text{N}$ channel of thickness 24 nm. In addition, temperature-dependent electronic transport measurements reveal that alloy disorder scattering is the dominant scattering mechanism in the AlGaN channel 2DEGs, with an alloy fluctuation potential of ≥ 1.8 eV for electrons in AlGaN.

AlN/AlGaN/AlN double heterostructures were grown on the Si-face of semi-insulating 6H-SiC substrates using a Veeco GEN10 MBE system equipped with one standard effusion cell for elemental Ga, two cells Al1 and Al2 for elemental Al, and a radio frequency plasma source for the active N species. N plasma power of 400 W, corresponding to a growth rate of $0.42 \mu\text{m}/\text{hour}$, was used. A $1 \mu\text{m}$ thick unintentionally doped (UID) AlN buffer layer was epitaxially grown on SiC with a nucleation layer of 50 nm that was grown in a slightly N-rich condition with Al (ϕ_{Al}) to active N flux (ϕ_{N}) ratio $\phi_{\text{Al}} : \phi_{\text{N}}$ of 0.9 while the remaining 950 nm AlN buffer layer was grown in metal-rich

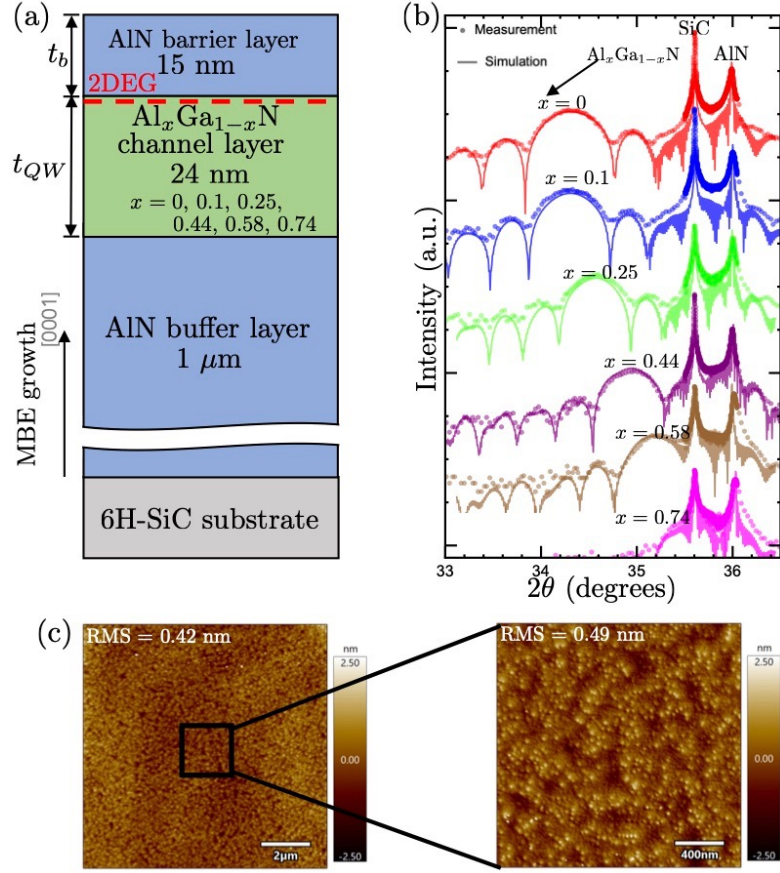


Figure 2.3: (a) Schematic and (b) XRD symmetric $\omega/2\theta$ scans of the AlN/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /AlN quantum well heterostructures with $0 \leq x \leq 0.74$. (c) $10 \mu\text{m} \times 10 \mu\text{m}$ and $2 \mu\text{m} \times 2 \mu\text{m}$ AFM micrographs of the AlN/ $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$ /AlN sample showing smooth surface morphology with sub-nm rms roughness.

conditions with $\phi_{\text{Al}} : \phi_{\text{N}}$ of 1.1. The N-rich nucleation layer blocks the Si up diffusion from the SiC surface and prevents it from incorporating in the active region.[151, 72] This was followed by the growth of $t_{\text{QW}} = 24 \text{ nm}$ thick strained AlGa N quantum well to host the 2DEG channel. The Al composition (x) in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel was systematically varied from $x = 0$ to $x = 0.74$ (calibrated by X-ray diffraction as discussed later) across six samples by changing the ϕ_{Al} with respect to ϕ_{N} while keeping the Ga flux (ϕ_{Ga}) constant. The relative flux conditions of $\phi_{\text{Al}} + \phi_{\text{Ga}} > \phi_{\text{N}}$, $\phi_{\text{Al}} < \phi_{\text{N}}$ were maintained to ensure N-limited (or metal-rich) AlGa N MBE growth conditions. An AlN

layer of thickness $t_b = 15$ nm was grown on the AlGa_xN channel as the top barrier. The AlN buffer layer and the top AlN barrier layer were grown using Al1 cell whereas the AlGa_xN channel layer was grown using Al2 cell to avoid growth interrupts. The entire heterostructure was grown at a constant substrate thermocouple temperature of 750°C. Figure 2.3(a) shows the schematic layer structures of the AlN/AlGa_xN/AlN double heterostructures with varying Al content in the AlGa_xN channel used for this study.

X-ray diffraction (XRD) was used to determine the structural quality of the epitaxial structures and the average Al composition x of the AlGa_xN channel. Figure 2.3(b) shows the measured symmetric (002) reflection XRD spectra of the six samples with increasing Al content x , along with the simulated diffraction patterns based on the layer structure shown in Figure 2.3(a). The AlGa_xN peaks are clearly resolved to the left of the substrate SiC peak for all the samples. The clearly visible thickness fringes suggest abrupt hetero-interfaces in the structure. Fitting measured spectra with the simulation confirmed the targeted thickness of the epi-layers while also yielding the average Al mole fraction x in the AlGa_xN channel layers as 0, 0.1, 0.25, 0.44, 0.58, and 0.74 for the six samples under study. The effect of strain in the AlGa_xN layer is taken into account to estimate the x values from XRD. All the samples exhibit similar smooth surface morphologies measured by atomic force microscopy (AFM) with rms roughness < 0.8 nm over a $10\ \mu\text{m} \times 10\ \mu\text{m}$ area. Figure 2.3(c) shows a representative AFM scan from the AlN/Al_{0.44}Ga_{0.56}N/AlN sample.

The in-plane lattice constant of a relaxed wurtzite AlN crystal $a_0^{\text{AlN}} = 3.112\ \text{\AA}$ is smaller than that of unstrained Al _{x} Ga _{$1-x$} N $a_0^{\text{AlGa}N} = (3.189 - 0.077x)\ \text{\AA}$, obtained from Vegard's law. Consequently, the c-plane of the AlGa_xN epitaxial layer grown over AlN experiences an in-plane compressive strain, $\epsilon_{xx}^{\text{AlGa}N} = (a^{\text{AlGa}N} - a_0^{\text{AlGa}N})/a_0^{\text{AlGa}N}$, where $a^{\text{AlGa}N}$ is the lattice constant of the strained AlGa_xN film on AlN. $\epsilon_{xx}^{\text{AlGa}N}$ depends both

on the Al composition x as well as the thickness of the AlGa N QW layer t_{QW} . Quantification of strain in the AlGa N channel layer is critical for HEMT heterostructure design as it dictates the maximum thickness of the AlN barrier layer that can be grown without cracking.[34] Moreover, it influences the carrier transport properties as it not only determines the piezoelectric polarization, which in turn affects the 2DEG carrier density, but it also modifies the electron effective mass and therefore, the mobility.

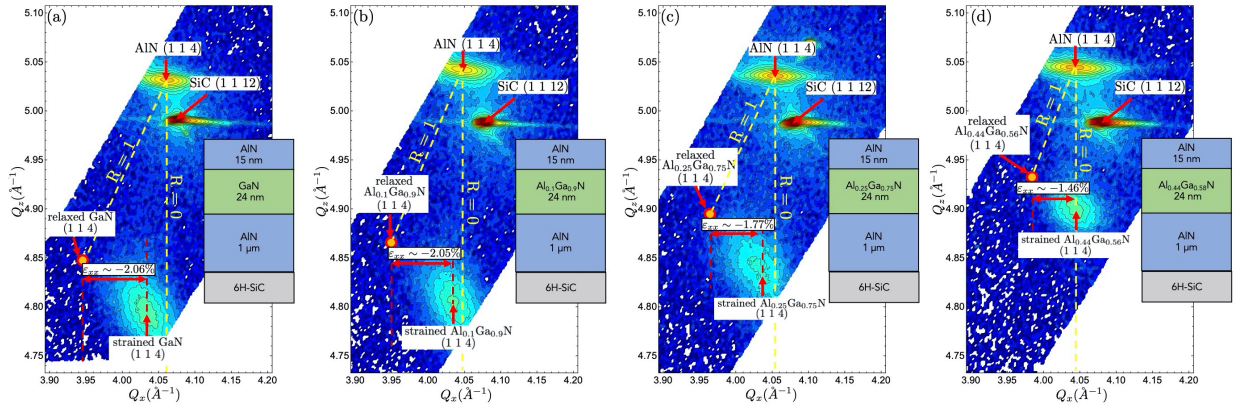


Figure 2.4: Asymmetric RSM scans of AlN/Al $_x$ Ga $_{1-x}$ N/AlN samples with (a) GaN, (b) Al $_{0.1}$ Ga $_{0.9}$ N, (c) Al $_{0.25}$ Ga $_{0.75}$ N and (d) Al $_{0.44}$ Ga $_{0.56}$ N quantum well channel layers. The dashed yellow lines indicate where the fully relaxed ($R = 1$) and fully strained ($R = 0$) Al $_x$ Ga $_{1-x}$ N layers with varying Al compositions should be. The Al $_x$ Ga $_{1-x}$ N RLPs get closer to the fully strained position with increasing x . The in-plane compressive strain (ϵ_{xx}) in the AlGa N layers, extracted with respect to their relaxed (114) position, decreases as the AlGa N layer gets more Al-rich.

To experimentally investigate the strain in the AlGa N QW as a function of its Al composition, reciprocal space mapping (RSM) using XRD was conducted on the AlN/AlGa N /AlN heterostructures around the SiC (1 1 12)/AlGa N (1 1 4) peaks to extract the in-plane lattice spacings of the AlGa N layer. RSMs for samples with GaN, Al $_{0.1}$ Ga $_{0.9}$ N, Al $_{0.25}$ Ga $_{0.75}$ N and Al $_{0.44}$ Ga $_{0.56}$ N QWs are shown in Figure 2.4. The extracted a -lattice constants are $a^{AlN} = 3.1089 \text{ \AA}$ for the AlN buffer layer and $a^{GaN} =$

3.1230 Å, $a^{Al_{0.1}Ga_{0.9}N} = 3.1160$ Å, $a^{Al_{0.25}Ga_{0.75}N} = 3.1135$ Å and $a^{Al_{0.44}Ga_{0.56}N} = 3.1089$ Å for the various strained AlGaN QW layers. With increasing Al composition, the maximum reflection intensity of AlGaN reciprocal lattice points (RLPs) progressively shifts from a partially relaxed ($0 < R < 1$) towards a fully strained ($R = 0$) position, as seen in Figure 2.4. Here the degree of relaxation $R = (a^{AlGaN} - a^{AlN}) / (a_0^{AlGaN} - a^{AlN})$ is calculated with respect to the AlN buffer layer. As the QW changes from GaN to $Al_{0.44}Ga_{0.56}N$, the AlGaN layer becomes more pseudomorphic and assumes the in-plane lattice constants of the underlying AlN layer. The signal from the top AlN barrier in the RSM is aliased by the stronger signal from the bottom AlN buffer layer.

The compositional dependence of the extracted strain ϵ_{xx} and the relaxation R in the AlGaN QW are shown in Figure 2.5. Data from other AlN/AlGaN/AlN samples with $Al_{0.58}Ga_{0.42}N$ and $Al_{0.74}Ga_{0.26}N$ QW are also included. It is seen that both the strain and the relaxation of the AlGaN QW decrease as x increases. The strain shows a monotonic reduction while the relaxation drops to 0 for $x \geq 0.44$. The dashed gray line in Figures 2.5(a) and 2.5(b) show the theoretical dependence of ϵ_{xx} and R with x if the AlGaN layer is grown pseudomorphically to the AlN buffer. These results indicate that higher composition ($x \geq 0.44$) AlGaN QW can be grown even thicker than 24 nm over AlN without significant relaxation, opening up opportunities for further improvements in the heterostructure design.

X-ray rocking curves (XRCs) along the AlGaN (0002) plane were measured for each of the six samples with varying Al concentrations in the AlGaN channel to characterize the full width at half maximum (FWHM) values as shown in Figure 2.6(a). The screw threading dislocation densities D_{screw} are related to the FWHM values through the relation $D_{screw} = \beta_{0002}^2 / 4.35 b_{screw}^2$, where β_{0002} is the XRC FWHM value in radian and b_{screw} is the Burger's vector length for $Al_xGa_{1-x}N$. The compositional dependence of

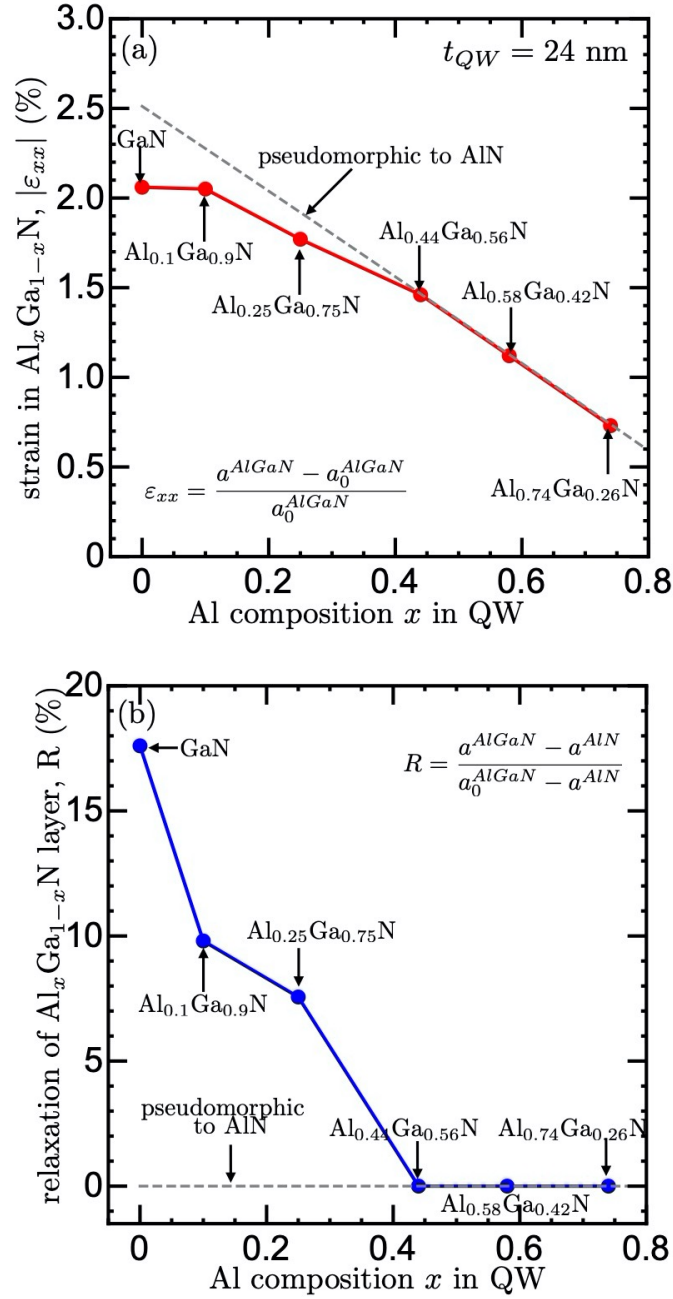


Figure 2.5: Experimental dependence of the (a) in-plane compressive strain ε_{xx} and (b) relaxation R in the $\text{AlGa}_x\text{Ga}_{1-x}\text{N}$ layer as a function of the Al concentration x in MBE-grown $\text{AlN}/\text{AlGa}_x\text{N}/\text{AlN}$ heterostructure grown on 6-H SiC. ε_{xx} and R are extracted from X-ray diffraction reciprocal space maps shown in Figure 2. ε_{xx} is calculated with respect to relaxed AlGa_xN in-plane lattice constant (a_0^{AlGa}) and R is calculated with respect to the AlN buffer layer lattice constant (a^{AlN}). The dashed gray lines indicate the theoretical compositional dependance of ε_{xx} and R in AlGa_xN QW layers fully-strained to the underlying AlN buffer layer.

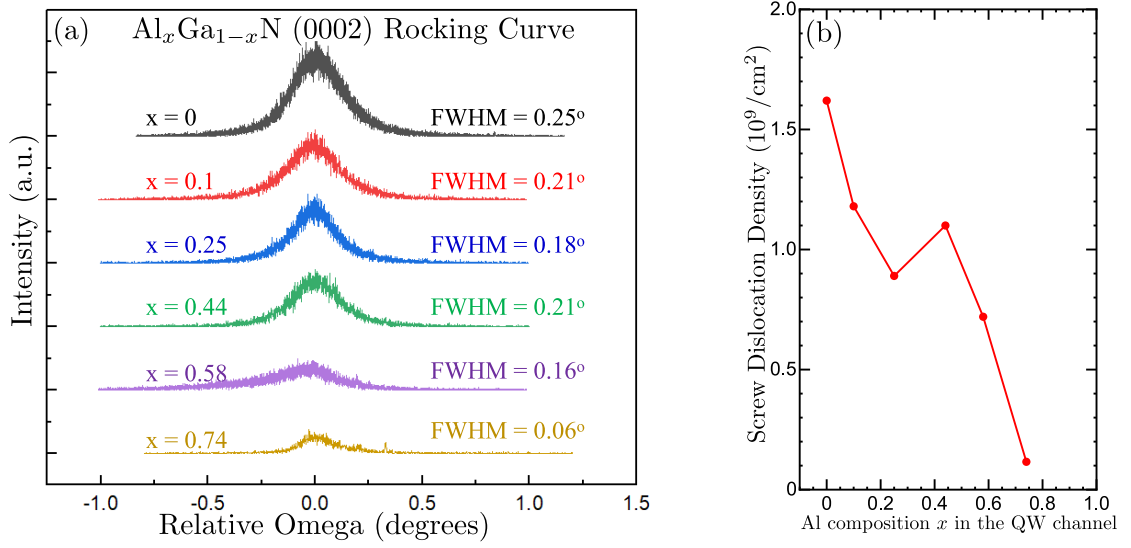


Figure 2.6: (a) X-ray rocking curves along the AlGa_N (0002) plane were measured for each of the six samples with varying Al concentrations in the AlGa_N channel. (b) Screw threading dislocation densities extracted from the FWHM values of the XRCs.

the extracted screw dislocation densities in the AlGa_N QW is shown in Figure 2.6(b). It is clearly seen that the dislocation densities in the AlGa_N QW show a decreasing trend with increasing Al composition. The Ga_N channel has a screw dislocation density of $\sim 1.6 \times 10^9/\text{cm}^2$ which decreases to $\sim 1.1 \times 10^8/\text{cm}^2$ for the $\text{Al}_{0.74}\text{Ga}_{0.26}\text{N}$ channel. This is to be expected because as the Al content of the channel increases, it becomes more pseudomorphically strained to the underlying AlN buffer layer, resulting in a low defect density. While X-ray diffraction provides an estimate of the dislocation density and the underlying trend, nano-characterization techniques such as transmission electron microscopy (TEM) will be performed in the future to get a more accurate assessment of the different crystal defects in these heterostructures.

Figure 2.7 shows the 300 K photoluminescence (PL) spectra of the AlN/AlGa_N/AlN double heterostructures with varying Al composition of the QW. The Ga_N QW sample was excited by a 325 nm He-Cd laser whereas the rest of the AlGa_N QW samples were

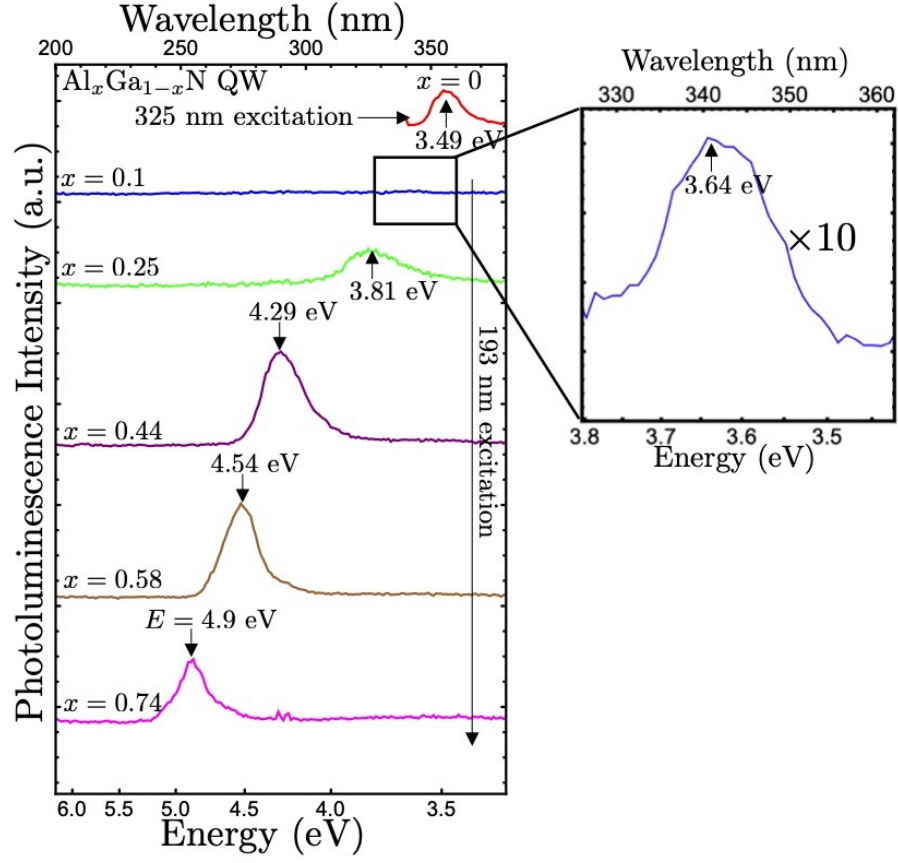


Figure 2.7: Photoluminescence spectra of AlN/AlGaIn/AlN double heterostructures with varying Al composition x of the AlGaIn QW at $T = 300$ K, showing photon emission from the AlGaIn QWs. The PL intensity of the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ QW sample was multiplied by a factor of 10 in the inset to show the emission peak clearly.

excited by a 193 nm ArF excimer laser. Band-to-band PL emission from the AlGaIn QW is observed for all six samples. The AlGaIn QW PL peaks at 355 nm (3.49 eV), 340 nm (3.64 eV), 325 nm (3.81 eV), 289 nm (4.29 eV), 273 nm (4.54 eV) and 253 nm (4.9 eV) for the GaN, $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$, $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$, $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ and $\text{Al}_{0.74}\text{Ga}_{0.26}\text{N}$ QW samples, respectively. It is evident that as the Al composition x of the QW channel increases, the interband transition PL peak blue-shifts giving a direct signature of the increasing bandgap of the channel. This also shows the tunability of the bandgap of the AlGaIn channel layer between GaN and AlN. The predicted energy

gap values for $x = 0, 0.1, 0.25, 0.44, 0.58$ and 0.74 are 3.42, 3.61, 3.94, 4.43, 4.83 and 5.34 eV respectively, taking into account a bowing parameter of 1 eV. [215] The difference between the measured and predicted values, specifically the PL peak broadening, intensity suppression and peak shifts are attributed to properties including variability in optical absorption coefficient, quantum confinement, strain, compositional fluctuation and polarization-induced quantum-confined Stark effect (QCSE).

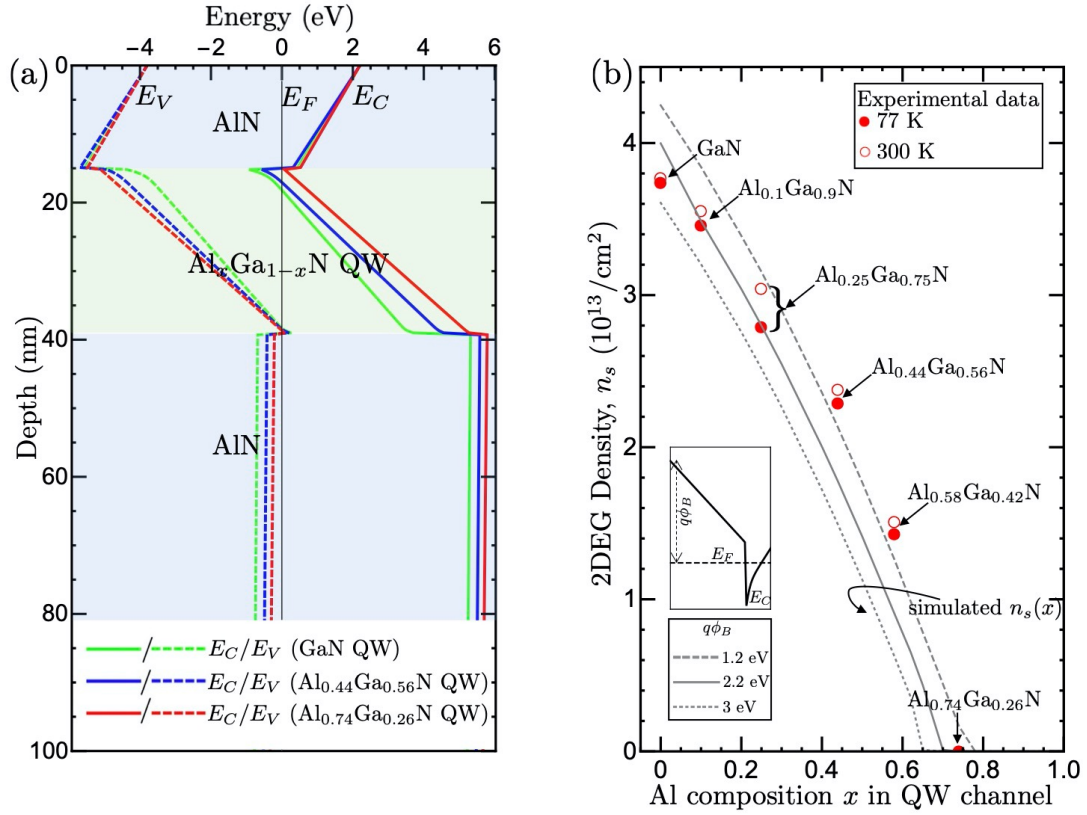


Figure 2.8: (a) 1D Schrödinger-Poisson energy band diagram simulation showing the control of the as-grown 2DEG in the AlGaIn channel by adjusting the Al composition in the channel. Green curve is the GaN channel, blue curve is the Al_{0.44}Ga_{0.56}N channel and red curve is the Al_{0.74}Ga_{0.26}N channel. (b) Measured 2DEG Hall densities at 77 K (filled circles) and 300 K (hollow circles) as a function of Al composition x in AlGaIn QW channel for different samples. The simulated 2DEG densities (gray lines) are also plotted as a function of Al composition for different surface barrier heights $q\phi_B$ (inset) and show good agreement with the experimental data.

Thus, the AlN/AlGaN/AlN samples have the desired structures in which the electrical transport properties of 2DEGs can be studied systematically as a function of Al composition x . As discussed previously, the sheets of charge $\pm q\sigma_\pi(x)$, located at the AlN/AlGaN heterointerfaces, induce a rearrangement of free carriers. Theoretically, this rearrangement generates a 2DEG at the top interface and a 2DHG at the bottom one. A self-consistent 1D Schrödinger-Poisson energy band diagram simulation for the heterostructures under study is shown in Figure 2.8(a) for three samples with GaN, Al_{0.44}Ga_{0.56}N and Al_{0.74}Ga_{0.26}N QW channels, with a surface barrier height $q\phi_B = 2.2$ eV. With increasing Al concentration x , the bandgap inside the QW widens, thereby pushing up the conduction band edge E_C with respect to the Fermi level E_F . The 2DEG density decreases commensurately with increasing x . Eventually, as shown in Figure 5(a), E_F should move into the bandgap, as is the case for Al_{0.74}Ga_{0.26}N QW channel. At and beyond that x , there should be no 2DEG in an as-grown heterostructure for the given layer thicknesses.

Hall-effect measurements were performed on the samples using soldered corner indium contacts to the AlGaN QW 2DEGs. The results of the Hall-effect measurements are summarized in Table 2.1. All the samples except the one with Al_{0.74}Ga_{0.26}N QW showed Hall conductivity indicating the presence of 2DEGs. As discussed earlier, the polarization induced 2DEG is most likely absent in Al_{0.74}Ga_{0.26}N QW sample as the polarization difference between the top AlN and Al_{0.74}Ga_{0.26}N layers is not large enough to induce the 2DEG for the given thicknesses of the layers. No direct evidence of the 2DHG formed at the bottom AlGaN/AlN interface was observed in the Hall-effect measurements for the samples reported here. Figure 2.8(b) compares the experimentally measured 2DEG Hall densities in the AlN/AlGaN/AlN samples to the simulated 2DEG densities n_s from a self-consistent 1D Schrödinger-Poisson calculation. The 2DEG densities $n_s(x)$ are calculated as a function of AlGaN channel composition x for different

Table 2.1: Structural details of the AlN/AlGaN/AlN double-heterostructures studied in this work, with the corresponding bandgap of the AlGaN channel measured via photoluminescence and their 2DEG densities n_s , mobilities μ measured via Hall-effect at 300 and 77 K. Sheet resistance R_s of $> 10^3$ k Ω per sq. indicates resistive samples in which the transport could not be extracted using Hall effect measurements.

Channel	Energy bandgap	n_s^{300K}	μ^{300K}	R_s^{300K}	n_s^{77K}	μ^{77K}	R_s^{77K}
Layer	from PL (eV)	($10^{13}/\text{cm}^2$)	($\text{cm}^2/(\text{V.s})$)	(k Ω per sq.)	($10^{13}/\text{cm}^2$)	($\text{cm}^2/(\text{V.s})$)	(k Ω per sq.)
GaN	3.49	3.78	401	0.41	3.75	614	0.27
Al _{0.1} Ga _{0.9} N	3.64	3.56	250	0.7	3.47	355	0.5
Al _{0.25} Ga _{0.75} N	3.81	3.05	45	4.55	2.8	52	4.29
Al _{0.44} Ga _{0.56} N	4.29	2.39	36	7.26	2.3	33	8.23
Al _{0.58} Ga _{0.42} N	4.54	1.52	24	17.13	1.44	21	20.66
Al _{0.74} Ga _{0.26} N	4.9	-	-	$> 10^3$	-	-	$> 10^3$

surface barrier heights $q\phi_B$ of 1.2, 2.2, and 3 eV. As the Al mole fraction in the channel increases, the measured 2DEG density decreases from $3.78 \times 10^{13}/\text{cm}^2$ in the GaN channel to the $\text{Al}_{0.74}\text{Ga}_{0.26}\text{N}$ channel sample which shows no 2DEG, in agreement with the simulated results. A surface barrier height $q\phi_B = 2.2$ eV results in the best fit to the experimental data. The surface Fermi level is not pinned in AlN and a fixed surface barrier height $q\phi_B$ may not necessarily explain the experimental data well over the entire range of samples with varying Al composition x in the AlGa_N QW channel. For AlGa_N/GaN HEMTs it has been previously observed that $q\phi_B$ is dependent on carrier concentration [105] and the AlGa_N barrier thickness [115]. The unpinned surface Fermi level in AlN barrier layer presents an attractive opportunity to employ work function engineering to tune threshold voltages of transistors.

A good electrostatic control over the 2DEG densities is thus demonstrated by varying the Al composition of the AlGa_N layer in as-grown heterostructures. The higher the Al composition x , the higher the AlGa_N channel bandgap and hence higher the expected electrical breakdown field. However, the 2DEG density decreases with an increase in x . A high 2DEG density is desired in RF HEMTs to obtain high on-currents and low access resistances. Hence, this trade-off between channel breakdown and on-current needs to be carefully optimized for designing an AlGa_N-channel HEMT. This study, therefore, provides valuable experimental data for guiding heterostructure and device design for AlGa_N-channel HEMTs for high-power, high-frequency applications.

A temperature-dependent electron transport study was performed for all the AlGa_N QW channel samples that showed conductivity. Figures 2.9(a) and 2.9(b) show the temperature-dependent Hall-effect measurement results from 300 K down to 10 K. In all samples, the 2DEG density does not show significant variation with temperature. This robustness of the 2DEG densities with temperature confirms their polarization-induced

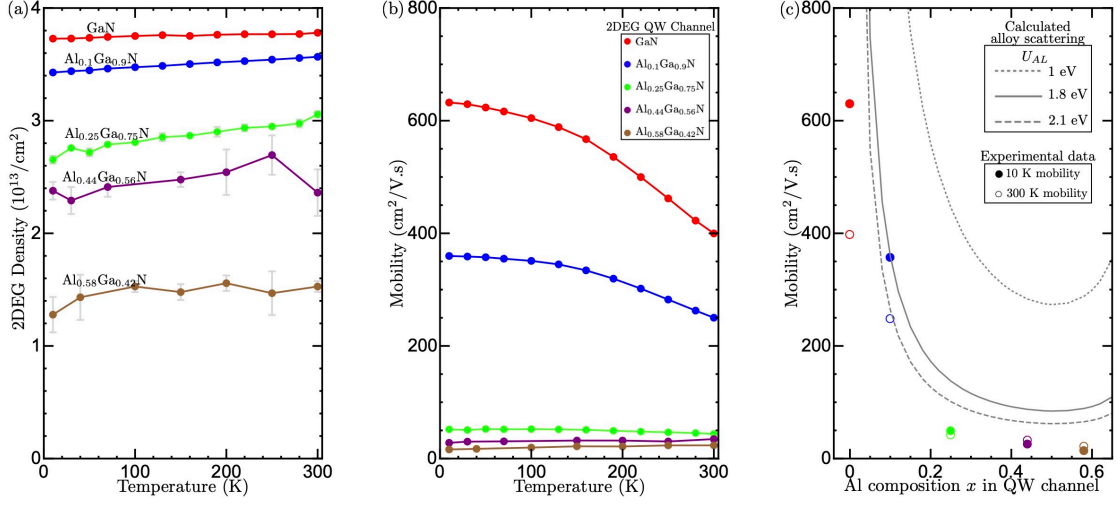


Figure 2.9: Temperature dependent (a) measured 2DEG Hall densities and (b) measured 2DEG Hall mobilities for samples with varying Al composition in the AlGaIn QW channel. (c) 10 K (filled circle) and 300 K (hollow circle) electron mobilities as a function of Al composition x in the AlGaIn QW channel. The gray curves show the calculated alloy scattering mobilities for different alloy scattering potentials confirm that the major scattering mechanism in high Al composition AlGaIn channel 2DEGs is alloy scattering. Color scheme for the plots shown in (b) is the same across the panels for different samples.

origin.

The electron mobility in the GaN and $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ QW channel samples increases monotonically upon lowering the temperature, as expected due to the freeze-out of phonon scattering. However, due to additional alloy scattering, the 10 K mobility in $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ QW is limited to $\sim 360 \text{ cm}^2/(\text{V.s})$ compared to $\sim 630 \text{ cm}^2/(\text{V.s})$ in GaN QW. The rest of the samples with $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$ and $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ channels show nearly constant mobilities $\lesssim 50 \text{ cm}^2/(\text{V.s})$ over the whole temperature range, indicating that temperature independent alloy scattering is the dominant scattering mechanism. Other scattering mechanisms such as dislocation scattering, surface charge scattering, and interface roughness scattering were found to be much weaker

than alloy scattering in the AlGaN channel for the whole temperature range.

The mobilities of MBE-grown $x \geq 0.25$ AlGaN channel HEMTs in this study are lower than the values reported previously in MOCVD-grown high Al composition AlGaN channel HEMT structures [15, 13, 210]. For example, Baca *et al.* [13] have measured a mobility of $250 \text{ cm}^2/(\text{V.s})$ in $\text{AlN}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ HEMT for a carrier density of $6 \times 10^{12}/\text{cm}^2$ and Xue *et al.* [210] report a mobility of $175 \text{ cm}^2/(\text{V.s})$ for a carrier density of $8.5 \times 10^{12}/\text{cm}^2$ in $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ HEMT structure. The observation of lower carrier mobilities in our films may partly be attributed to higher alloy scattering due to comparatively higher electron densities in our HEMT heterostructures. It is also possible that the MBE-grown AlGaN films in the current study suffer from relatively higher lateral alloy fluctuations, hence causing AlN/GaN energy barriers for lateral electron transport. [17] However, we do not expect alloy fluctuations so large that carriers would be localized in quantum dot like regions. The fact that carriers are mobile and undergo drift transport indicates that for the most part, the fluctuations are low.

For electrons in the AlGaN QW, the mobility decreases with the increasing Al composition (decreasing by up to 90% in higher composition AlGaN compared to GaN) due to the combined effects of alloy scattering and the increase in the Γ valley conduction band edge electron effective mass. Quantitatively, under a single parabolic conduction band approximation, the alloy disorder limited mobility μ_{alloy} of 2D electron carriers in an alloy channel with composition x is given by [23]

$$\mu_{\text{alloy}}(n_s, x) \approx \frac{q\hbar^3}{m^*(x)^2 \Omega_0(x) U_{AL}^2 x(1-x)} \cdot \frac{16}{3b(n_s(x), x)}, \quad (2.1)$$

where $\hbar$ is the reduced Planck's constant and $m^*(x)$ is the effective mass of elec-

trons in AlGa_N of composition x , interpolated between the Γ valley effective mass of GaN ($0.2m_0$) and AlN ($0.4m_0$) where m_0 is the free electron effective mass. $b(n_s, x) = [(33m^*(x)q^2n_s)/(8\hbar^2\epsilon_0\epsilon_s)]^{1/3}$ is the variational Fang–Howard wavefunction parameter that quantifies the spatial spread of the 2DEG. $\Omega_0(x) = \sqrt{3}/2 \cdot a_0^{\text{AlGaN}}(x)^2 c_0^{\text{AlGaN}}(x)$ is the volume of the wurtzite unit cell, where a_0^{AlGaN} and c_0^{AlGaN} are the interpolated in-plane and out-of-plane lattice constants of AlGa_N. U_{AL} is the alloy fluctuation potential and is typically estimated by fitting to experimental mobility measurements. In the absence of experimental data, U_{AL} is approximated to be the conduction band offset ΔE_C , or bandgap difference ΔE_g between the constituents of the ternary alloy [65, 24] which in our case are GaN and AlN. For AlGa_N, U_{AL} has been estimated to be between 1.3–2.2 eV by various theoretical and experimental methods [84, 172, 24, 132, 146]. The series of polarization-induced, undoped AlN/AlGa_N/AlN 2DEG samples used in this study offer an opportunity to quantify U_{AL} for AlGa_N to understand the physical limits of 2DEG mobilities in AlGa_N channel HEMTs.

Using Equation 2.1, μ_{alloy} is calculated for AlN/Al _{x} Ga _{$1-x$} N/AlN heterostructures as a function of Al content $x = 0$ to 0.8 for various short-range alloy scattering potentials $U_{AL} = 1, 1.8$ and 2.1 eV. For mobility calculations, $n_s(x)$ is obtained from 1D Schrödinger-Poisson solver using a surface barrier height $q\phi_B$ of 2.2 eV as discussed earlier in Figure 5(b). The results of calculated μ_{alloy} are plotted in Figure 2.9 (c) along with the measured 10 K and 300 K Hall mobilities in the AlN/AlGa_N/AlN samples as a function of Al composition x . Compositional dependence of the measured 10 K mobilities in the AlGa_N channel fall on U-shaped curve characteristic of alloy scattering. Upon comparing experimental data with calculated μ_{alloy} (gray curves in Figure 2.9 (c)), it is predicted that $U_{AL} \gtrsim 1.8$ eV. It should be noted that the 2DEG mobilities in these AlN/AlGa_N/AlN double heterostructures could have been adversely affected by the 2DHG formed at the bottom AlGa_N/AlN heterojunction due to proximity phe-

nomena such as Coulomb drag effect, as has been suspected earlier for AlN/GaN/AlN heterostructures. [116, 152]

In summary, this chapter presents a systematic study of MBE-grown AlN/AlGaN/AlN double heterostructures with thin and strained $\text{Al}_x\text{Ga}_{1-x}\text{N}$ quantum well channels surrounded by AlN. The material characteristics of the heterostructures and the transport properties of the 2DEGs in AlGaN channels have been examined as a function of the Al composition $0 \leq x \leq 0.74$. Photon emission from the AlGaN QWs was observed in the photoluminescence spectra. The bandgap increased with x ranging from 3.49 eV to 4.9 eV. The density of the 2DEG could be manipulated from 0 – $3.7 \times 10^{13}/\text{cm}^2$ by changing x while keeping the thicknesses of the layers constant. Thus, these AlGaN channel HEMT heterostructures lay the groundwork for new generations of high-power RF and mm-wave HEMTs. These structures would also be useful for pushing the breakdown voltages higher for power switching applications. More importantly, the AlN platform allows for the integration of nitride RF and mm-wave amplifiers with components such as p-channel FETs, and RF and mm-wave filters as described by Hickman *et al.* [71].

2.4 Future Directions

1. Pathways to improve low-field mobility in AlGaN channel 2DEGs

As shown by the systematic study in this chapter, the low-field mobility in AlGaN channel 2DEGs is a strong function of alloy composition, and it degrades with increasing Al composition x . How do we increase the mobilities of these 2DEGs?

- Since the mobility in the AlGaN channel is intrinsically bound by the limits set by the statistical disorder in the alloy system, the low-field conductivity in such alloyed channels can be potentially boosted by switching to a

$(\text{GaN})_n/(\text{AlN})_m$ "digital alloy" scheme. Such a superlattice alloying method for AlGa_N-channel has been recently proposed theoretically by Pant *et al.* [147], to diminish the in-plane disorder scattering while still maintaining the high breakdown characteristics. It is important to note that the mobility could be impacted significantly by the interface roughness scattering in such thin GaN channels, which has not been taken into account in the calculations shown in Ref. [147].

- The mobility is also expected to improve by moving to bulk single-crystal AlN substrates which have less defects and dislocations compared to AlN films grown on foreign substrates such as Si, SiC and sapphire. Recently, high-quality AlN homoepitaxy has been demonstrated both on the Al-face [37, 109] and N-face [174] of native AlN substrates which can enable further advancements in AlGa_N channel HEMTs.
- Lastly, most of the work to date has been focused on metal-polar AlGa_N channel transistors. The N-polar AlGa_N/AlN heterostructure, which unlike the metal-polar AlN/AlGa_N/AlN heterostructure hosts a 2DEG in the Al-GaN channel *without* an accompanying 2DHG, offers the possibility of even further mobility enhancement.

2. Extremely high Al composition AlGa_N channel for enhancement mode operation

Even though the as-grown heterostructure with Al_{0.74}Ga_{0.26}N channel presented in this chapter is highly resistive, it can potentially enable normally-off operation with high threshold voltage which is desirable for power switching and energy conversion applications. Previous reports [63, 19] have theoretically simulated the enhancement mode operation in such high-composition AlGa_N HEMTs, however, the experimental demonstration of such devices remains to be realized yet.

Clever device engineering would be needed to alleviate the effects of increased access region resistance originating from the reduced polarization difference between barrier and channel in such E-mode HEMTs. As an example, selective-area ion implantation of Si in the access region of the AlGa_N channel could help solve this problem.

CHAPTER 3

ALN/ALGAN/ALN HIGH ELECTRON MOBILITY TRANSISTORS

3.1 Introduction

In the previous chapter, tunable, high-conductivity 2DEGs were demonstrated in the AlN/AlGaN/AlN heterostructure. These 2DEGs are used as a channel layer for fabricating n-channel transistors or HEMTs on the AlN platform, which are the focus of this chapter.

As discussed in the introductory chapter, semiconductors with a significantly larger energy bandgap than silicon are needed for efficient, ultra-high-voltage (> 20 kV) power-conversion electronics. While the wide bandgap semiconductors such as SiC and GaN have had commercial success in power electronics [164, 87], ultra-wide bandgap (UWBG) (bandgaps > 3.4 eV) semiconductor materials offer the possibility of electronics with even higher operating voltages [194]. Moreover, these UWBG semiconductors can also enable high-power RF electronics thanks to their high breakdown fields and capability to operate at high temperatures. UWBG semiconductor candidates include diamond [205], Ga₂O₃ [187], and AlGaN [89].

Because AlGaN has the distinguishing feature of polarization-induced doping to form 2-dimensional electron gases (2DEGs), work on AlGaN channel high electron mobility transistors (HEMTs) has blossomed in recent years, with several results appearing in the literature [14, 209, 56, 94] both for power and RF electronics. In this chapter, we first utilize the AlN/AlGaN/AlN epitaxial structures to fabricate HEMT devices. A compositional dependence study of electrical characteristics of Al_xGa_{1-x}N quantum well channel-based AlN/AlGaN/AlN high electron mobility transistors (HEMTs) with

$x = 0.25, 0.44$, and 0.58 , is presented. The use of selectively regrown n-type GaN ohmic contacts results in contact resistance that increases as the Al content of the channel increases. The DC HEMT device characteristics reveal that the maximum drain current densities progressively reduce from 280 mA/mm to 30 mA/mm to 1.7 mA/mm for $x = 0.25, 0.44$, and 0.58 , respectively. This is accompanied by a simultaneous decrease (in magnitude) in threshold voltage from -5.2 V to -4.9 V to -2.4 V for the three HEMTs. This systematic experimental study of the effects of Al composition x on the transistor characteristics provides valuable insights for engineering AlGaIn channel HEMTs on AlN for extreme electronics at high voltages and high temperatures. Finally, the RF operation of UWBG channel AlN/Al_{0.25}Ga_{0.75}N/AlN HEMTs with a record high f_T/f_{max} of $67/166 \text{ GHz}$ is demonstrated.

3.2 DC devices: A comparative study across AlGaIn channels

Past studies on AlGaIn channel HEMTs have primarily focused on the growth and device performance of HEMTs with specific Al composition in the AlGaIn channel. While using higher Al content AlGaIn to achieve a wider bandgap channel to enhance the breakdown voltage is desirable, several device engineering trade-offs must be taken into account when designing AlGaIn channel HEMT heterostructures for various applications. Making ohmic contacts to the AlGaIn channel becomes increasingly challenging for high Al concentration AlGaIn. Furthermore, for a fixed AlGaIn barrier composition, the polarization difference between the barrier and the channel diminishes as the Al composition of the channel increases, resulting in decreased polarization-induced 2DEG densities. This reduced polarization contrast leads to low on-currents, high access resistances, and a positive shift in threshold voltage for HEMT devices. Moreover, alloying reduces the thermal conductivity and electron mobility in the channel compared

Table 3.1: Summary of the device characteristics of AlN/AlGa_N/AlN quantum well channel HEMTs studied in this work with the 2DEG densities n_s , mobilities μ and sheet resistance R_s measured via Hall-effect at 300 K.

Channel Al composition	n_s^{300K} ($10^{13}/\text{cm}^2$)	μ^{300K} ($\text{cm}^2/(\text{V.s})$)	R_s^{300K} ($\text{k}\Omega$ per sq.)	R_C ($\Omega\cdot\text{mm}$)	I_D^{max} (mA/mm) @ $V_G = 2$ V	I_{on}/I_{off} -	V_T (V)
25%	3.05	45	4.55	0.23	280	$> 10^5$	-5.2
44%	2.39	36	7.26	9.3	30	$> 10^5$	-4.9
58%	1.52	24	17.13	212.1	1.7	$\sim 10^5$	-2.4

to the binary constituents GaN and AlN. Therefore, it is crucial to identify the tradeoffs in the choice of the AlGa_N channel composition x to obtain optimal characteristics of HEMT devices.

For this purpose, a series of three AlGa_N channel compositions ($x = 0.25, 0.44$, and 0.58) of AlN/AlGa_N/AlN QW channel HEMTs were fabricated, and their DC device characteristics are compared. Epitaxial regrowth formation of heavily Si-doped n-GaN contacts to the strained AlGa_N channel is studied, and the resulting compositional dependence of the contact resistance is presented. Following that, the long channel devices demonstrated maximum drain currents $I_D^{max} = 280, 30$, and 1.7 mA/mm for the three HEMTs with increasing Al mole fractions in the channel from 0.25 , 0.44 , and 0.58 , respectively. A positive threshold voltage shift is also observed when the Al mole percentage in the channel increases.

The HEMT samples were grown using MBE on Si-face of 6H-SiC substrates, as described in the previous chapter of the dissertation. In chapter 2, we reported a compositional dependence study of polarization-induced 2DEG properties in AlN/AlGa_N/AlN heterostructures with the strained QW $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel compositions ranging from $x = 0$ to $x = 0.74$, spanning energy bandgaps of the conducting HEMT channels from

3.49 eV to 4.9 eV measured by photoluminescence. Three samples from this study with 15 nm AlN barrier / 24 nm AlGaIn channel / 1 μm AlN buffer layer structures having Al mole fraction $x = 0.25, 0.44$, and 0.58 were chosen for HEMT device fabrication and comparison of their device characteristics. A summary of the Hall-effect measurements at room temperature is listed in Table 3.1. The use of *thin* and *compressively strained* AlGaIn QW channels surrounded by an AlN buffer below and an AlN barrier layer on the top should leverage the advantages of the AlN material platform [71, 152, 68, 149, 34]. The AlN barrier layer maximizes the conduction band offset, thereby increasing the 2DEG density at the interface with AlGaIn and reducing gate leakage current. The high thermal conductivity of AlN buffer layer provides an efficient heat conduction path away from the active region of the device. Overall, this AlN/AlGaIn/AlN material stack has a very high bandgap, allowing access to higher breakdown electric fields and operating temperatures than conventional GaN HEMT stacks [125, 124].

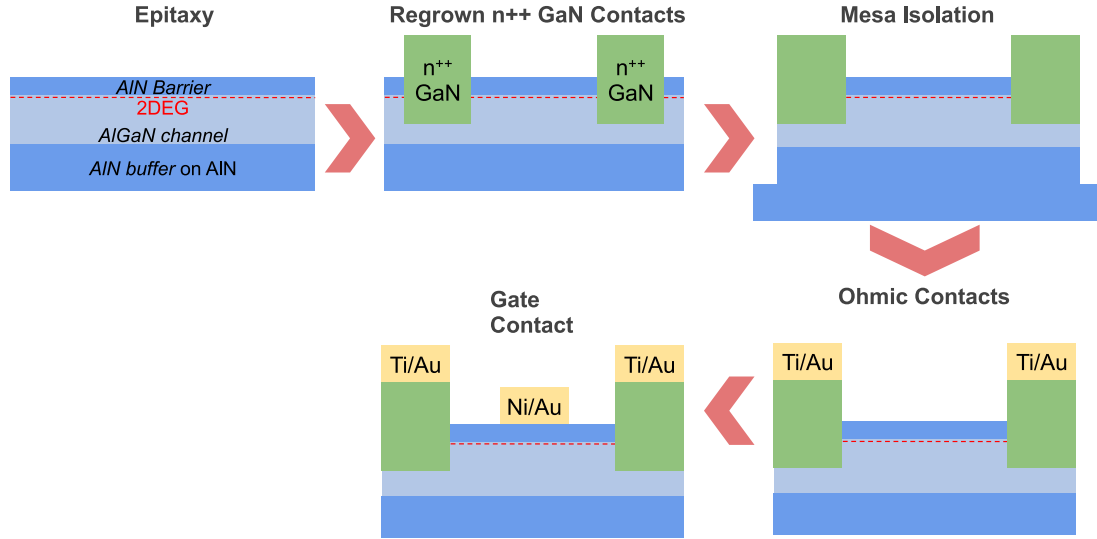


Figure 3.1: Fabrication process flow for QWHEMT devices.

Following a realigned gate-last process, all three samples were co-processed to minimize user and tool variances, ensuring fair comparison. First, the as-grown samples were

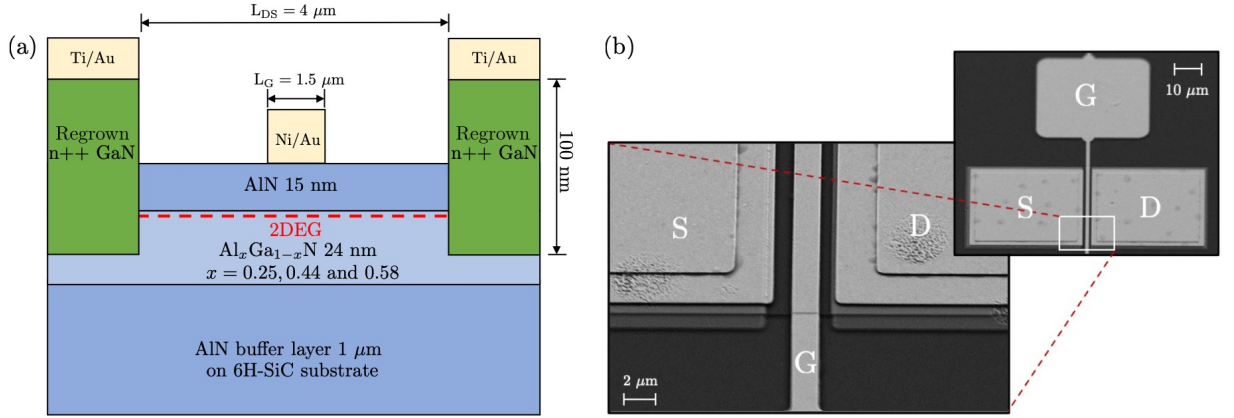


Figure 3.2: (a) Cross-sectional schematic illustration of the device structure. (b) Top-view SEM image of a portion of a typical device. HEMT fabrication was performed by EK Kim and Dr. Austin Hickman.

patterned with SiO₂/Cr hard mask and etched by BCl₃ inductively coupled plasma (ICP) to expose the 2DEG sidewalls. Source/drain ohmic contact regions were then formed by regrowing a 100 nm thick heavily Si doped ($\sim 10^{20} \text{ cm}^{-3}$) GaN layer using plasma-assisted MBE. Following the regrowth, the SiO₂/Cr hard mask was stripped in buffered HF, and device isolation was achieved by BCl₃ ICP etch. Non-alloyed ohmic contacts were formed by depositing 50/100 nm of Ti/Au via electron-beam evaporation after a short dip in buffered HF to remove native oxides and ensure clean metal-semiconductor contact. Lastly, rectangular gates were defined by photolithography, aligned to the regrowth patterns, and metalized by Ni/Au (50/100 nm) evaporation on the AlN barrier surface to form Schottky contacts. The full process flow for the fabrication is shown in Figure 3.1. The cross-section and scanning electron microscope images of a fully processed HEMT are shown in figures 3.2(a) and 3.2(b), respectively. All HEMTs presented in this study feature a source-to-drain distance $L_{DS} = 4 \mu\text{m}$, $W_G = 50 \mu\text{m}$ device width, and a rectangular gate placed in the middle of the source-to-drain spacing with a gate length $L_G = 1.5 \mu\text{m}$.

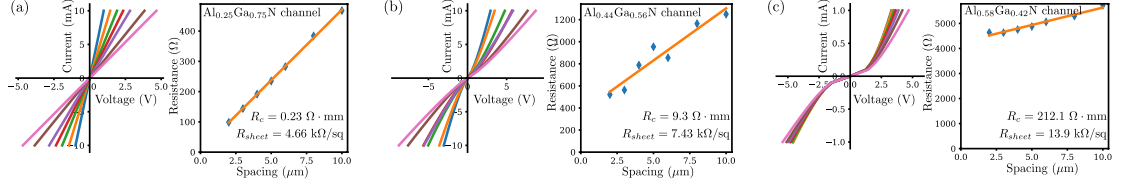


Figure 3.3: Two terminal current-voltage (I-V) characteristics using TLM patterns with MBE-regrown n^{++} -GaIn contact along with the linear TLM analysis for AlN/AlGaIn/AlN quantum well channel HEMTs with (a) $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, (b) $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$, and (c) $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ channels respectively.

Following the device fabrication, contact resistance R_C from the metal pad to the 2DEG and the 2DEG channel sheet resistance R_{sh} were extracted by the transfer length method (TLM), as shown in figure 3.3. The TLM measurements performed on a sample with the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ channel revealed linear I-V characteristics and $R_C = 0.23 \, \Omega\cdot\text{mm}$, which is the lowest value reported on AlGaIn channel HEMTs with Al composition equal to or higher than 25%. The TLM analysis also revealed $R_{sh} = 4.66 \, \text{k}\Omega\cdot\text{mm}$, consistent with Hall-effect measurements performed on the as-grown sample before device fabrication as shown in Table 3.1. On the other hand, the same measurements performed on the samples with a higher Al composition AlGaIn channel revealed non-linear I-V characteristics with significantly higher $R_C = 9.3 \, \Omega\cdot\text{mm}$ and $212.1 \, \Omega\cdot\text{mm}$, for $x = 0.44$ and $x = 0.58$, respectively.

This increased R_C and Schottky-like behavior is attributed mainly to the decreasing electron affinity of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ as a function of x [58]. The low electron affinity leads to the formation of a higher Schottky barrier height between n^+ -GaIn and AlGaIn, which inhibits electron transport across the interface as a result of a poor tunneling probability ($\sim e^{-\sqrt{2m^*(q\phi_b)/\hbar^2} \cdot W}$, where m^* is the effective electron mass, $\hbar$ is the reduced Planck's constant, ϕ_b is the Schottky barrier height and W is the tunneling width) [18]. Furthermore, due to a lower carrier concentration in the AlGaIn channel, the tunneling

width and barrier height would be larger for a high Al composition AlGa_N channel. Other possible explanations of poor ohmic contacts include increasing lattice mismatch between n⁺⁺-Ga_N and Al_xGa_{1-x}N as a function of x , thereby degrading the crystal quality of regrown n⁺⁺-Ga_N. The formation of native oxides on the AlGa_N sidewalls might also impede the electron flow. Although piranha pre-treatment was performed on all samples to remove surface oxide before re-loading into the MBE chamber for the regrowth, the AlGa_N surface oxidizes rapidly in ambient conditions, forming an effective metal-oxide-semiconductor structure. Al atoms in AlGa_N have been reported to be more reactive with O₂ compared to Ga atoms, and therefore high Al composition AlGa_N might suffer from the accelerated oxidation rate [200].

Figure 3.4 shows the 3-terminal output characteristics and the log scale transfer characteristics of Al_xGa_{1-x}N channel HEMTs with $x = 0.25, 0.44$, and 0.58 . All HEMTs, regardless of x , revealed good gate control and relatively sharp pinch-off characteristics with an on/off ratio exceeding 10^5 . A higher gate leakage (I_G) current was observed for samples with lower Al composition in the channel ($I_G \sim 2 \times 10^{-3}$, 7×10^{-5} , and 3×10^{-5} mA/mm for $x = 0.25, 0.44$, and 0.55 , respectively). This observation of a reduction in gate leakage as the Al content of the channel increases is interesting and can be explained by comparing the tunneling probability of electrons from the gate to the 2DEG channel in reverse bias.

To first order, the lower conduction band offset between AlN and the AlGa_N channel for higher Al composition of the channel should increase the *forward-bias* gate current, but *not* the reverse-bias gate current responsible for breakdown, for the following reason. At high reverse-bias voltage on the gate, near and beyond the threshold, electrons from the metal tunnel into the 2DEG channel through a voltage-dependent triangular

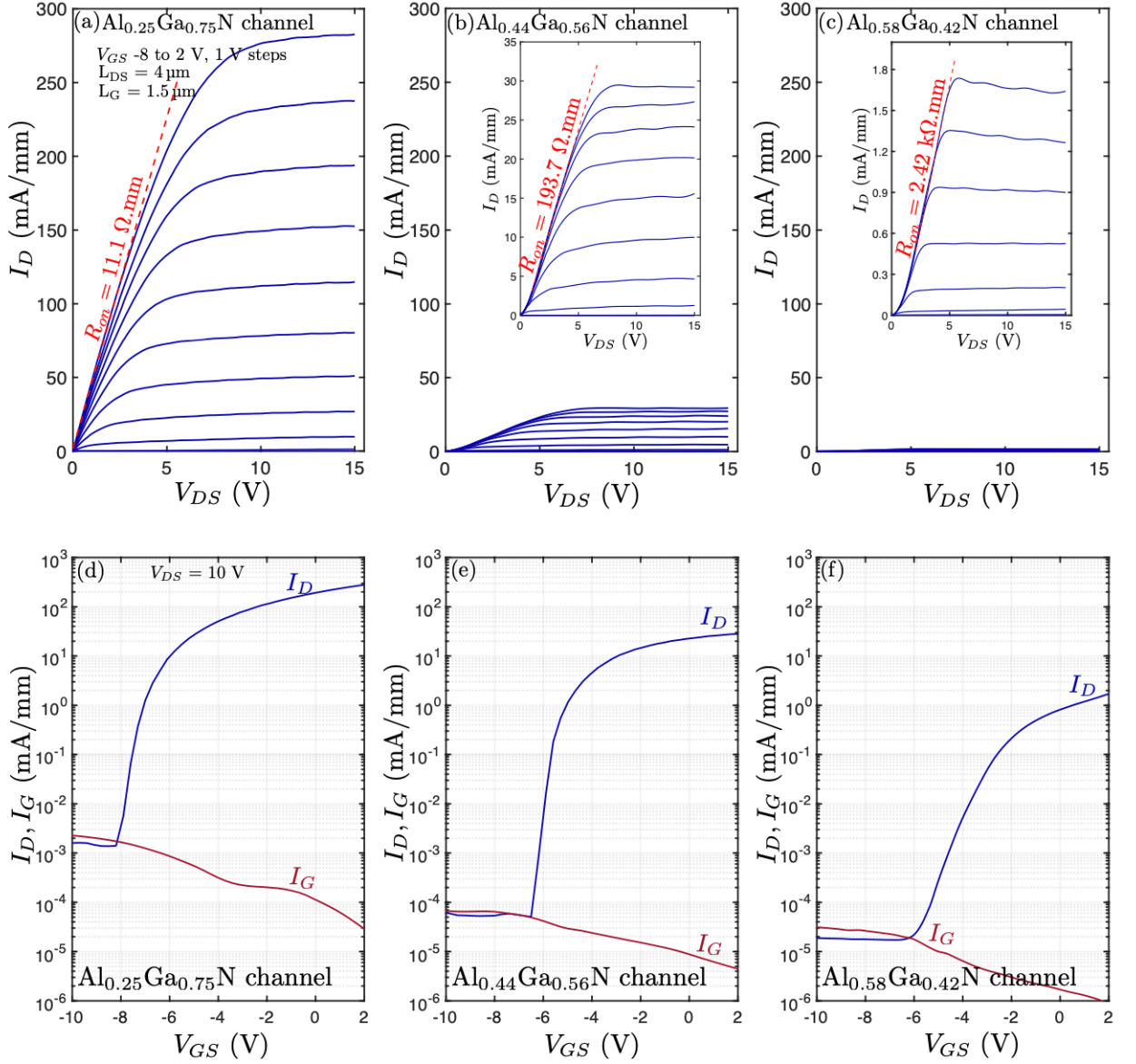


Figure 3.4: I_D - V_{DS} output characteristics of (a) $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, (b) $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$, and (c) $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ QW channel HEMTs yielding maximum drain currents $I_D^{max} = 280, 30, 1.7 \text{ mA/mm}$ respectively. Log-scale transfer curves show five orders of on-off modulation, limited by gate leakage for (d) $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, (e) $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$, and (f) $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ channel HEMTs respectively. Device geometries and bias conditions are stated in figures (a) and (d).

potential barrier by the Fowler-Nordheim (FN) tunneling mechanism. At low reverse-bias voltages on the gate, the leakage is dominated by the trap-assisted Frenkel-Poole emission (FPE) mechanism [57]. If the Schottky barrier height at the metal/AlN contact interface is the same for the three AlGaN QW channel HEMTs, the trap-assisted emission and direct FN tunneling mechanisms are strong functions of the field in the AlN barrier under reverse bias near the metal/AlN interface, and the AlN/AlGaN interface and band offset does not play the dominant role.

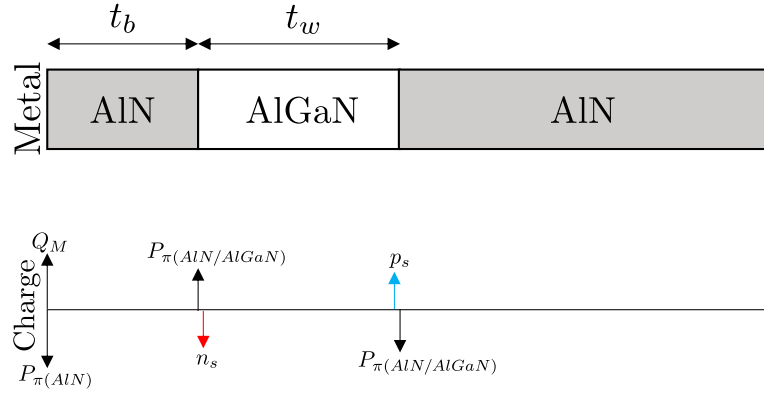


Figure 3.5: Charge diagram of the AlN/AlGaN/AlN heterostructure.

The vertical electric field F_b in the AlN barrier is related to the electric field F_w in the AlGaN quantum well via Gauss's law from the charge-diagram shown in Figure 3.5 as

$$F_b = \frac{q(P_{\pi(\text{AlN})} - P_{\pi(\text{Al}_x\text{Ga}_{1-x}\text{N})} - n_s(V_{GS}))}{\epsilon_{\text{AlN}}\epsilon_0} - \frac{\epsilon_{\text{AlGaN}}}{\epsilon_{\text{AlN}}}F_w. \quad (3.1)$$

Here, $P_{\pi(\text{AlN})} \sim 5.5 \times 10^{13}/\text{cm}^2$ is the AlN polarization charge, $P_{\pi(\text{Al}_x\text{Ga}_{1-x}\text{N})} \sim (2.1 + 2.1x + 1.3x^2) \times 10^{13}/\text{cm}^2$ is the AlGaN polarization charge, ϵ_{AlN} is the dielectric constant of AlN, ϵ_{AlGaN} is the dielectric constant of AlGaN and n_s is the 2DEG density obtained from a self-consistent 1-D Poisson Schrodinger simulation as a function of gate voltage V_{GS} . If there is a 2DEG at the top interface of AlGaN channel and a 2DHG at the bottom interface, the intrinsic field in AlGaN F_w is $\sim E_{g(\text{AlGaN})}/qt_w$, where $E_{g(\text{AlGaN})} = (3.4 + 2.6x)$ eV is AlGaN energy bandgap and t_w is the thickness of AlGaN

quantum well. Assuming, $\epsilon_{AlN} \approx \epsilon_{AlGaN}$, F_b simplifies to

$$F_b = \frac{q(P_{\pi(AlN)} - P_{\pi(Al_xGa_{1-x}N)} - n_s(V_{GS}))}{\epsilon_{AlN}\epsilon_0} - \frac{E_{g(AlGaN)}}{qt_w}. \quad (3.2)$$

As a negative gate voltage is applied, the 2DEG depletes, until there is no charge remaining under the gate $n_s \rightarrow 0$ when $V_{GS} = V_T$. At this point, the electric field in the AlN barrier saturates to

$$F_{sat} = \frac{q(P_{\pi(AlN)} - P_{\pi(Al_xGa_{1-x}N)})}{\epsilon_{AlN}\epsilon_0} - \frac{E_{g(AlGaN)}}{qt_w} = (4.7 - 4.8x - 2.3x^2) \text{ MV/cm}. \quad (3.3)$$

The calculated vertical field levels off to $F_b \rightarrow F_{sat}$ as a more negative gate bias $V_{GS} < V_T$ is applied. From Ref. 22 of the main manuscript, we know that the leakage current through the gate barrier for FPE follows $J_{FPE} \propto e^{\sqrt{F_b}}$ and the FN tunneling current density follows $J_{FN} \propto F_b^2 e^{-1/\sqrt{F_b}}$. Clearly, both tunneling mechanisms result in an increased leakage current density with an increasing field in the barrier. For the AlGaIn channel HEMTs, the saturation electric field in the AlN barrier F_{sat} at sufficiently high reverse bias decreases with increasing Al composition x as shown in Equation 2. Therefore, both J_{FPE} and J_{FN} should *decrease* with increasing x resulting in a *lower* leakage for a higher Al mole fraction in the channel. This is consistent with our experimental observations. *It is interesting to note here that, somewhat counterintuitively, both J_{FPE} and J_{FN} do not depend on the conduction band offset at the AlN barrier/ $Al_xGa_{1-x}N$ channel interface.*

The decrease in F_b as the Al content of the channel increases is better illustrated by a self-consistent 1-D Poisson Schrodinger energy band diagram simulation under a negative gate bias of $V_{GS} = -9$ V as shown in Figure 3.6. The magnitude of the electric fields in the AlN barrier from the simulation is 6.47, 5.22, and 4.27 MV/cm for $Al_{0.25}Ga_{0.75}N$, $Al_{0.44}Ga_{0.56}N$, and $Al_{0.58}Ga_{0.42}N$ channels, respectively which are

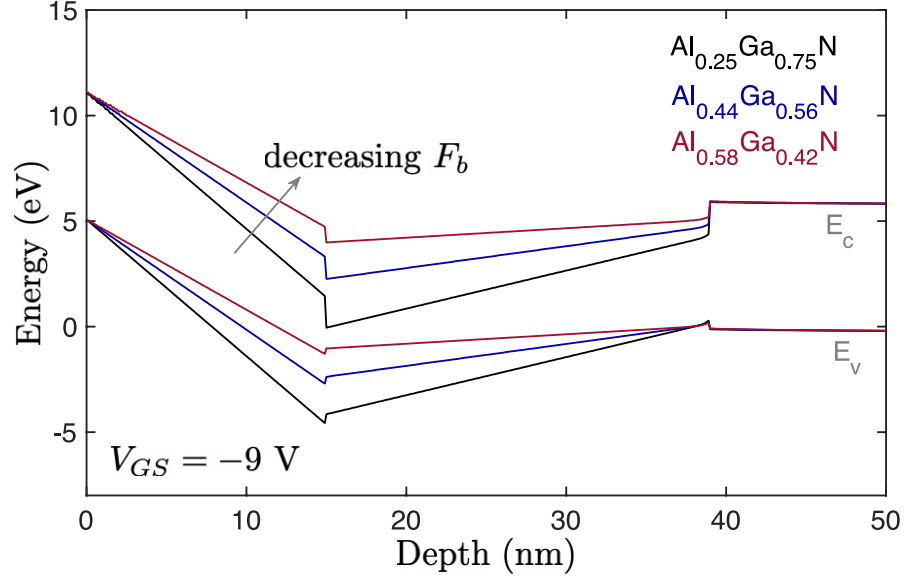


Figure 3.6: 1D Schrödinger-Poisson energy band diagram simulation for the AlN/AlGaN/AlN HEMT heterostructures under a negative gate bias of $V_{GS} = -9$ V showing the decrease in electric field in AlN barrier F_b as the Al composition in the AlGaN channel increases.

consistent with the analytical model presented before. Therefore, we conclude that the higher electric field in the AlN barrier is the main reason for increased gate leakage in the lower composition AlGaN channel HEMTs.

Another possible reason for the lower gate leakage observed in higher Al composition AlGaN channel might be due to the high parasitic resistances. Electrons are injected from the gate metal into the channel, but due to the high access and contact resistance, the injected electrons cannot readily flow through the drain contact and as a result, accumulate in the channel. This, in turn, reduces the electric field in the barrier and fewer electrons get injected from the gate metal, therefore lower gate leakage is observed. It is possible that the device isolation process which causes the gate metal to contact the 2DEG channel on the mesa sidewall can form a parasitic gate leakage path. This mesa sidewall gate leakage can contribute to the increase in the total gate leakage for lower Al composition channels. To avoid the mesa sidewall leakage current, planar ion

implantation can be used for selective area isolation in the future.

The $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ channel HEMTs exhibited drain current density exceeding 280 mA/mm with excellent saturation and the on-resistance $R_{on} = 11.1 \, \Omega \cdot \text{mm}$. HEMTs with $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$ and $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ channel, on the other hand, showed contact-limited maximum drain current density of 30 mA/mm and 1.7 mA/mm, with $R_{on} = 193.7 \, \Omega \cdot \text{mm}$ and $2.42 \, \text{k}\Omega \cdot \text{mm}$, respectively. The degradation in on-currents with increasing Al content in the channel is attributed to increasing contact resistance, diminishing electron density, and reduced electron mobility (Table 3.1) due to increased alloy scattering.

For the $\text{AlN}/\text{AlGa}\text{N}/\text{AlN}$ heterostructure, the threshold voltage V_T may be approximated as $qV_T = q\phi_b - \Delta E_C + qF_b t_b$, where q is the magnitude of the electron charge, ϕ_b is the Schottky barrier height at the Ni/barrier interface, ΔE_C is the conduction band offset at the barrier/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ interface, and F_b and t_b are the electric field and thickness of the barrier. Since ΔE_C decreases as x increases, [204] given by $\Delta E_C(x) = (1.8 - 1.171x - 0.63x^2) \, \text{eV}$, a positive shift in V_T is expected with increasing x . Similarly, an increase in x reduces the magnitude of the positive polarization bound charge at the top $\text{AlN}/\text{AlGa}\text{N}$ hetero-interface, resulting in a decreased electric field in the barrier. This change in the electric field as x increases also contributes to the overall positive shift in V_T . Figure 3.7 shows the transfer characteristics of the HEMTs in the linear scale for the three samples measured at drain voltage $V_{DS} = 10 \, \text{V}$. The threshold voltages are extracted to be $V_{T1} = -5.2 \, \text{V}$, $V_{T2} = -4.9 \, \text{V}$, and $V_{T3} = -2.4 \, \text{V}$ from linear fits of transfer I-V curves for the $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$ and $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ QW channel HEMTs respectively.

The tunability of V_T with x observed in this series of samples is understood from the as-grown 2DEG density variation with x . The threshold voltage in these quantum well channel HEMTs can be approximated as the ratio of the 2D charge density (qn_s) to the

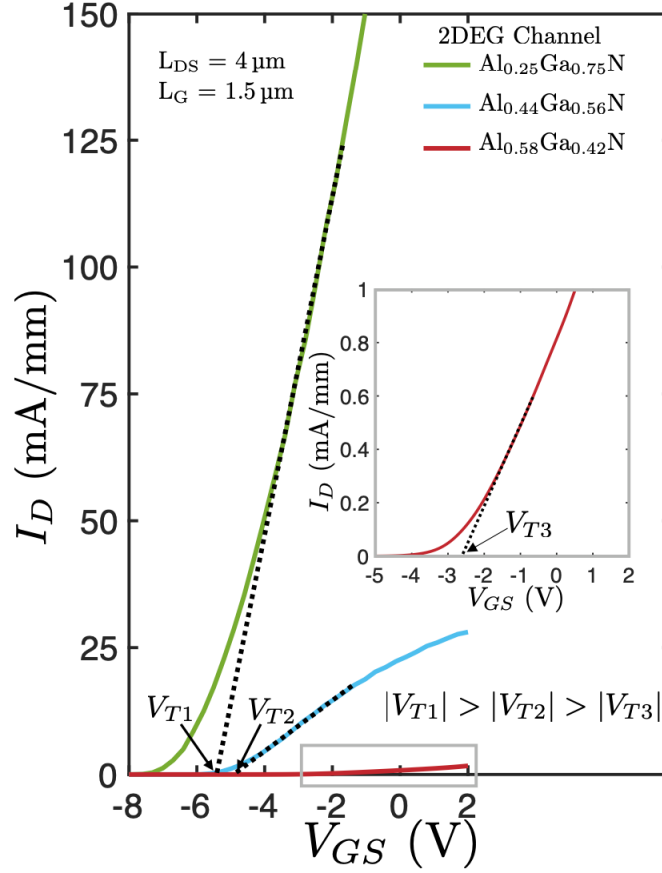


Figure 3.7: Linear-scale transfer curves show normally-on operation with threshold voltages $V_{T1} = -5.2$ V, $V_{T2} = -4.9$ V, and $V_{T3} = -2.4$ V for $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$, and $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ QW channel HEMTs respectively, measured at drain voltage $V_{DS} = 10$ V. Inset zooms into the transfer curve of the $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ QW channel HEMT.

intrinsic gate capacitance per unit area (C_{GS}) as $V_T = -qn_s/C_{GS} = -qn_s t_b / \epsilon_{\text{AlN}} \epsilon_0$, where ϵ_{AlN} is the relative dielectric constant of the AlN barrier and ϵ_0 is the permittivity of free space. Since n_s decreases as x increases due to the reduced polarization difference, based on the as-grown Hall 2DEG density (see Table 3.1), V_T is calculated to be -8.2 , -6.2 , and -4.1 V for $x = 0.25$, 0.44 , and 0.58 respectively. While we observe the same trend of increasing threshold voltage with x in our study, the discrepancy between the experimental and calculated threshold voltages is attributed to the presence of interface

traps at the gate metal/AlN interface and partial oxidation of the AlN surface.

Following this trend in V_T , a heterostructure with even higher Al composition $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel would result in nearly zero conductivity under equilibrium, which opens up the potential for realizing enhancement mode operation without employing commonly used techniques for shifting V_T , such as fluorine ion implantation [31] or insertion of p-type GaN underneath the gate [198]. The challenge, however, lies in simultaneously achieving a high electron density in the access region while having no 2DEG density at the AlN/AlGaN heterointerface under the gate, which may be solved via selective-area ion implantation of Si.

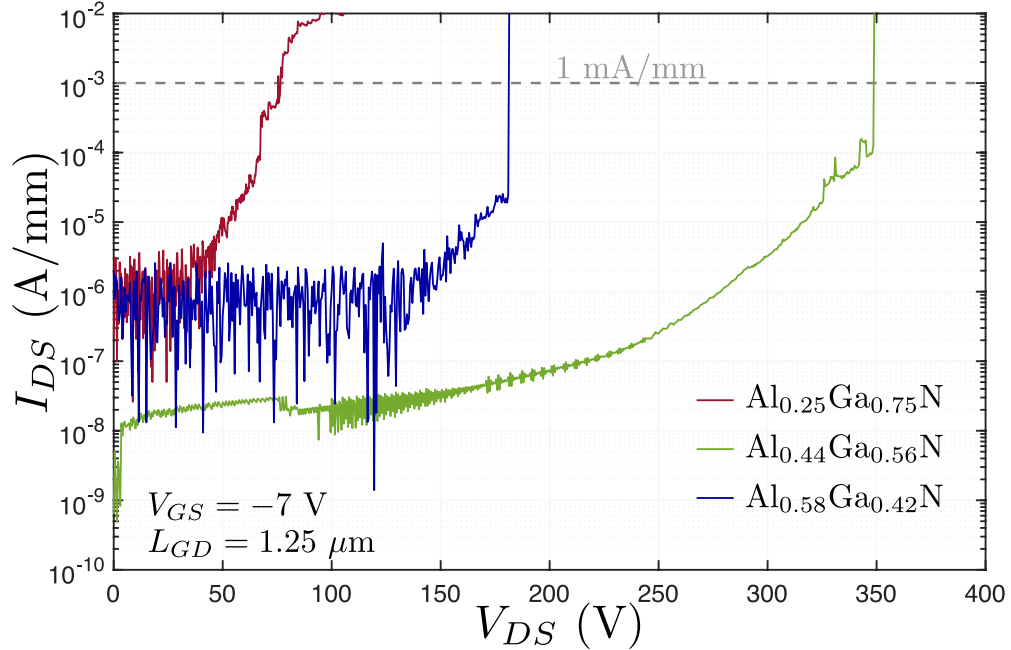


Figure 3.8: Three terminal off-state breakdown characteristics of the three Al-GaN QW channel HEMTs with gate-to-drain spacing of $1.25 \mu\text{m}$ at $V_{GS} = -7 \text{ V}$. The breakdown voltages are 83.5, 355.5, and 188 V for $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$, $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$, and $\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}$ channels, respectively.

To investigate the breakdown characteristics, the gate voltage was set below the threshold voltage ($V_{GS} = -7 \text{ V}$), and V_{DS} was increased until HEMT breakdown oc-

curred. The breakdown voltage metric is defined as $I_D \geq 1$ mA/mm. The devices were covered in Fluorinert during the measurement process. Figure 3.8 shows the three terminal off-state breakdown characteristics for the three AlGa_N QW channel HEMTs with $L_{GD} = 1.25$ μ m. The breakdown voltages for Al_{0.25}Ga_{0.75}N, Al_{0.44}Ga_{0.56}N, and Al_{0.58}Ga_{0.42}N channels are 83.5, 355.5, and 188 V respectively, which correspond to average electric fields of 0.67, 2.84, and 1.5 MV/cm at the breakdown. During the measurement process and before the breakdown, the drain current is roughly equal to the gate current for all three HEMTs with different Al compositions in the channel. This suggests that the gate-drain leakage is the primary factor responsible for the breakdown and not avalanche or channel breakdown, and is far from the material limits of AlGa_N.

It is important to note that for a fair comparison of breakdown voltages across AlGa_N channel HEMTs with different Al compositions, the 2DEG density must be of comparable magnitude because the peak electric field around the drain-side gate edge increases with 2DEG density [170]. Interestingly, the highest breakdown voltage is observed for the Al_{0.44}Ga_{0.56}N channel HEMT, even higher than the Al_{0.58}Ga_{0.42}N channel, despite having a higher 2DEG density and a smaller energy band gap. The reason for this is currently under investigation, but no clear answer has not been found yet.

Previous studies on AlGa_N channel HEMTs have demonstrated contact-limited current, and various measures have been taken to address ohmic contact limitations. Overall, there are three main approaches demonstrated so far: alloy contact, ion implantation, and heavily doped semiconductor contact. For example, for contacting via metal ohmic stacks, Yafune *et al.* [211] demonstrated a contact resistance of 85 Ω ·mm on AlN/Al_{0.6}Ga_{0.4}N heterostructure with Zr/Al/Mo/Au after rapid thermal annealing at 950°C. It was shown that the Ti/Al-based metal stacks, frequently utilized in GaN technology, do not work well on Al-rich AlGa_N. A Zr-based alloy contact enables more ef-

ficient metal diffusion over the AlGa_N barrier than a Ti-based alloy contact [212, 211]. Nanjo *et al.* [137], on the other hand, realized good contacts through Si ion implantation with a 1150°C anneal for Al_{0.4}Ga_{0.6}N/Al_{0.2}Ga_{0.8}N HEMT heterostructure.

However, the most promising results for attaining the lowest contact resistances to Al-rich AlGa_N channel HEMTs have been obtained using heavily doped semiconductor contacts, typically with the help of an etch and regrowth approach similar to the one used in the present work. Previous reports have also shown the use of heavily doped regrown GaN for contacting the AlGa_N channel, akin to the regrowth contact strategy used routinely for RF GaN HEMTs. For example, Abid *et al.* [2] used MBE to regrow n-type doped GaN in the source-drain regions and measured a R_C of 21 $\Omega \cdot \text{mm}$ for AlN/Al_{0.5}Ga_{0.5}N HEMT. Douglas *et al.* [50] reported R_C of 62 $\Omega \cdot \text{mm}$ for Al_{0.85}Ga_{0.15}N/Al_{0.66}Ga_{0.34}N HEMT, and Baca *et al.* [13] reported R_C of 1900 $\Omega \cdot \text{mm}$ for AlN/Al_{0.85}Ga_{0.15}N HEMT, both using selective MOCVD epitaxy to regrow n⁺⁺-GaN to make contacts. Recently, Maeda *et al.* [123] have demonstrated a record-low contact resistance of 0.43 $\Omega \cdot \text{mm}$ using regrown n⁺⁺-GaN (electron concentration $\sim 2.6 \times 10^{20} \text{ cm}^{-3}$) contacts to AlN/Al_{0.5}Ga_{0.5}N HEMT structure grown using pulsed sputtering deposition (PSD). This lower contact resistance compared to that of our Al_{0.44}Ga_{0.56}N and Al_{0.58}Ga_{0.42}N channel QW HEMTs may partly be attributed to better 2DEG side-wall coverage and a higher electron density of regrown GaN prepared by PSD. A high electron density in regrown GaN results in a higher Fermi level position above the conduction band edge, thereby reducing the Schottky barrier height.

Nevertheless, the n⁺⁺-GaN contacting method to the AlGa_N channel HEMTs suffers from an inherent Schottky barrier at that lateral hetero-interface, which can become unfavorable as the Al composition of the channel increases, as shown by our systematic study. This problem can potentially be overcome by using a heavily doped reverse-

graded regrown AlGa_N contact layer instead of n^{++} -Ga_N to flatten the conduction band edge between ohmic metal and the AlGa_N channel. For instance, to achieve good ohmic contacts to their Al_{0.75}Ga_{0.25}N/Al_{0.6}Ga_{0.4}N HEMT, Xue *et al.* [210] performed an MBE regrowth starting with 100 nm of n^{++} -Al_{0.6}Ga_{0.4}N followed by 50 nm of heavily doped reverse-composition graded AlGa_N ($x = 0.6 \rightarrow 0$), which yielded a R_C of 7.5 $\Omega \cdot \text{mm}$.

To summarize this section, we have presented a systematic study of AlN/Al_{*x*}Ga_{1-*x*}N/AlN HEMTs with $x = 0.25, 0.44$, and 0.58 . While HEMTs with Al_{0.25}Ga_{0.75}N channel exhibited a relatively high maximum drain current density of 280 mA/mm, higher Al composition Al_{*x*}Ga_{1-*x*}N channel HEMTs showed diminished drain current densities of 30 mA/mm and 1.7 mA/mm for $x = 0.44$ and 0.58 , respectively, as a result of lower 2DEG densities and higher parasitic resistances. Al_{0.25}Ga_{0.75}N channel HEMTs with regrown contacts exhibited record low contact resistance of 0.23 $\Omega \cdot \text{mm}$, but achieving low contact resistance was found to be challenging for HEMTs with higher Al composition AlGa_N channel. The change in electron affinity of AlGa_N results in a tunable threshold voltage from -5.2 V to -2.4 V for $x = 0.25$ to $x = 0.58$. AlGa_N HEMTs with higher Al content may enable efficient enhancement mode operation with a positive threshold voltage. These results showing the dependence of electrical characteristics of AlN/AlGa_N/AlN HEMTs on Al composition provide insightful information that will help determine suitable Al content and other design parameters for RF and power switching applications.

3.3 RF operation of AlN/Al_{0.25}Ga_{0.75}N/AlN HEMTs

AlGa_N HEMTs show potential for next-generation high-power RF applications with the promise of a high Johnson's figure of merit ($JFOM = V_{br} \times f_T$) compared to the

incumbent GaN HEMT technology. Therefore, it is critical to increase the device's three-terminal off-state breakdown voltage V_{br} while ensuring a high unit gain cutoff frequency f_T in order to achieve superior RF performance. Previous theoretical studies have suggested that the saturation velocity v_{sat} of AlGaIn alloys is comparable to GaN. This indicates that for equivalent device dimensions, the maximum achievable f_T^{max} in HEMTs, which is determined by the ratio of saturation velocity to gate length, should be similar for AlGaIn and GaN channels. With a higher breakdown field and similar saturation velocity, AlGaIn channel transistors are therefore expected to deliver higher power density at high frequencies.

While it might seem intuitive to maximize the Al content in the AlGaIn channel HEMTs for superior RF performance due to higher breakdown voltage, such consideration has to be balanced with other design concerns. For example, when the Al content increases, the low-field mobilities and carrier densities in the AlGaIn channel decrease, increasing the sheet resistance and, as a result, the parasitic delay, thereby reducing f_T and f_{max} . Moreover, it becomes difficult to make ohmic contacts to the AlGaIn channel as the Al concentration of AlGaIn grows. So, an optimal Al mole fraction of the AlGaIn channel needs to be chosen that simultaneously maximizes f_T , f_{max} , and V_{br} to demonstrate an improvement over incumbent GaN HEMT technology.

Although AlGaIn-channel transistors are making rapid progress in long-channel devices designed for power-switching applications, there are limited reports of their RF performance. Xue *et al.* [210] reported a record f_T/f_{max} of 40/58 GHz for $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ HEMTs. The highest output power of Al-rich AlGaIn to date, 2.7 W/mm at 10 GHz albeit at a low PAE of 4%, was achieved in microchannel $\text{Al}_{0.65}\text{Ga}_{0.35}\text{N}/\text{Al}_{0.4}\text{Ga}_{0.6}\text{N}$ HFET structures [209].

In this section, we report a highly scaled T gate $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ QW HEMT, for im-

proved RF performance. We demonstrate devices with simultaneously high I_D^{max} (> 900 mA/mm) with low R_{on} ($= 6.5 \text{ } \Omega \cdot \text{mm}$), high average breakdown field strength (> 2 MV/cm) and record-high $f_T/f_{max} = 67/166$ GHz for any AlGaIn channel HEMT. We demonstrate high average breakdown voltage without any field plate technique which could potentially provide cost advantages for high-voltage RF applications.

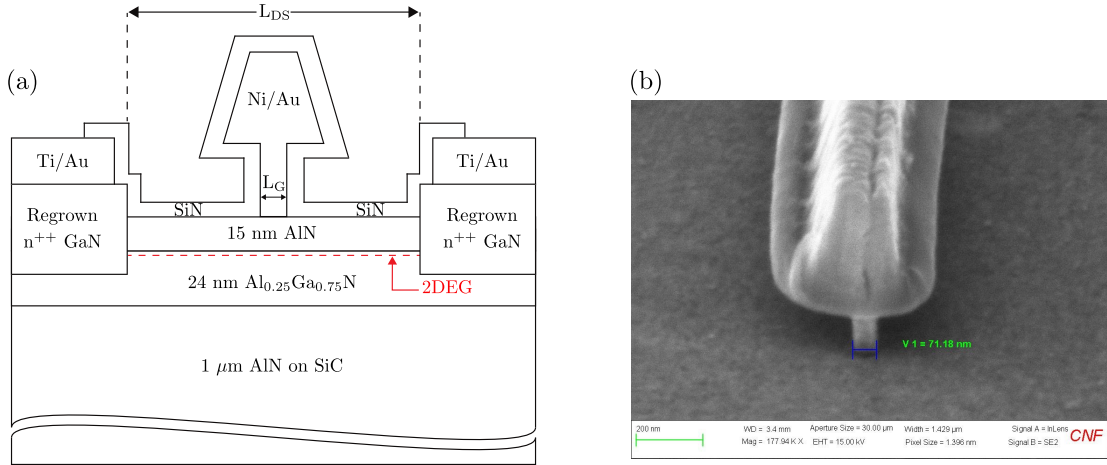


Figure 3.9: (a) Cross-sectional representation of a fully processed AlN/ $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ /AlN HEMT with a T-gate. (b) SEM image of a T-gate with $L_G = 70$ nm.

The fabrication process used for the QW HEMTs in this study is an extension of the process presented in the previous section. To explore the RF performance of AlN/AlGaIn/AlN HEMTs, an electron beam lithography (EBL) defined T-shaped gate was introduced in place of a rectangular gate previously defined by photolithography, and a SiN passivation layer was added for an improved dispersion control. A tri-layer resist stack was patterned by EBL, and a Schottky contact was formed by sputtering 10 nm Ni and evaporating 300 nm Au. The HEMTs were then passivated with 100 nm low-power plasma-enhanced chemical vapor deposition SiN. Figs. 3.9(a) and 3.9(b) show the final HEMT cross-section and a scanning electron microscope (SEM) image of a T-gate, respectively. The reported HEMTs feature a source-to-drain spacing $L_{DS} = 600$

nm, $W_G = 2 \times 25 \mu\text{m}$ device width, and a T-shaped gate placed in the middle of the source-to-drain spacing with a gate length $L_G = 70 \text{ nm}$.

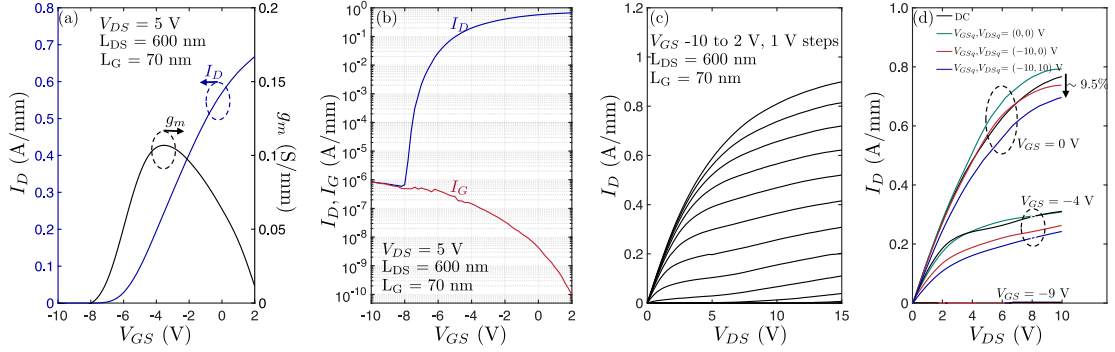


Figure 3.10: The (a) linear and (b) log transfer characteristics for AlN/Al_{0.25}Ga_{0.75}N/AlN HEMT showing a peak $g_m = 0.11 \text{ S/mm}$. The (c) output measurements demonstrate maximum drain current $I_D = 0.9 \text{ A/mm}$. (d) Pulsed $I_D - V_D$ measurements for a 500 ns pulse, at a bias of $V_{GS} = 0 \text{ V}$, -4 V , and -9 V .

After the device fabrication, a contact resistance from the top metal pad to 2DEG (R_c) and a sheet resistance (R_{sh}) were extracted by the linear transfer length method (TLM). The extracted $R_{sh} = 4.66 \text{ k}\Omega/\text{sq}$ closely matches with that measured on the as-grown sample via Hall-effect, indicating minimum process damage. The regrown n^{++} GaN non-alloyed ohmic contacts exhibited $R_c = 0.23 \Omega\cdot\text{mm}$, which is the lowest value among all AlGa_N channel HEMTs reported in the literature. Figs. 3.10(a) and 3.10(b) show the transfer curves measured at a drain bias $V_{DS} = 5 \text{ V}$, revealing an on/off ratio exceeding 10^6 with sharp pinch-off characteristics and a peak transconductance $g_m = 0.11 \text{ S/mm}$. The output curves in fig. 3.10(c) show a maximum drain current $I_D = 0.9 \text{ A/mm}$ at a gate bias $V_{GS} = 2 \text{ V}$ and an on-resistance $R_{on} = 6.5 \Omega\cdot\text{mm}$. The observed DC output conductance (G_{DS}) is higher than that of previously reported AlN/GaN/AlN HEMTs with a similar gate length [68], suggesting the presence of short channel effects (SCE). The cause of SCE is most likely a thicker AlN barrier used in this study, resulting in a low channel aspect ratio (L_G/d , d = gate-to-channel distance) less than 4.5 [166].

Further supported by negligible G_{DS} observed in AlGaN HEMTs with a longer gate length on the same chip as reported in the previous section, the short channel effect is expected to be suppressed upon thinning down the top AlN barrier.

To investigate the dynamic and transient behavior, pulsed I-V measurements were performed using 4225-PMU modules with a Keithley 4200. 500 ns long pulses and a 1 ms period were used, and the drain current density at $V_{GS} = 0$ V, -4 V, and -9 V was pulsed from different biasing conditions, $(V_{GSq}, V_{DSq}) = (0$ V, 0 V), (-10 V, 0 V), and (-10 V, 10 V), to assess current collapse and knee walkout. The AlGaN channel HEMTs demonstrated appreciable RF dispersion, with an average of $\sim 10\%$ current collapse (shown in Fig. 3.10(d)). The possible sources of current dispersion include the surface states and a formation of a 2-dimensional hole gas or a filling of hole traps located near the valence band edge at the bottom GaN/AlN interface with a net negative polarization charge [188, 203]. To suppress RF dispersion in future devices, proper control of surface states with an in-situ passivation layer and Si- δ doping in the AlN back barrier to compensate positive charges may be necessary [34].

RF characterization was performed using an Agilent 8722ES network analyzer and Infinity GSG probes. After the Short-Open-Load-Through calibration, scattering parameters were measured in the frequency range of 100 MHz to 40 GHz, and parasitic elements were de-embedded using on-wafer open and short structures. f_T and f_{max} were extracted from scattering parameters by extrapolating $|h_{21}|^2$ and a unilateral gain U , respectively, following the -20 dB/dec slope. As shown in Fig. 3.11, the HEMTs biased at $(V_{GS}, V_{DS}) = (-4$ V, 10 V) for maximum transconductance demonstrated a record-high $f_T/f_{max} = 67/166$ GHz for any AlGaN channel HEMTs. The high speed observed in Al_{0.25}Ga_{0.75}N channel HEMTs is attributed to a low contact resistance, which has been reported to be challenging to achieve with higher Al composition AlGaN channel,

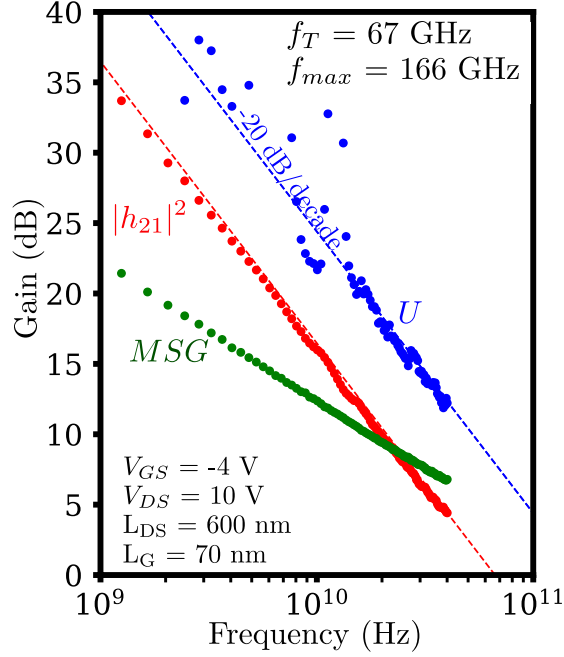


Figure 3.11: The small-signal characteristics for HEMT with $L_G = 70$ nm, with a resulting $f_t/f_{max} = 67/166$ GHz.

as well as a short gate length and low access resistance as a result of more aggressive lateral device scaling.

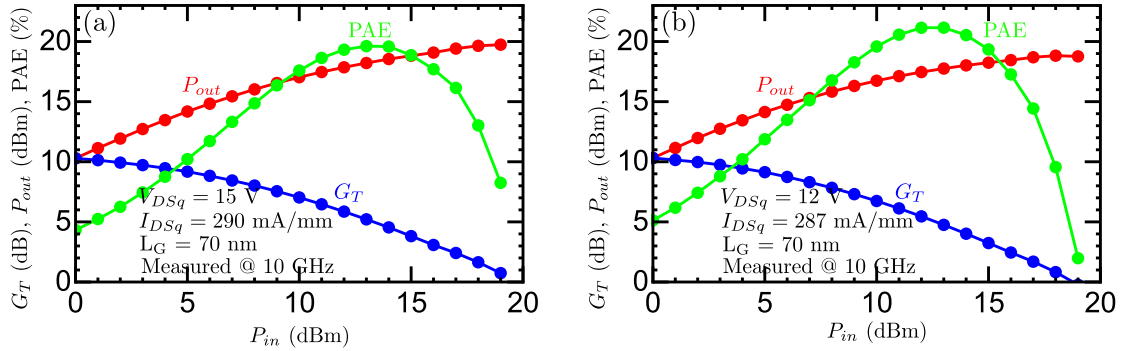


Figure 3.12: Load-pull power sweep at 10 GHz for a $2 \times 25 \mu\text{m}$ device biased in class AB operation for two bias points (a) $V_{DSq} = 15$ V, $I_{DSq} = 290$ mA/mm and (b) $V_{DSq} = 12$ V, $I_{DSq} = 287$ mA/mm. A saturation output power $P_{out} = 2$ W/mm is obtained at 10 GHz.

A Maury load-pull system at 10 GHz was used for large signal continuous wave RF

measurements. After finding the impedance for maximum output power density (P_{out}) by tuning an external load, the input power was swept to measure gain, P_{out} , and power-added efficiency (PAE). CW large signal load-pull measurement was performed at class AB operation with two bias conditions as shown in Fig. 3.12. As shown in Fig. 3.12 (a), a saturation output power $P_{out} = 2$ W/mm is obtained at 10 GHz. The maximum PAE is measured to be $\sim 20\%$ and the power gain G_T is 5.2 dB at this condition.

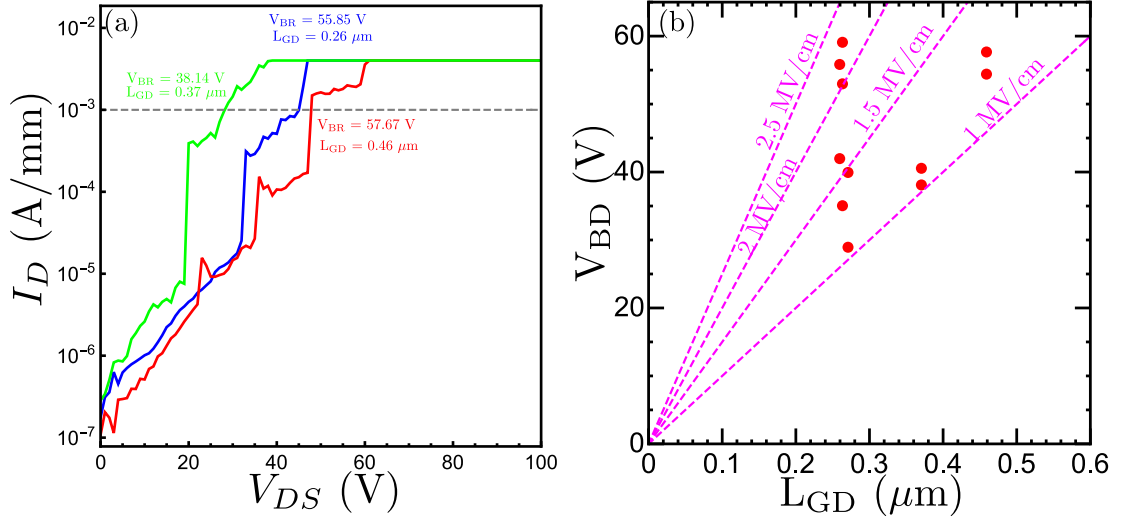


Figure 3.13: (a) Hard breakdown of three sub-micron channel HEMTs with varied gate-to-drain separations. (b) Breakdown voltage scaling as a function of gate-drain separation.

The three-terminal off-state breakdown voltage was measured by increasing V_{DS} until hard breakdown of the HEMT occurred with the gate voltage set below the threshold voltage, $V_{GS} \sim -10$ V. The breakdown voltage metric used in this study is defined as the drain voltage at which the drain current (I_D) exceeds 1 mA/mm. To explore the potential for high-frequency applications, sub-micron channel lengths were examined for breakdown. Fig. 3.13(a) shows the three terminal off-state breakdown of three AlGaIn QW channel HEMTs with varied gate-drain distances. Among all devices, a breakdown voltage of 59 V was measured for a HEMT with a 260 nm gate-drain distance. This

corresponds to an average breakdown field exceeding 2 MV/cm. Fig. 3.13(b) shows the scaling of breakdown voltage as a function of L_{GD} , all the measured HEMTs show $E_{avg} > 1$ MV/cm, demonstrating the potential of QW HEMTs for extremely high-power operation in RF applications.

3.4 Future Directions

1. Extreme temperature operation of AlGaN channel HEMTs

Ultra-wide bandgap semiconductors such as AlGaN are suitable for high temperature, harsh environment applications due to their inherent low intrinsic carrier concentration ($n_i \propto e^{-E_g/2k_bT}$, where E_g is the bandgap and k_b is Boltzmann's constant) and stability. Therefore it is reasonable to evaluate whether Al-rich AlGaN may be more promising for high-temperature electronics than GaN devices and materials.

Typically in GaN channel HEMTs, the 2DEG mobility is a strong function of the temperature because the dominant scattering mechanism is due to optical phonons, which is strongly temperature dependent. Therefore at a high temperature, characteristics of GaN channel HEMTs degrade from the room temperature characteristics (such as a decreasing drain current). On the other hand, the temperature dependence of 2DEG mobility in AlGaN channel HEMTs is nearly negligible, since the temperature-independent alloy scattering is the dominant scattering mechanism.

While all the transistor device results presented in this chapter were at room temperature, we also report some preliminary high temperature transfer and output characteristics of AlGaN HEMTs at temperatures ranging from 25 to 200 °C as shown in Figure 3.14, which is the upper limit of the equipment used for the mea-

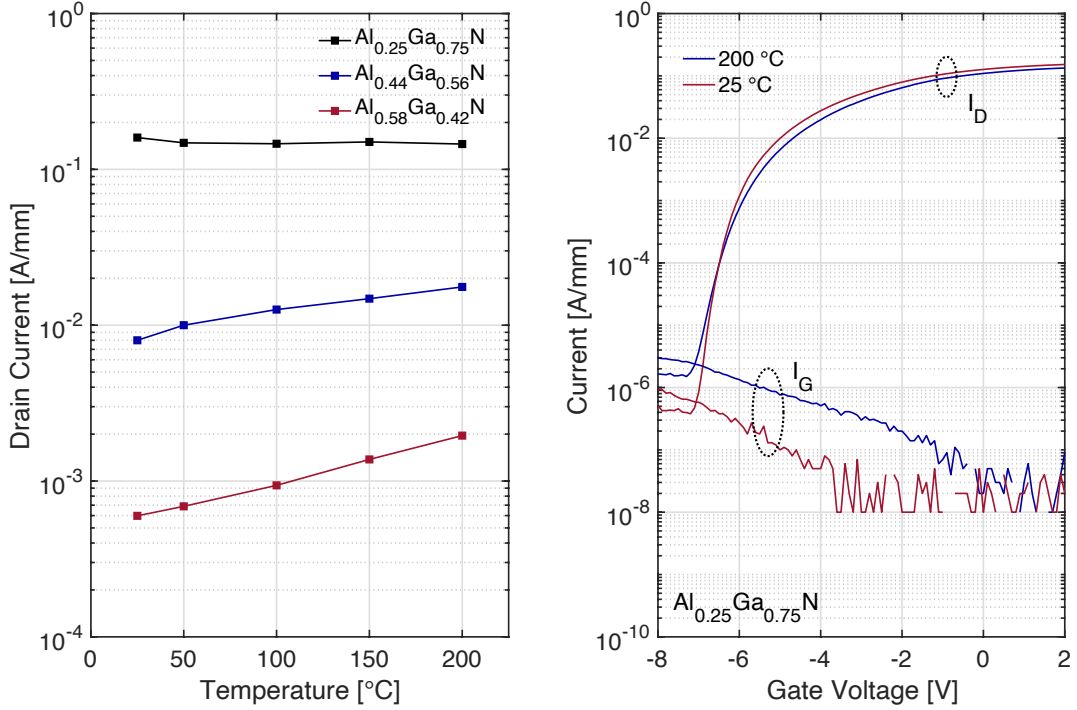


Figure 3.14: High temperature DC operation of AlGaIn channel HEMTs

surement in our laboratory. The thermal stability of HEMT device characteristics is clearly demonstrated where it is seen that little to no decrease in drain current for Al_{0.25}Ga_{0.75}N channel HEMTs up to 200 °C is observed.

For Al_{0.44}Ga_{0.56} and Al_{0.58}Ga_{0.42} channel HEMTs, the drain currents were observed to *increase* at higher temperatures. This increase in drain current for the higher Al composition channels is mainly attributed to the decrease in contact resistance at elevated temperatures. For these two samples, the Schottky-like source and drain contacts are the dominating factor limiting the current flow, rather than the 2DEG mobility. Therefore the observed higher drain current is likely to be the result of an increased rate of thermionic emission across the contacts at elevated temperatures. We expect a stable operation over the large range of tempera-

tures upon improving the contacts, but a detailed temperature-dependent analysis of the comparative transistor characteristics of the AlGa_{0.3}N quantum well channel HEMTs is proposed for future work.

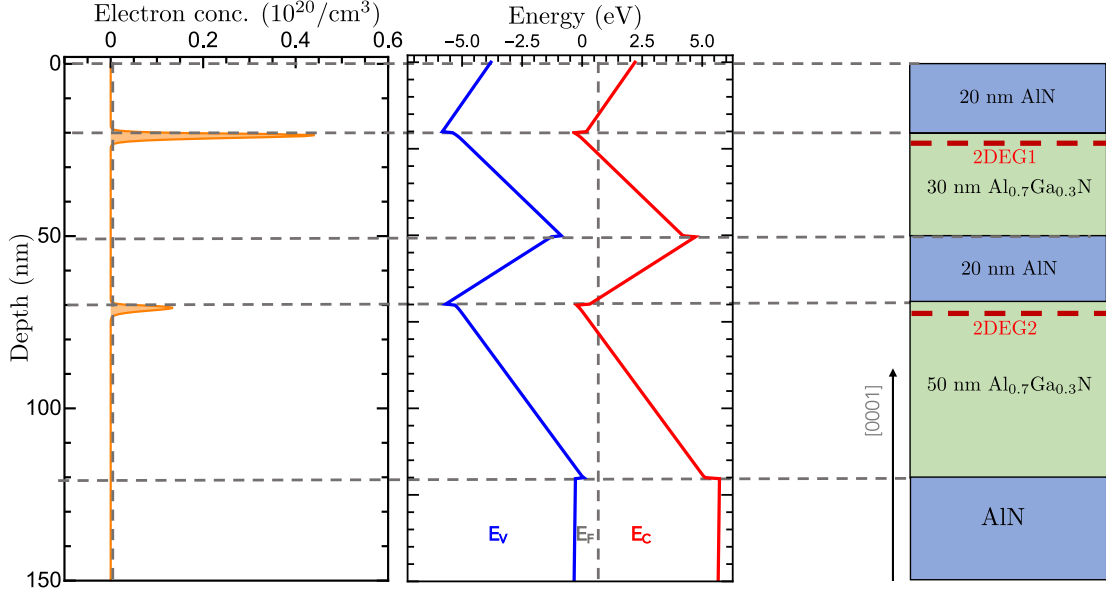


Figure 3.15: Layer structure and energy band diagram of double channel AlN/Al_{0.7}Ga_{0.3}N heterostructure.

2. Double/Multiple channel AlGa_{0.3}N HEMTs

To boost the current density in AlGa_{0.3}N channel HEMTs, the number of parallel conducting channels in the devices can be increased by realizing a vertically stacked multi-channel arrangement. As shown in Figure 3.15, the new device consists of two (or more) 2DEG channels enabled by two AlN/Al_{0.7}Ga_{0.3}N epilayers. The 2DEG charge density located at the two AlN/Al_{0.7}Ga_{0.3}N heterointerfaces are calculated to be $6.5 \times 10^{12}/\text{cm}^2$ and $3.5 \times 10^{12}/\text{cm}^2$. Hence, the total charge is almost $\sim 10^{13}/\text{cm}^2$ for the two channels, thus improving the sheet resistance compared to single quantum well structures. The whole heterostructure stack has an extremely wide energy bandgap > 5 eV, thus making it suitable for high-power and high-temperature electronics.

However, the gate control of double-channel devices becomes a new problem in comparison with single-channel devices. In order to overcome this, it is possible to structure the multiple channels into nanowires in the gate region of the device and form a 3D gate electrode (tri-gate) [223, 119, 122] on them for controlling the parallel channels through the sidewall portions of the nanowire.

CHAPTER 4

**SINGLE-CRYSTAL ALN SUBSTRATE ENABLED HIGH POWER
ELECTRONICS ON N-POLAR ALN: MOLECULAR BEAM HOMOEPITAXY
OF N-POLAR ALN**

4.1 Introduction

In chapters 2 and 3 of this dissertation, the metal-polar AlN/AlGaN/AlN heterostructure has been studied which generates a 2DEG at the positive polarization interface. These structures grown on 6H-SiC substrates have achieved high n-type conductivity in some of the widest bandgap semiconductors to date which enabled high performance RF HEMTs on the AlN platform.

The output power, PAE, and cutoff frequency of nitride HEMTs is limited by the ability to extract heat from the thermal hot spot formed at the drain side of the gate where the lateral electric field peaks and electrons reach their highest kinetic energies (e.g. see [54]). The highest performance RF and mm-wave HEMT power amplifiers today use nitride semiconductor heterostructures on SiC substrates. The SiC substrate is available in large area and high crystalline quality, and has among the highest thermal conductivities ($\sim 350 - 400$ W/m·K) for efficient heat removal. Furthermore, its 6H crystal structure also allows a reasonable lattice matching with AlN and GaN for the heterostructures desired for the HEMT.

Among substrates attractive from a thermal point of view, bulk GaN substrates are available. Thermal conductivity of up to 280 W/(m·K) is achievable in pure single-crystal GaN, and wafer size is growing over time. While conductive single-crystal GaN substrates are appealing for vertical power devices [142, 41, 38], they are not compet-

itive for mm-wave HEMTs. This may seem counter-intuitive, given that using a GaN bulk substrate will almost certainly reduce thermal boundary resistances. The issue occurs because thick epitaxial layers are required to place the HEMT channel far enough away from the growth interface to prevent carrier trapping, while the unintentional doping of GaN by MOCVD and MBE in a few micron thick layers is in the range $N_d \sim 10^{16} / \text{cm}^3$. This high density of mobile electrons is too lossy for RF and mm-wave electronics.

Even if a solution could be developed, the larger problem is that the back-barrier is GaN itself. The lack of a back-barrier with a higher energy bandgap than GaN inhibits lateral scaling in a GaN channel HEMT. When the gate length is reduced to the 10 – 100 nm window in order to raise the f_T and f_{max} , the lack of a back-barrier causes severe short-channel effects such as drain-induced barrier lowering (DIBL), resulting in an increase in output conductance and a drop in HEMT gain.

The SiC substrate has become the preferred substrate due to its large-area and high thermal conductivity. Direct growth of GaN on SiC poses chemical incompatibilities (such as gallium meltback etching of SiC). Today, at least a ~ 200 nm AlN layer is commonly grown on SiC substrates before the formation of GaN and Al(Ga)N or Al(Sc)N barrier layers for high performance HEMTs as demonstrated in previous chapters of this dissertation as well. This enables the inclusion of AlGaN back barriers with low Al content, albeit these structures have thermal restrictions due to the relatively low thermal conductivity of AlGaN due to alloy scattering of acoustic phonons (see [80]). Even if we replace the AlGaN back barrier with AlN, which is the basis of our metal-polar AlN-based HEMTs, the heat flow from the channel to the substrate still passes over many heterointerfaces, one of which being the AlN/SiC interface. The AlN/SiC thermal boundary resistance (TBR) of $0.2 \text{ GW/m}^2 \cdot \text{K}$ is a current bottleneck in high-power

HEMTs. What is the remedy to this inherent technological issue? The TBR can be eliminated by growing AlN buffer layers on bulk AlN substrates.

4.2 Advantages of using single crystal AlN substrates

One of the major challenges in developing III-nitride epitaxy has been the lack of native substrates. Nitride epilayers then are grown on a foreign substrate, leading to films with high densities of dislocations due to lattice mismatch. The high dislocation density can contribute to reduced performance in III-nitride HEMTs. The lack of native substrates is because, unlike other material families like Si, GaAs, SiC, and recently Ga₂O₃, nitrides cannot easily be grown as large, single crystal boules from the melt via the Czochralski method or a similar bulk synthesis method.

While single crystal GaN substrates are now commercially available, the growth of bulk AlN, which has more desired thermal properties as well as a larger bandgap and smaller lattice constant, has historically proven difficult. Recently, several techniques have been developed to synthesize large-area, usually two-inch diameter, bulk wafers of high-quality single crystalline aluminum nitride at a commercial scale. One such technique is based around the physical vapor transport (PVT) method, where AlN powder is used as a precursor, which is sublimated at high temperatures and the vapor is carried via thermal gradients to a heated seed crystal. Primarily driven by UV LEDs and laser development, these PVT grown bulk AlN substrates were instrumental in the demonstration of first UV-C laser diode [221]. Single crystal bulk AlN substrates provide a number of potential advantages to a lateral transistor thanks to its low dislocation densities of 10^4 - $10^5/\text{cm}^2$ and high thermal conductivity of $\sim 340 \text{ W/m.K}$. So, not only will bulk AlN substrate help in eliminating TBR, AlN is more attractive as a choice of

substrate compared to GaN or SiC due to its excellent thermal conductivity, but more importantly, due to its larger energy bandgap of 6.2 eV compared to 3.4 eV of GaN and 3.3 eV of SiC. Unlike GaN, unintentionally doped AlN is extremely electrically resistive. The key motivators for using single crystal AlN substrates for AlN-based transistor technology can be summarized as follows:

- **Efficient heat removal from active region:** Because heat removal from SiC substrates is reaching its limits, Figure 4.1 depicts temperature rise estimates based on interface thermal boundary resistance while accounting for the phonon density of states (DOS) mismatch between the buffer layer and the substrate. This calculation is similar to the one described in [71], and it is based on a simplistic model of heat dissipation by a HEMT modeled as a wire dissipating 1 W of power into a 1 μm thick buffer layer on a 50 μm thinned substrate. The heat flow can be considered to be cylindrical due to the dimensions. The calculation unambiguously reveals that a bulk, single-crystal AlN substrate and an AlN buffer layer will result in the lowest channel temperature among the considered cases. Even if large-area diamond substrates were available and AlN was grown on them, that would still perform worse than AlN buffer layer on bulk AlN. The removal of thermal boundary resistance between the buffer layer and the substrate is the primary reason. Moreover, due to the lower dislocation density in bulk AlN, phonon scattering by dislocations in the crystal is suppressed, thereby not contributing significantly to the rise in the channel temperature.
- **Improved carrier transport due to less dislocations:** Growth of AlN on substrates where lattice and thermal mismatch is present (such as Si, SiC etc.) leads to a high threading dislocation density (TDD) of the order of 10^9 - $10^{10}/\text{cm}^2$ and other defects. These defects act as scattering centers and traps for carriers and hamper the performance of electronic devices. The charge accumulation along

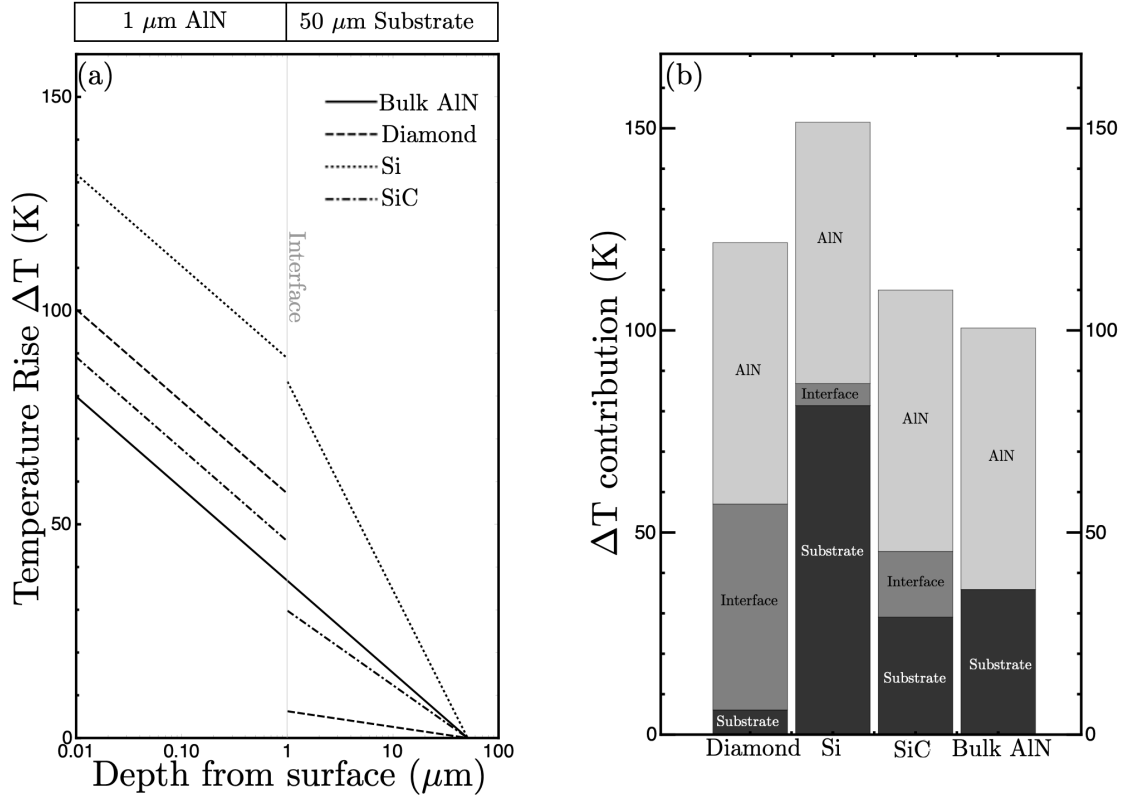


Figure 4.1: (a) Calculated decrease in temperature of HEMT channels near the surface due to the elimination of the thermal boundary resistance using bulk AlN substrates compared to attempted recent options. The x -axis is in logarithmic scale. (b) Calculated ΔT (K) contributions from various layers and interfaces for AlN buffer layer grown on different substrates. Note that there is no contribution from interface in the case of AlN buffer layer grown on bulk AlN.

dislocations and the resulting electric field scatters the carriers in the active region. At high carrier densities, these dislocations are screened by the accumulation of electrons around the dislocation. However, at low charge densities, the presence of insufficient electrons to screen these dislocations results in high dislocation scattering. Thus, this dislocation scattering can lead to very low electron mobilities near pinch-off, which can be detrimental for deep class AB amplifier operation. Dislocation scattering can be greatly diminished by using bulk AlN

substrates with orders of magnitude lower TDD ($<10^4/\text{cm}^2$). Moreover, these dislocations also contribute to deep-level bulk traps which cause current collapse under high operation biases. This can again be minimized by moving to bulk AlN substrates.

- **Higher breakdown voltage through reduced gate leakage:** Coulombic electron scattering is not the exclusive factor affecting device performance in high TDD nitride devices. Defects originating from crystal growth, are a very crucial factor that affect gate Schottky leakage current. These defects act as conducting paths and lead to gate leakage current, lowering breakdown voltage by hot-carrier induced impact ionization. Since parasitic conduction (leakage) through the (Al,Ga,In)N barrier reduces the operation efficiency, HEMT performance hinges on the epitaxial quality of these layers. The breakdown voltage can thus be improved by using single crystal AlN substrates which would suppress the vertical leakage due to low TDD.

4.3 Al-polar versus N-polar AlN

Motivated by the above advantages of high-quality bulk AlN substrates and their recent availability [74], there have been numerous efforts in the field to explore their effect on electronic lateral device performance. Metal-polar GaN HEMTs growth on bulk AlN from Fujitsu have demonstrated output powers upto 15 W/mm [144] and 24.4 W/mm [102] in X-band. The demonstration of very high mesa breakdown fields of ~ 11.5 MV/cm in AlGaN channel HEMT by Khachariya *et al.* [94] was also on bulk AlN substrates.

The first step to achieving III-N HEMTs based on the bulk AlN platform is the

demonstration of AlN homoepitaxy on single-crystal AlN substrates. Due to the absence of inversion symmetry, the metal-polar (0001) and N-polar (000 $\bar{1}$) surfaces of wurtzite III-nitrides are not equivalent. Epitaxial films grown on the metal-face and the N-face exhibit different surface morphologies, optical properties, and growth kinetics. [134, 67] So, bulk AlN substrates offer two possible polar orientations for growth. Successful molecular beam homoepitaxy of *metal*-polar AlN on single-crystal AlN substrates has been recently demonstrated [37, 109]. Key to the homoepitaxial MBE growth of AlN on the metal-face of AlN substrates was the development of an aluminum-assisted *in situ* substrate cleaning process. The homoepitaxial growth of AlN on bulk AlN substrate maintained its high quality and low dislocation density without a structural boundary between them, as confirmed by transmission electron microscopy (TEM) [37].

Ideally, a zero TBR (or infinite thermal boundary conductance) is expected in such a homoepitaxial AlN film on bulk AlN substrates, but chemical impurities such as oxygen at the interface could increase the TBR. Experimental measurements of the thermal boundary conductance using the frequency-domain thermoreflectance method reported an ultra-high thermal boundary conductance value exceeding $\sim 1 \text{ GW}/(\text{m}^2\cdot\text{K})$ for $1 \mu\text{m}$ metal-polar AlN grown on the bulk AlN substrate, which is five times higher than all reported state-of-the-art thermal boundary conductance for GaN HEMTs as shown in Figure 4.2 [4]. Further increases in the thermal boundary conductance are expected upon reduction in oxygen concentration and other impurities at the interface which could be a key enabler for increasing output powers for RF HEMTs at high frequencies.

Building on these growth advancements on the Al-face of bulk AlN, GaN/AlN high-density 2DHGs and AlN/GaN/AlN 2DEGs have been shown recently using MBE on bulk AlN substrates. However, the N-face of bulk AlN substrates has largely been unexplored. In chapters 2 and 3, the focus was on the metal-polar AlN-based HEMT

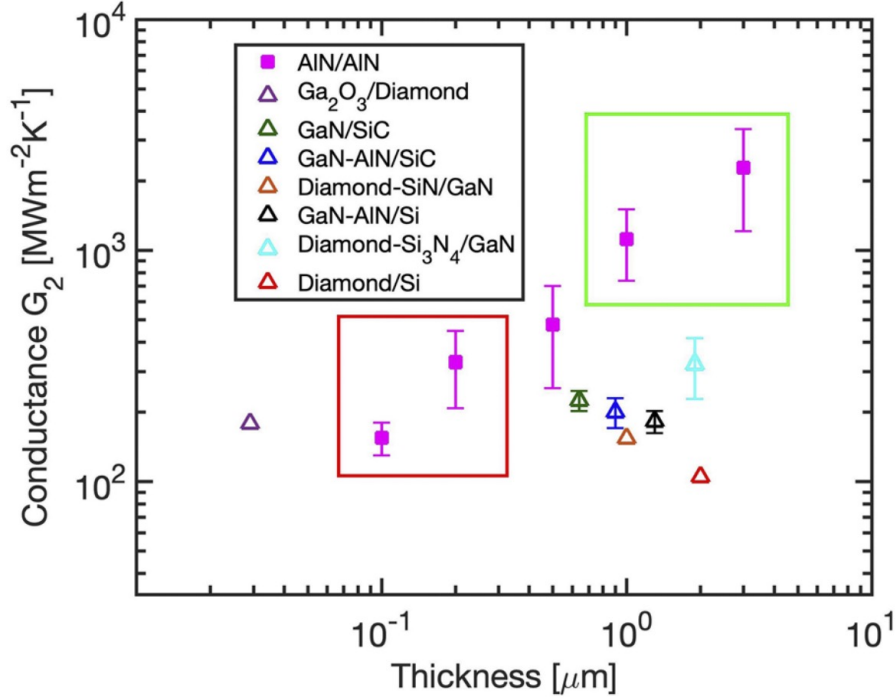


Figure 4.2: Measured thermal boundary conductances for various nitride HEMT interfaces. Ideally one expects the TBR to be eliminated in AlN homoepitaxial layer grown on bulk AlN, taking the thermal boundary conductance (TBC) to infinity. But the presence of oxygen impurities at the epitaxial growth interface limits the TBC to $\sim 1 \text{ GW}/(\text{m}^2.\text{K})$, which is still the highest measured among existing nitride HEMT boundary conductances. Figure reproduced from [4]

heterostructures and devices; here we argue why the N-polar AlN platform is attractive for next-generation power and RF electronics.

Nitrogen-polar HEMTs have a reversed structure compared to the typical metal-polar HEMTs. The main difference between metal- and N-polar HEMTs is that in N-polar HEMTs, the 2DEG is located closer to the device surface, on top of a higher bandgap barrier layer [201]. This better positioning of the 2DEG results in several advantages. First, the higher bandgap material acts as an effective back-barrier, keeping electrons confined more effectively in the channel [154], leading to improved performance in both the on and off states, especially in highly scaled transistors. Secondly,

low-resistivity ohmic contacts can be made to the channel through the lower bandgap and lower surface potential material [45]. The third advantage of N-polar HEMTs is that they can be scaled more aggressively, as the 2DEG is located between the gate metal and the gate-barrier interface, reducing the effective gate-channel distance [148]. This allows for independent control of the gate-channel distance and charge carrier density, within the limits of available material compositions and thickness. In contrast, in metal-polar devices, using a thinner barrier reduces the gate-channel distance but also decreases the charge carrier density in the channel [175]. Finally, using the N-polar materials enhancement-mode devices can be fabricated more easily by adding an additional barrier layer on top of the channel, thereby depleting the channel [127].

Because of the above-mentioned advantages, the current state-of-the-art performance has been achieved using N-polar GaN/AlGa_N HEMTs with output powers above 8 W/mm at up to 94 GHz [161]. While the transistors based on the N-polar GaN platform have proven to be a useful device technology with their excellent performance in W-band (75-110 GHz) in the past decade[201, 93], the replacement of N-polar GaN with N-polar AlN as the buffer layer can enable further advancements. N-polar AlN can enable the formation of two-dimensional electron gas (2DEG) with AlN back-barriers, with the promise of enhanced thermal management, reduced buffer leakage and short channel effects [202, 112, 110]. High conductivity 2DEG channels with high-density 2DEGs induced at the heterointerface with AlN can then be expected.[202, 112, 180]

Therefore the growth of smooth, high-quality N-polar AlN films is technologically relevant for developing high electron mobility transistors (HEMTs) built on the wide-bandgap III-nitride materials platform for high-power mm-wave electronics. Moreover, a homoepitaxial platform for N-polar AlN could offer new possibilities in deep-ultraviolet (UV) laser diodes and light-emitting diodes [221, 199]. Besides suppressing

optical losses due to the reduction in dislocation and point defect densities by growth on single-crystal AlN [191], the N-polarity can improve the light output in deep-UV emitters by enhancing the injection efficiency [197].

4.4 Molecular Beam Homoepitaxy of N-polar AlN on single crystal AlN substrates

Homoepitaxial growth of high quality N-polar AlN is an important first step for N-polar RF and power electronics on the AlN platform. Growth of N-polar wurtzite AlN on foreign substrates such as Si, SiC and sapphire by metal-organic vapor phase epitaxy (MOVPE), sputtering and molecular beam epitaxy (MBE) have been reported [92, 189, 46, 143, 108, 111, 75, 169]. Recently, MBE homoepitaxy of N-polar AlN grown on AlN templates on sapphire has also been demonstrated [220]. A limited number of reports exist on the growth of N-polar AlN on native AlN substrates.[75] This is because single crystal AlN substrates with epi-ready N-face have not been readily available.

Growth of N-polar nitrides is particularly challenging compared to their metal-polar counterparts. The first challenge is that the adsorption efficiency of impurities such as oxygen is higher in N-polar surfaces than metal polar ones.[225, 190, 213, 126] Second, a low surface diffusivity [224, 139] on the N-polar face is thought to inhibit step-flow-growth mode.

In this section, we report the MBE homoepitaxy of N-polar AlN films on bulk N-polar AlN substrates. Taking inspiration from the *in situ* cleaning techniques of thermal annealing and Al assisted cleaning developed for Al polar AlN [37, 109], an *in situ* cleaning method for the surface of bulk N-polar AlN is developed, before perform-

ing epitaxy. Careful monitoring of *in situ* reflection high-energy electron diffraction (RHEED) helps to repeatably obtain clean N-face AlN surfaces free of contaminants and enables a meaningful study of homoepitaxy of N-polar AlN.

Subsequently, AlN homoepitaxy is performed by PA-MBE. The surface morphology after epitaxy is found to be strongly dependent on the Al droplet coverage during growth where the condition with the highest Al droplet accumulation is found to produce parallel atomic steps. On the other hand, at low Al droplet coverage, it is observed that the surface suffers from pits and spiral hillocks. This is likely because Al droplets facilitate adatom diffusion on the N-face. KOH etching study is used to confirm the N-polarity of the homoepitaxial films while also revealing a low density of Al-polar inversion domains whose properties are discussed in detail. Finally, secondary ion mass spectrometry (SIMS) analysis of the smooth homoepitaxial N-polar AlN films indicates low chemical impurity densities for hydrogen and silicon near the detection limit, whereas oxygen and carbon show higher densities of incorporation.

4.4.1 Challenges associated with N-face AlN substrate preparation

2-inch diameter N-polar AlN (000 $\bar{1}$) bulk substrates prepared by Asahi Kasehi were used in this study. The dislocation densities of these substrates were less than 10^4 cm^{-2} signifying high structural quality. The substrates have surface defects arising from the chemical-mechanical polishing (CMP) process used on the N-face of AlN to prepare it for epitaxy. Figure 4.3 shows an AFM image of the N-face of the single crystal AlN substrate prior to cleaning and epitaxy. The surface morphology is largely smooth with a root-mean-square (rms) roughness between 1-2 nm over a $10 \mu\text{m} \times 10 \mu\text{m}$ area. But scratches and particulate debris from the CMP process covering the surface are ob-

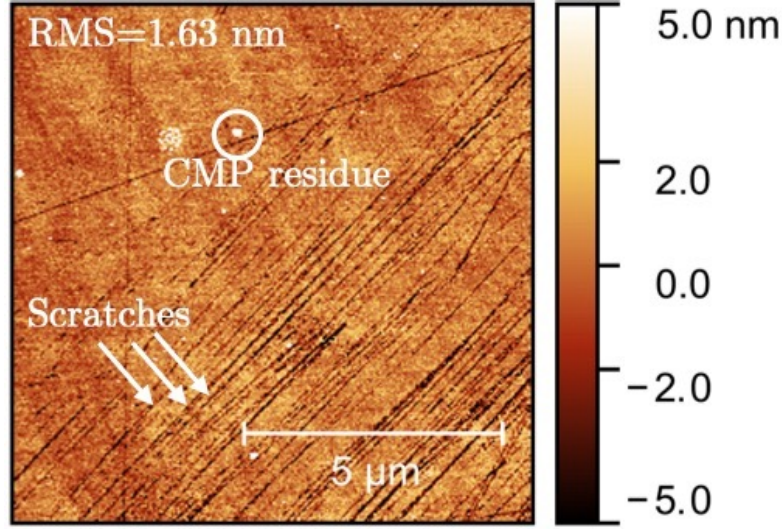


Figure 4.3: AFM micrograph of the surface of the N-face of an as received bulk AlN substrate. The surface has particulate residue and scratches from the CMP process.

served, as indicated in Fig. 4.3. The wafers were diced into $7 \times 7 \text{ mm}^2$ pieces and cleaned *ex-situ* in acetone, isopropyl alcohol and deionized water. They were then mounted on a faceplate and transferred into the load-lock chamber of a Veeco GEN10 plasma-MBE system and degassed at 200°C for 8 h. No other *ex situ* cleaning procedures (e.g. using strong acids such as Piranha, H_2SO_4 etc.) were used here since it was found that such treatments damage the surface of N-face AlN as shown in Figure 4.4. This is in stark contrast to the *ex situ* cleaning of the Al-face of bulk AlN substrates where acid treatment reveals the atomic steps on the surface instead [109].

4.4.2 *In situ* substrate cleaning

In situ cleaning of the substrates was performed in the MBE growth chamber using a combination of thermal deoxidation and Al assisted thermal desorption at a substrate temperature of $\approx 1100^\circ\text{C}$. Evolution of the surface during the *in situ* cleaning of the

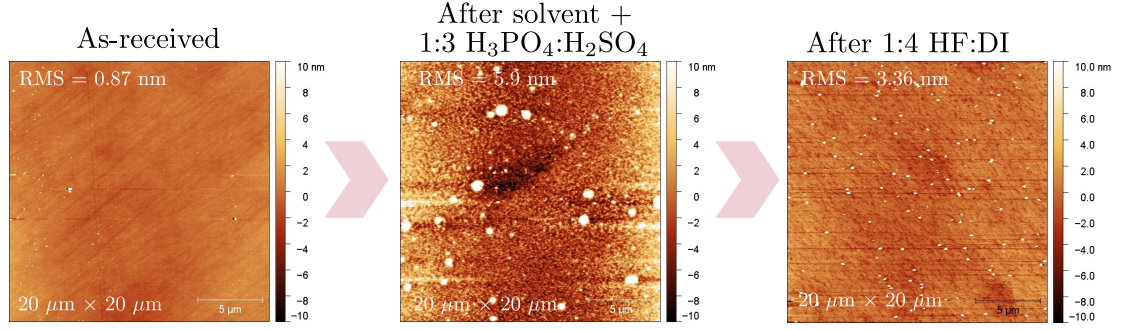


Figure 4.4: Summary of surface evolution during acid-treatment process on the N-face for bulk AlN substrates. The same ex situ cleaning procedure that is typically used for cleaning Al-face of bulk AlN substrates was used here. The surface of N-polar AlN substrate becomes rough after the acid treatment.

AlN substrate, as well as during and after the homoepitaxy of AlN were monitored by RHEED. Firstly, changes in the AlN substrate surface during thermal deoxidation process were studied. The substrates were heated up to a thermocouple temperature of 1100°C. As the temperature of the substrate was increased from 400°C to 1100°C, the RHEED pattern of the sample evolved from dim and diffuse to bright and spotty signifying that the thermally volatile oxides and hydroxides are removed from the surface, as shown in Figure 4.5. The surface becomes less amorphous as a result of this thermal deoxidation process, but further *in situ* chemical cleaning was found to be necessary to remove thermally non-volatile oxides and impurities.

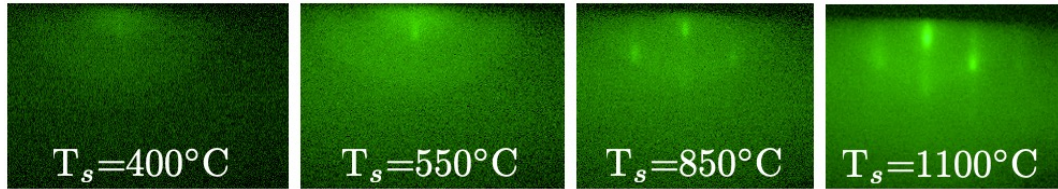


Figure 4.5: Evolution of the RHEED patterns of the AlN substrate taken along $\langle 11\bar{2}0 \rangle$ azimuth during thermal deoxidation as the substrate temperature is progressively increased from 400°C to 1100°C.

While holding the substrate at a thermocouple temperature of 1100°C, *in situ* Al

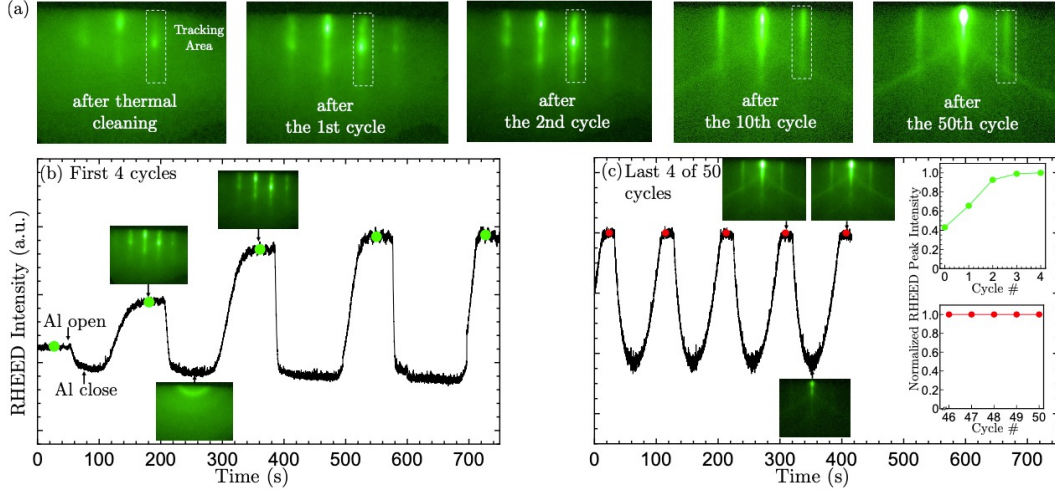


Figure 4.6: (a) RHEED patterns of the AlN substrate at various stages during the 50 Al polishing cycles. RHEED intensity vs time of the boxed area in (a) is shown in (b) for the first four cycles and (c) for the last four cycles. Inset RHEED images in (b) and (c) show the diffraction patterns during the 2nd and 50th Al polishing cycles respectively. The inset in (c) shows the evolution of normalized RHEED peak intensity after each cycle as a function of the cycle number. All the RHEED patterns were taken along the $\langle 11\bar{2}0 \rangle$ azimuth.

assisted surface cleaning was then performed to prepare for epitaxy. This process involved exposing the surface to an aluminum metal flux $\phi_{Al} = 15.9$ nm/min for 30s, and then holding the substrate at a high temperature long enough for the deposited Al to desorb; this adsorption and desorption, which Cho *et al.* developed for the cleaning of Al polar bulk AlN substrates [37] and Lee *et al.* called Al polishing [109], was repeated for ~ 50 cycles. Though the procedure of Al polishing of N-polar AlN is similar to the Al-polar single crystal AlN, a few characteristic differences are observed in the nature of RHEED evolution during the course of Al assisted cleaning.

Figure 4.6 shows the evolution of the RHEED pattern and the variation of RHEED intensity during the Al polishing cycles. Fig. 4.6(a) depicts the gradual transformation of the diffraction pattern from spotty and diffuse after thermal cleaning, to bright and streaky after 50 cycles of Al polishing. Fig. 4.6(b) and Fig. 4.6(c) track the temporal

evolution of the RHEED intensity of the boxed area in Fig. 4.6(a), during the first four and last four cycles of Al polishing, respectively. In each cycle, the intensity first drops when Al is deposited. Subsequently, when Al is desorbed, the intensity increases and eventually saturates to the peak value of the cycle. This is similar to the observations made for Al-polar AlN. [37, 109] The first three cycles are distinct as the corresponding peak/saturation intensity progressively increases over them, after which the saturation intensity remains unchanged for the remaining cycles. This gradual increase in the saturation intensity over the initial few cycles can be explained by the removal of amorphous contaminants such as oxides and hydroxides of Al and various other impurity alloys of Al, O and N from the surface of the substrate during Al polishing, thereby improving the crystallinity of the surface.

The RHEED images in Fig. 4.6(b) also show how the Al metal reacts with the contaminated surface of the substrate during the 2nd cycle of Al polishing. Starting with a spotty and diffuse RHEED pattern before the Al adsorption, the RHEED pattern exhibits diffuse Debye rings when Al reacts with the surface. These rings indicate the formation of a polycrystalline complex which is removed from the surface as Al is desorbed, revealing a visibly brighter and streakier RHEED pattern, implying a smoother and cleaner surface. This process of Al assisted cleaning is repeated for 50 cycles until no further change is observed in the evolution of RHEED intensity as a function of time as seen in the last four cycles of Al polishing in Fig. 4.6(c). It is noteworthy that when the surface of AlN is sufficiently clean, the Al adsorption and desorption behaves differently compared to when the surface is contaminated. The RHEED images in Fig. 4.6(c) show how the cleaned AlN surface behaves during Al adsorption and desorption in the final (50th) cycle. The RHEED pattern is initially bright and streaky. Upon Al adsorption the RHEED pattern becomes dark due to Al adlayer formation and Al droplet accumulation without forming any polycrystalline complex. The streaky pattern

Table 4.1: Growth conditions with nitrogen plasma power at 400 W and 1.85 sccm flow rate

Condition	Substrate Temperature ($^{\circ}\text{C}$)	ϕ_{Al} (nm/min)	Al/N Ratio
A	1055	12.7	1.84
B	1055	19.6	2.84
C	1000	19.6	2.84

is recovered upon Al desorption. This change in the behavior during Al adsorption accurately signals when the surface is free of contamination, along with the RHEED pattern changing from spotty-diffuse before Al polishing to bright-streaky after 50 cycles as shown in Fig. 4.6(a).

4.4.3 N-polar AlN growth and characterization

AlN homoepitaxy was performed directly after the *in situ* cleaning. Surface morphologies of AlN grown in various metal-rich growth conditions (see Table 4.1) were explored for pit-free and smooth homoepitaxy. The nitrogen plasma power was held at 400 W with 1.85 sccm flow rate, corresponding to a growth rate of 6.9 nm/min ($= \phi_N$) where ϕ_N is the N flux. Al metal was provided from a standard effusion cell. AlN films of thicknesses ~ 500 nm were grown in three conditions shown in Table 4.1. The epitaxial process was started by first opening the Al shutter for 20 s to wet the surface. Then Al and N fluxes were provided simultaneously during the epitaxial growth. To end the growth, the plasma is turned off, both Al and nitrogen shutters are closed, and the substrate is heated to 50°C higher than the growth temperature to desorb excess Al.

It was found that the surface morphology of homoepitaxial N-polar AlN is strongly dependent on the amount of excess Al on the surface during growth. Excess Al droplets

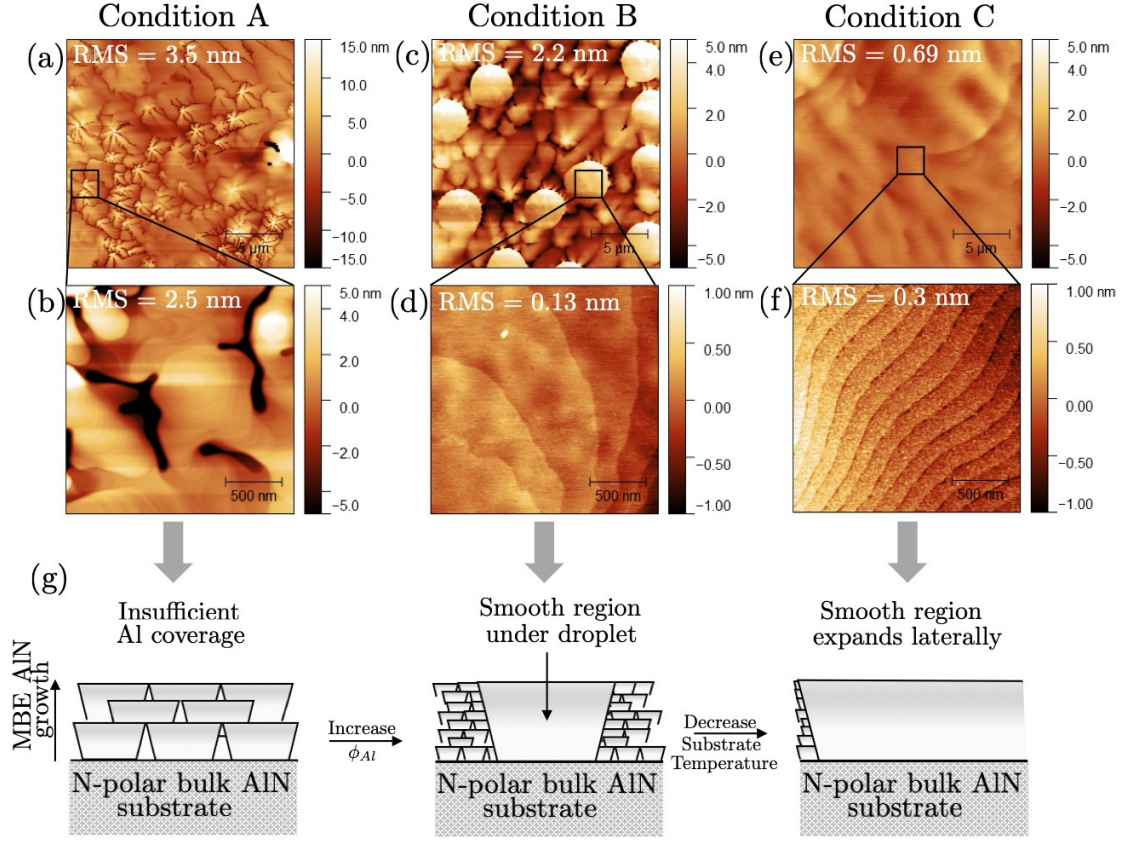


Figure 4.7: AFM micrographs of AlN grown on N-polar AlN bulk substrates under various metal-rich growth conditions (see Table 4.1). AFM images in (a), (c) and (e) show $20 \times 20 \mu\text{m}^2$ area scans and (b), (d) and (f) show $2 \times 2 \mu\text{m}^2$ area scans of 500 nm AlN grown under conditions **A**, **B** and **C** respectively. (g) Schematic of MBE growth of N-polar AlN under various growth conditions.

can be controlled by the ϕ_{Al} impinging on the surface, as well as by controlling the Al droplet desorption rate, which is a function of the substrate temperature. Condition **A** in Table 4.1 should lead to the lowest droplet accumulation because it is at the highest investigated substrate temperature of 1055°C and the lowest impinging Al/N ratio. Due to the insufficient Al coverage, a large number of pits were observed in the surface morphology of this sample, as well as spiral hillocks [Figs. 4.7(a) and 4.7(b)]. The sample grown in condition **B** at the same substrate temperature of 1055°C as condition

A, but at a ϕ_{Al} that is almost 1.5 times higher than that of condition **A**, reveals two distinct regions in the surface morphology. Smooth circular areas with clear atomic steps, and rough regions characterized by surface pits and spiral hillocks [Figs. 4.7(c) and 4.7(d)] are observed. The size and shape of the smooth regions indicate that it is possible that the diffusion of the adatoms is improved under the Al droplets, resulting in smooth morphology, indicating that the regions of AlN growth under Al droplets show two-dimensional (2D) growth mode. The spiral hillocks observed in conditions **A** and **B** could be formed due to threading dislocations induced by a relatively high density of surface impurities on the AlN substrate, (Fig. 4.10) which can make the formation of Al adlayer unstable, resulting in lower diffusion length of the adatoms. Similar defects have been observed for AlN grown on Al-polar AlN without proper deoxidation [37]. It is also possible that in growth conditions **A** and **B** where Al accumulation is not sufficient enough for step-flow growth mode, it is energetically favorable to form hillocks. In these conditions, the surface energy of the semi-polar facets would be lower than that of the N-polar surface, resulting in the formation of such hillocks. While keeping the ϕ_{Al} same as in condition **B**, the substrate temperature is reduced to 1000° C in condition **C** to reduce the Al desorption rate and to increase Al accumulation. It is observed that this sample shows a smooth surface with clear atomic steps over a large surface area [Figs. 4.7(e) and 4.7(f)]. The density of the smooth circular regions that were observed in condition **B** increased under condition **C** because of larger Al accumulation. The smooth regions coalesced to enable smooth homoepitaxial growth with clean and wide atomic terraces on the surface and rms roughness < 0.7 nm over a $20\ \mu\text{m} \times 20\ \mu\text{m}$ area. This observation is in sharp contrast with the MBE growth of typical group III-nitrides for which the presence/absence of the metallic droplets do not influence the growth modes as long as a complete metallic adlayer is formed on the surface [99, 101, 100]. For the samples in this study, therefore, it is likely that a relatively high density of surface

impurities, which presumably segregate from the substrate surface, hinder the formation of Al adlayer thus requiring Al droplets for smooth surface morphology. A similar effect has been reported in MBE-grown Mg-doped GaN where Mg affects the growth kinetics by making Ga-adlayer unstable [133].

Based on the surface morphologies observed, Fig. 4.7(g) schematically shows the probable epitaxial evolution of the MBE growth of N-polar AlN under each of the conditions. Further transmission electron microscopy studies would help to understand the nucleation interface as well as the various growth modes better. Thus, the growth at substrate temperature of $\sim 1000^\circ \text{C}$, with $\phi_{\text{Al}} \sim 19.6 \text{ nm/min}$, $\phi_{\text{N}} \sim 6.9 \text{ nm/min}$ and $\phi_{\text{Al}}/\phi_{\text{N}} \sim 2.84$ on the cleaned N-polar AlN surface is found to lead to smooth homoepitaxy.

Next, we confirm that the epitaxial layers retain the N-polarity of the underlying single-crystal AlN substrate. Wet chemical etching by KOH was used to determine the lattice polarity and its spatial homogeneity in the as grown AlN epitaxial layers. KOH etching is sensitive to the polarity of (Al,Ga)N. The etching rate and morphological features post etching depend strongly on the chemical nature of the surface [113, 62, 61]. The N-polar surface reacts and etches in KOH, leaving hexagonal pyramids bounded by more chemically stable $\{1\bar{1}0\bar{1}\}$ crystallographic planes. The metal polar surface remains fairly inert to KOH and only shows defect-selective etch behavior with hexagonal pits generated around dislocations after etching [120]. Fig. 4.8 shows 45° tilted aerial scanning electron microscopy (SEM) scans of a 500 nm epitaxial layer grown under condition C on bulk N-polar AlN, after etching in 50 wt% KOH aqueous solution at 80°C for 10 seconds. The surface is vigorously etched and the etch is nearly uniform in most regions, as seen in Fig.4.8 (a). It forms hexagonal pyramids of heights ranging from 400-600 nm as seen in Fig.4.8 (c). This indicates that nearly the entire epitaxial

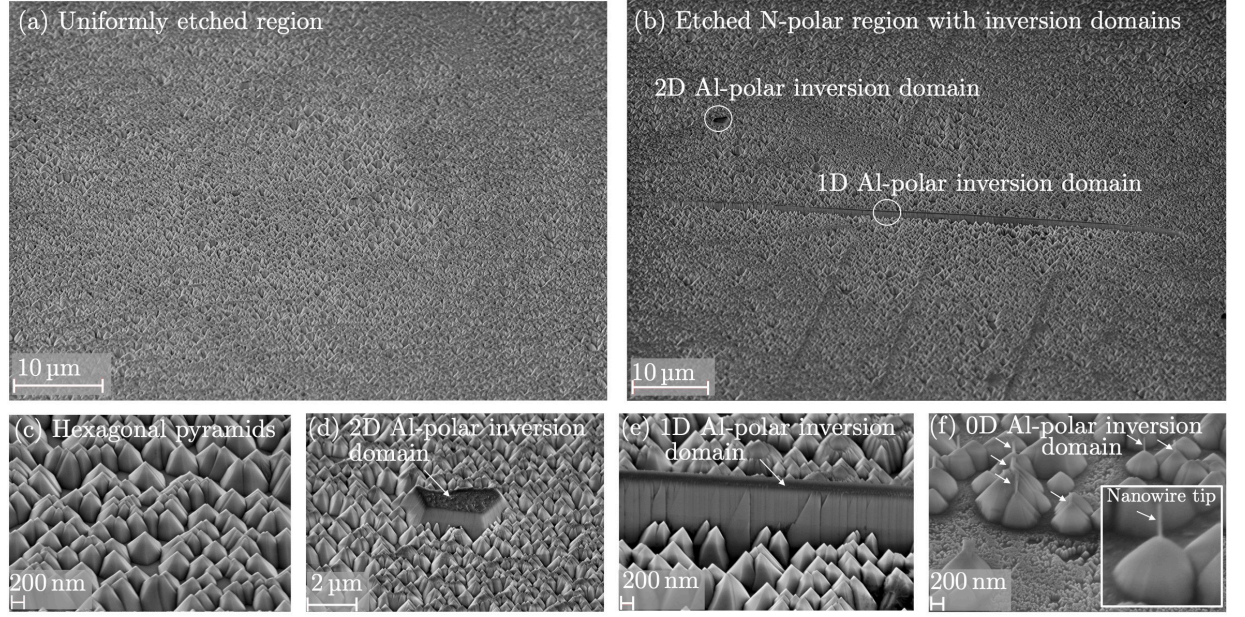


Figure 4.8: Tilted aerial SEM images of (a) uniformly etched N-polar AlN in KOH, (b) etched region with inversion domains, (c) hexagonal pyramids in the uniformly etched region, (d) 2D Al-polar inversion domain, (e) 1D Al-polar inversion domain and (f) 0D Al-polar inversion domain. Inset of (f) shows a zoomed-in image of an inversion nanowire tip.

film maintained the N-polarity of the substrate.

The etching process also revealed a low density of inversion domains as seen in Fig.4.8 (b) which are regions that were not etched by KOH. Three types of inversion domains were identified in the sample. They are classified on the basis of their shape and size, as 2D, 1D, and 0D Al-polar inversion domains as shown in Figs.4.8 (d)- 4.8(f). It is difficult to estimate the density of 2D and 1D Al-polar inversion domains as they are quite sporadic and sparsely spaced in the field of view of the SEM but their combined density is $\sim 1 \times 10^4/\text{cm}^2$. 0D Al-polar inversion domains are less common than 2D and 1D ones but wherever they are revealed after etching, they appear in clusters as seen in Fig.4.8 (f).

In spite of the scarce occurrence of these inversion domains, their properties and possible origins are briefly discussed. They are believed to have formed right at the nucleation stage of AlN on the substrate. They propagate through the entire thickness of the epitaxial film during growth, growing in the Al-polar orientation as opposed to the N-polarity of the majority of the film. The formation of these inversion domains is linked to improper substrate surface preparation before epitaxy. A 2D Al-polar inversion domain as shown in Fig.4.8 (d), has a plateau like feature, approximately 1-2 μm in lateral dimensions and a height of approximately 500 nm (the thickness of the epi-layer). 1D Al-polar inversion domains as seen in Fig.4.8 (e) are several tens of microns long wall-like features. They most likely are the remains of scratches after the CMP process (Fig. 4.3) of the as-received substrates. Fig.4.8 (f) shows 0D Al-polar inversion domains indicated by arrows which are Al-polar nanowire tips protruding from the apex of hexagonal N-polar pyramids. They are similar to the ones reported in previous works on N-polar AlN films on sapphire [78, 73]. Jasinski *et al.* [78] attributed the occurrence of such inversion domains in MOCVD N-polar AlN films grown on sapphire substrates to tiny Al-polar inversion domains nucleating at the substrate, and growing faster than the surrounding N-polar matrix that they are embedded in. It is likely that surface impurities such as oxygen, and particulate residues from CMP on the substrate surface (Fig. 4.3) contribute to the polarity inversion by acting as nucleating sites for 2D and 0D inversion domains. It has been demonstrated that oxygen plays a critical role in switching N-to-Al-polarity in AlN grown on sapphire, where the formation of aluminum-oxynitride ($\text{Al}_x\text{O}_y\text{N}_z$) acts as the inversion domain boundary [181, 182]. Even though the density of inversion domains present in our film is quite low, their presence can have negative impact on the electronic and photonic properties of devices made on the N-polar AlN platform. Therefore, continuous improvements in substrate preparation, cleaning and growth recipes are necessary to suppress their formation.

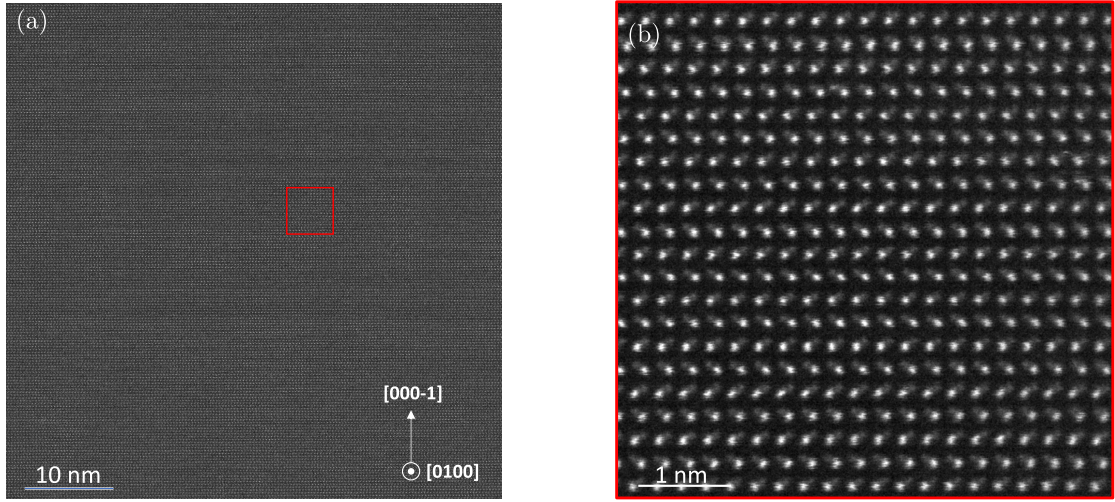


Figure 4.9: Cross-sectional STEM images of MBE-grown N-polar AlN film on bulk AlN substrates. (a) HAADF-STEM image showing the overview of the AlN/AlN interface around 1 μm deep from the surface. No boundary visible between the substrate and epitaxial AlN layer, confirming ideal homoepitaxy. The red square in (a) marks the region where the corresponding magnified image (b) is taken. N-polarity of the homoepitaxial film is confirmed from the arrangement of Al and N atoms in (b). STEM images courtesy Naomi Pieczulewski and Dr. David A. Muller.

Next, scanning transmission electron microscopy (STEM) measurements were performed to study the atomic structure and directly probe the polarity of a 1 μm -thick AlN film grown in the optimized condition **C**. The growth interface is examined at a depth of around 1 μm from the surface. Figure 4.9(a) shows the high-angle annular dark field STEM (HAADF-STEM) images of the homoepitaxial film near the substrate-film interface and no distinguishable boundary is observed. The atomic resolution image of the MBE-grown AlN epilayer in Figure 4.9(b) shows a very well-ordered N-polar AlN crystal structure in the epilayer, with no visible defects.

A sample with 500 nm of N-polar AlN grown in conditions similar to condition **C** (See Table 4.1) was investigated by SIMS. Figure 4.10 shows that the Si and H im-

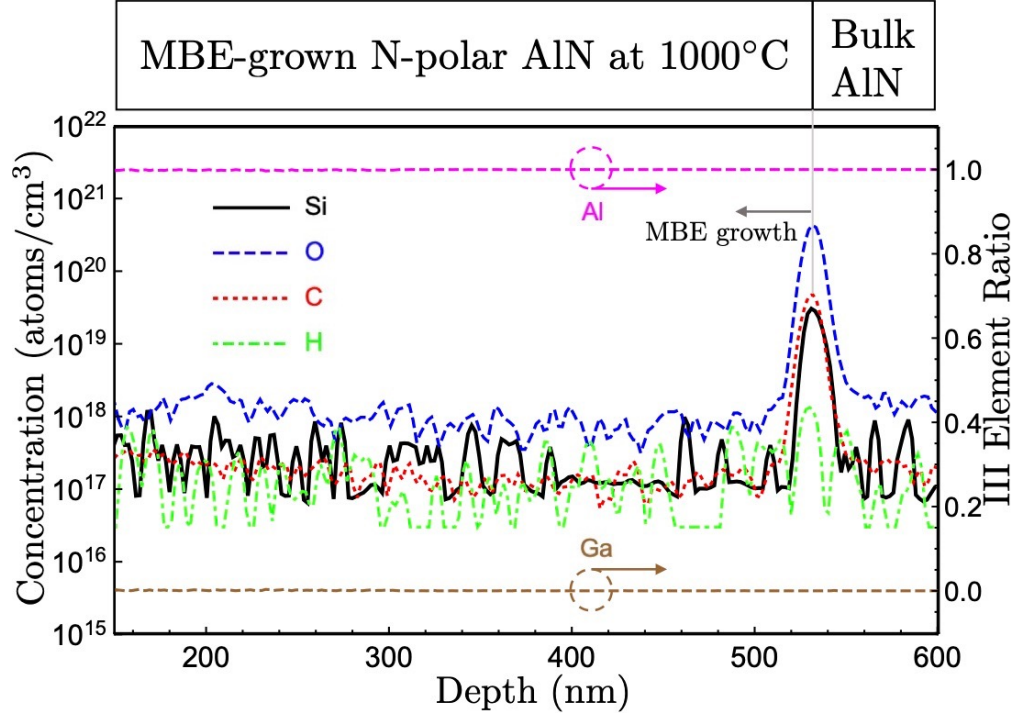


Figure 4.10: Secondary ion mass spectrometry profile of silicon, oxygen, hydrogen, and carbon in the N-polar AlN epitaxial films grown by PA-MBE. The peak concentrations for O, C and Si are $\sim 4.5 \times 10^{20}$ atoms/cm³, $\sim 4.8 \times 10^{19}$ atoms/cm³ and $\sim 3.2 \times 10^{19}$ atoms/cm³ respectively. The III element ratio is specified on the right axis. The Ga content is less than 1% throughout the film, suggesting that there is no Ga contamination in the AlN.

purities are near, or below the detection limit throughout the 500 nm epitaxial layer away from the nucleation interface. O and C impurities show higher concentrations of $\sim 8 \times 10^{17}$ atoms/cm³ and $\sim 2 \times 10^{17}$ atoms/cm³ respectively (the detection limits are 2×10^{17} atoms/cm³ for Si and O, $1-2 \times 10^{17}$ atoms/cm³ for H, and $6-7 \times 10^{16}$ atoms/cm³ for C). Previously reported values for O and C impurity incorporation levels for epitaxial Al-polar AlN films were about $1-2 \times 10^{17}$ atoms/cm³ and $4-5 \times 10^{16}$ atoms/cm³ respectively, grown on the Al-face of single crystal AlN from the same substrate provider [109]. Similar observations of higher O and C impurity incorporation in N-polar nitride films compared to metal-polar ones have been reported for both MOCVD AlN on sap-

phire [189], and also for MOCVD GaN [184] previously. Previous experimental and theoretical studies have indicated that oxygen atoms favorably adsorb on N-polar GaN and AlN surfaces than on metal-polar ones because the adsorption energy at high oxygen coverage is significantly lower for the N-polar surfaces compared to their metal-polar counterpart [225, 190, 213, 126]. Carbon impurities in the epitaxial N-polar nitride films cause the generation of surface pits in films grown on N-polar GaN substrate [207].

It is evident from Figure 4.10 that there is a buildup of impurities at the growth interface. In addition to the residual impurities left over from polishing and processing performed before epitaxy, impurities may also accumulate on the surface during exposure to atmosphere. Peaks for O, C and Si were observed at the nucleation interface with concentrations of $\sim 4.5 \times 10^{20}$ atoms/cm³, $\sim 4.8 \times 10^{19}$ atoms/cm³ and $\sim 3.2 \times 10^{19}$ atoms/cm³ respectively. It was observed that thermal annealing of Al-polar AlN single crystal substrate prior to homoepitaxy at $\sim 1450^\circ\text{C}$ can nearly remove all carbon from the substrate surface [37]. Thus, such high temperature annealing can be possibly employed to suppress C incorporation in N-polar AlN in future.

In conclusion, these results indicate that *in situ* thermal deoxidation and Al-assisted cleaning enables the smooth epitaxial growth of N-polar AlN on single crystal AlN substrates. It is shown that the surface morphology of homoepitaxial N-polar AlN is sensitive to the amount of Al droplet accumulation during the metal-rich MBE growth. Excess Al enhances the adatom surface migration process, leading to a 2D growth mode over a large area, while exhibiting parallel smooth atomic steps. These findings will enable the epitaxial growth of heterostructures for future electronic and photonic device applications based on the single-crystal N-polar AlN platform.

CHAPTER 5

POLARIZATION-INDUCED ELECTRON GASES ON N-POLAR ALN PLATFORM

5.1 Introduction

In the last chapter, we discussed the high-quality homoepitaxy of N-polar AlN on bulk AlN substrates. High quality in this case is quantified by low dislocation density and a smooth surface both on the micro and the macro scale. The lack of device-quality epitaxial layers has previously prevented the demonstration of N-polar AlN-based devices. Although low dislocation densities have been achieved in N-polar layers in the past, surface roughness has been a serious obstacle. There are two effects, hexagonal hillocks and step-bunching, which cause macro-scale roughening of an N-polar surface, thus rendering the material unusable for devices [216, 91]. Thus, enabled by the Al-assisted cleaning process described in the previous chapter, the homoepitaxy of N-polar AlN can now serve as the foundation for a plethora of heterostructures that can host electron gases as indicated in Figure 5.1.

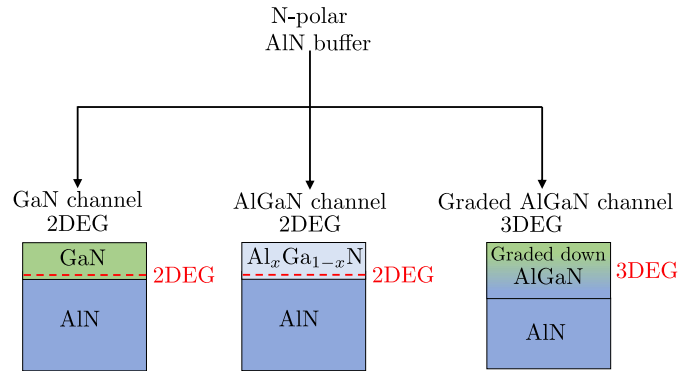


Figure 5.1: Various heterostructure realizations to obtain electron gases on the N-polar AlN platform.

In this chapter, we present structures ranging from the undoped N-polar GaN/AlN 2DEGs, N-polar AlGaN/AlN 2DEGs, and N-polar graded AlGaN/AlN 3DEGs.

5.2 The Undoped N-polar GaN/AlN 2DEGs

5.2.1 Epitaxial growth and characterization

N-polar GaN/AlN is the simplest structure for generating a 2DEG and is the n-type analog of the metal-polar GaN/AlN 2D hole gas. If a thin layer of N-polar GaN is grown on a relaxed AlN substrate, the net interface polarization difference, $[(P_{sp}^{GaN} + P_{pz}^{GaN}) - P_{sp}^{AlN}] \cdot \hat{n} = \sigma_\pi$ is positive in sign and should induce electrons. A mobile 2D electron gas of sheet density roughly equal to the fixed interface polarization charge $\sigma_\pi \sim 5 \times 10^{13}/\text{cm}^2$ is expected to form at the heterojunction, depending on the thickness of the GaN layer. Figures 5.2(a) and (b) show the simulated energy band diagrams and electron densities at the GaN/AlN interface using a self-consistent 1D Schrodinger–Poisson solver, assuming a surface barrier height of ~ 0.3 eV for N-polar GaN [76, 49].

In this section, we report the observation of polarization-induced 2DEGs in undoped pseudomorphic N-polar GaN/AlN heterostructures on free-standing N-polar AlN substrates. We use plasma-assisted molecular beam epitaxy for the study of the 2DEGs in this work, though the results are thought to be achievable by other growth techniques. Prior to the growth of epi-layers, *in situ* Al-assisted surface cleaning, similar to that outlined in the previous chapter was first performed in the MBE growth chamber to remove native oxides and other chemical impurities from the substrate, which would otherwise lead to polarity inversion and defect generation during epitaxy, from the highly reactive N-polar AlN surfaces. This Al-assisted surface cleaning has been found to be critical

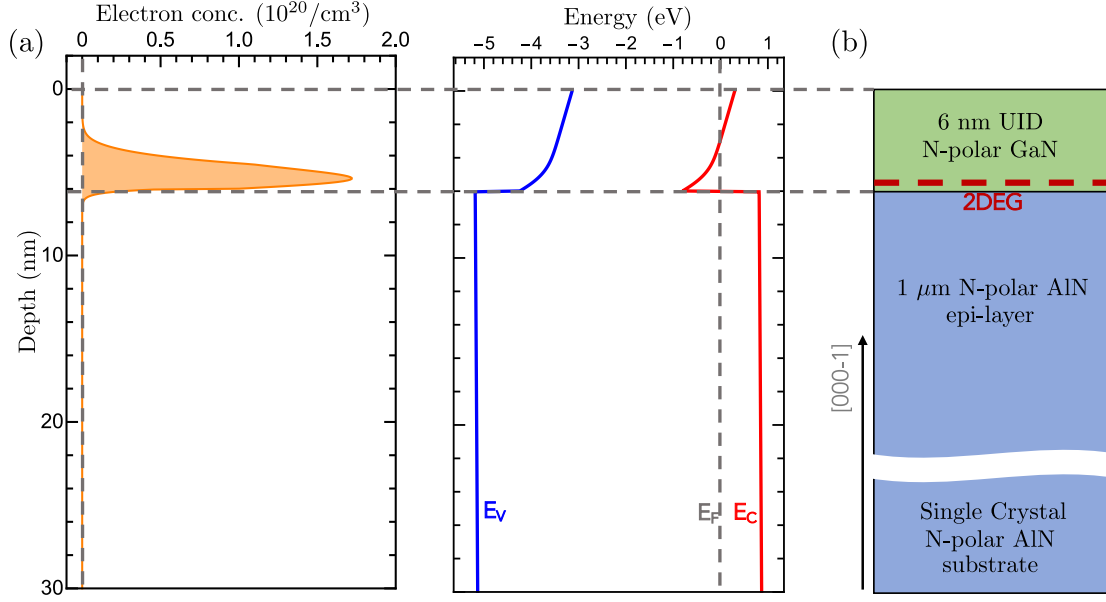


Figure 5.2: (a) The 2DEG carrier profile and (b) energy band diagram of the N-polar GaN on AlN for the (c) layer structure with 6 nm GaN on 1 μm AlN on N-polar AlN bulk substrate.

for the MBE-grown epilayer to inherit and maintain the N-polarity of the substrate and not flip to metal polarity.

After the Al-assisted cleaning, the homoepitaxial growth of 1 μm thick N-polar AlN was performed on the N-face of single crystal AlN substrates at a substrate temperature of $\sim 1000^\circ\text{C}$, after which the substrate temperature was lowered to $\sim 780^\circ\text{C}$ for the growth of ~ 6 nm GaN channel layer in metal-rich conditions. A schematic of the epitaxial structure is shown in Fig. 5.2(c).

RHEED reconstruction of GaN surfaces provides a direct determination of crystal polarity. Specifically, with Ga coverage and at low temperatures (below 300°C), metal-polar GaN surfaces show “ 1×1 ” reconstruction, whereas 3×3 , 6×6 , and $c(6 \times 12)$ reconstructions have been reported for N-polar GaN surfaces [177, 178]. At the end of the GaN growth, the sample was rapidly cooled down to observe GaN surface RHEED

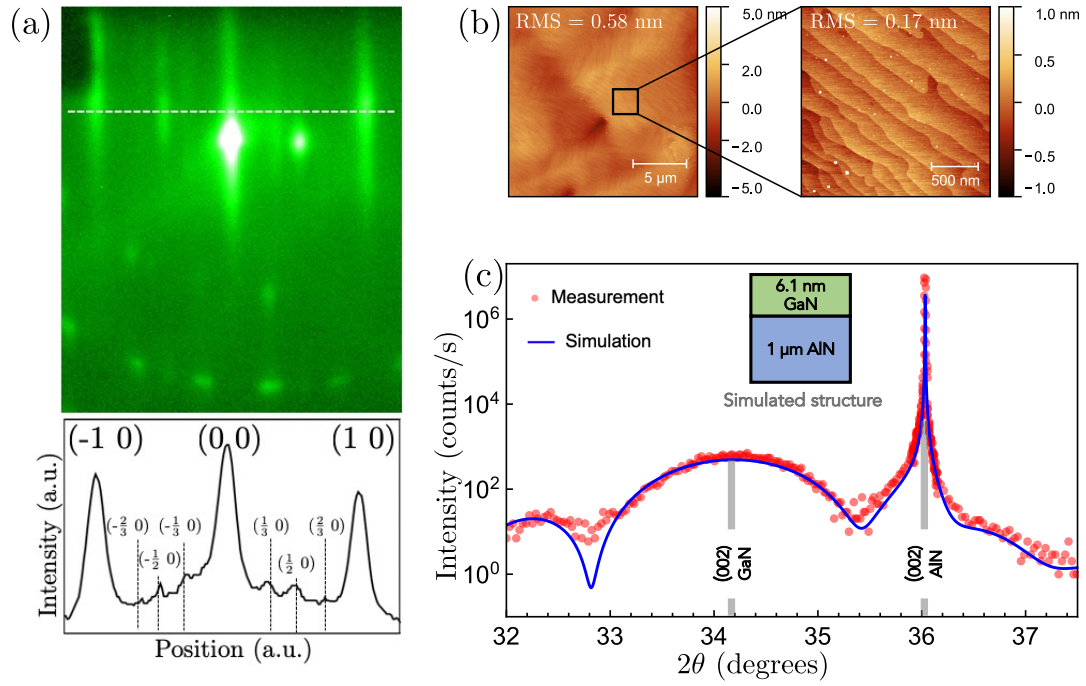


Figure 5.3: (a) $c(6 \times 12)$ RHEED reconstruction pattern observed from the top GaN surface at a substrate temperature of $350\ ^\circ\text{C}$ and below post-growth. The line-cut intensity profile across the RHEED pattern is also shown. (b) AFM scans of the as-grown surface showing smooth parallel atomic steps. The RMS roughnesses are $\sim 0.58\ \text{nm}$ and $\sim 0.17\ \text{nm}$ for the $20\ \mu\text{m}^2$ and $2\ \mu\text{m}^2$ scans, respectively. (c) XRD 2θ scan across the symmetric (002) reflection and the simulated data, confirming the targeted thickness and sharp interfaces.

reconstruction which revealed clear $c(6 \times 12)$ reconstruction at around a temperature of $350\ ^\circ\text{C}$ and below as shown in Figure 5.3 (a) which is indicative of a N-polar GaN film.

The as-grown surface has a smooth surface morphology with a root mean square (rms) roughness of $0.58\ \text{nm}$ over a $20\ \mu\text{m} \times 20\ \mu\text{m}$ area as seen in Figure 5.3(a). The surface exhibits parallel atomic steps and no spiral hillocks or surface pits are observed signifying the high structural quality of epi-layers with low density of dislocations. Figure 5.3(b) shows the measured X-ray diffraction scan of the sample, along with the simulated diffraction pattern based on the layer structure shown in the inset of the fig-

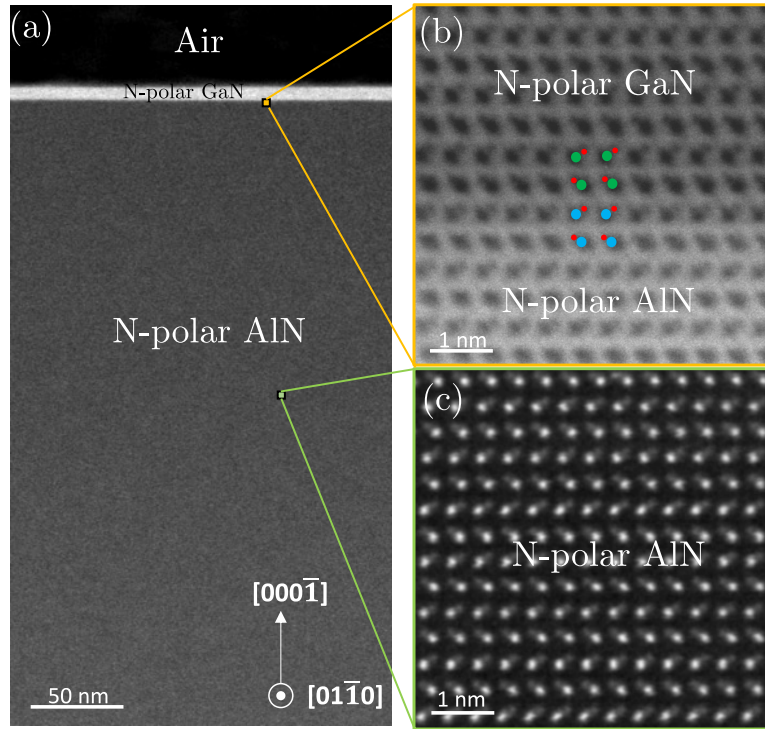


Figure 5.4: (a) HAADF-STEM image showing an overview of N-polar GaN/AlN interface. (b) Annular Bright Field (ABF-STEM) image of the GaN/AlN interface where the N-polarity can be determined by the overlaid crystal structure. Ga, Al, and N correspond to green, blue, and red atoms, respectively. (c) HAADF-STEM image of AlN buffer layer, showing its N-polarity. STEM images courtesy Naomi Pieczulewski and Dr. David A. Muller.

ure. A good agreement between the measured and simulated result is observed, and the clearly visible interference fringes suggest an abrupt heterointerface.

HAADF-STEM images of the same 6 nm GaN film on AlN (Fig. 5.4(a)) show that the GaN layer is uniform in thickness and that the GaN/AlN interface is atomically sharp. The wide-area image also confirms that the coherently sharp interface between the GaN and AlN (~ 1 -2 ML) is maintained over large areas of the wafer, which is essential for a high mobility and high uniformity of the polarization-induced 2D electron gas over the entire wafer. Fig. 5.4(b) shows a zoomed-in lattice image of the crystal

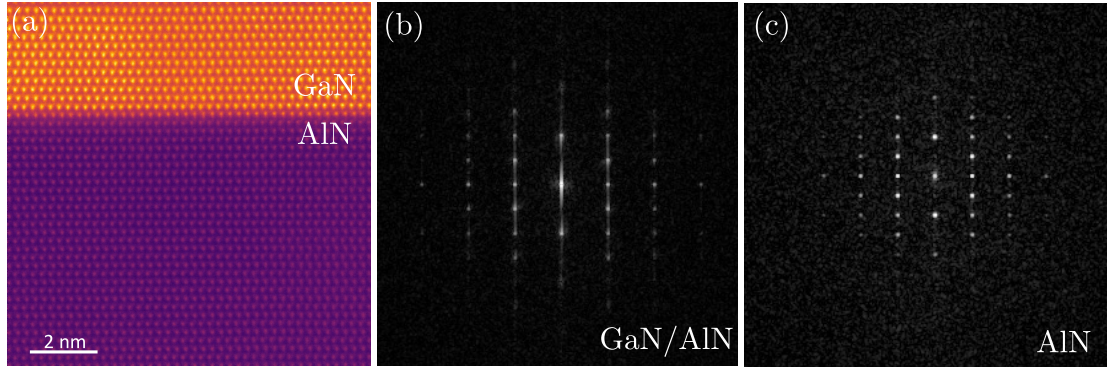


Figure 5.5: (a) False colored HAADF-STEM image showing N-polar GaN/AlN interface. (b) Fast Fourier Transform (FFT) of the entire image (a). (c) FFT of only the AlN region of the image (a). Multiple diffraction peaks are not observed in the GaN/AlN interface. STEM images courtesy Naomi Pieczulewski and Dr. David A. Muller.

heterointerface which shows that the GaN layer is coherently strained to the AlN layer. The atomic resolution image further confirms that the structure is indeed N-polar. Fig. 5.4(c) shows the N-polarity of the AlN buffer layer. Figs. 5.5(b) and (c) show fast Fourier transforms of regions from the GaN/AlN interface as well as just the AlN buffer layer of Figure 5.5(a) respectively. The absence of extra diffraction peaks in Figure 5.5(b) compared to Figure 5.5(c) shows that the GaN layer is completely strained to the underlying AlN.

Temperature-dependent photoluminescence measurements in Fig. 5.6 show that the interband emission peak from the GaN channel red-shifts as the temperature is increased. The bandgap of the compressively strained GaN channel shifts from 344 nm (3.60 eV) at 77 K to 346 nm (3.58 eV) at 295 K signifying the expected bandgap shrinkage for band-to-band transition. Blue shift in the bandgap of the GaN channel compared to bulk GaN is potentially due to compressive strain and quantization effects. Notably, a clear emission peak from the underlying AlN epi-layer is observed at ~ 206 nm (6 eV) at low temperatures. Figures 5.3, 5.4, 5.5 and 5.6 thus collectively show that the

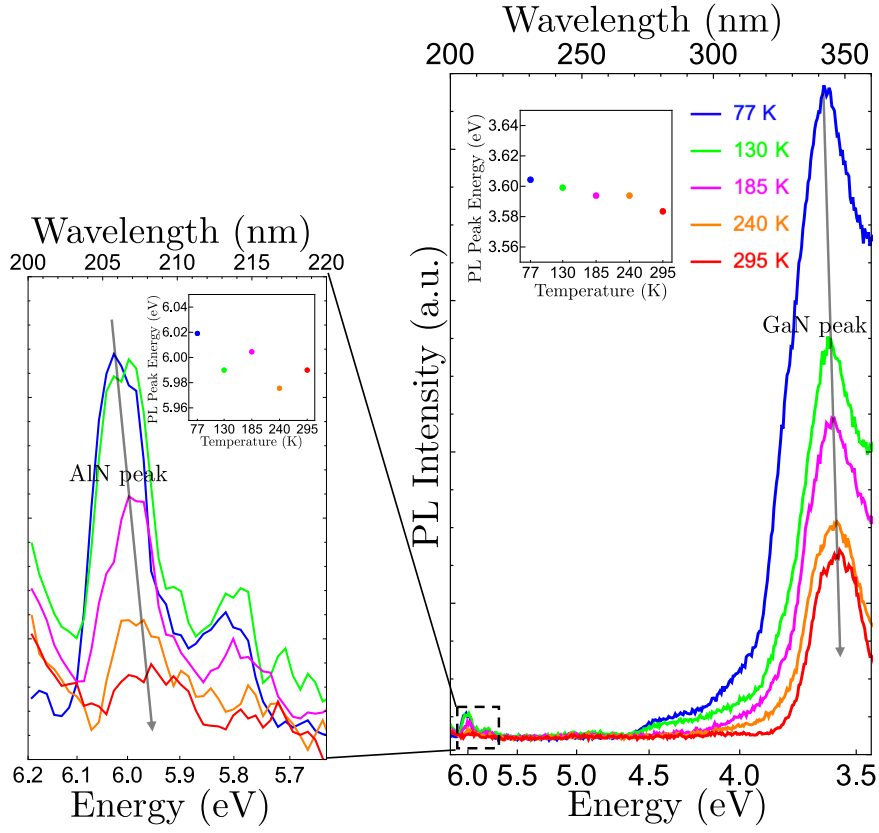


Figure 5.6: Temperature-dependent photoluminescence spectra of the as-grown N-polar GaN/AlN heterostructure using 193 nm laser excitation.

heterostructure is structurally and chemically in a form that should exhibit the undoped polarization-induced 2D electron gas, and the transport studies discussed next indicate indeed this is the case.

The temperature-dependent Hall-effect transport properties measured from 10 to 300 K are shown in Figs. 5.7(a) and 5.7(b) for two samples with GaN channel thicknesses of 6.1 nm and 7.1 nm respectively. Electron densities in both the samples do not show any significant variation as a function of temperature with the 6.1 nm and 7.1 nm GaN channels having carrier densities of $4 \times 10^{13}/\text{cm}^2$ and $5 \times 10^{13}/\text{cm}^2$ respectively as expected from the simulation in Fig. 5.2(a). This confirms the polarization-induced nature of the 2DEGs in this study. The Hall-effect mobilities in the N-polar GaN channels

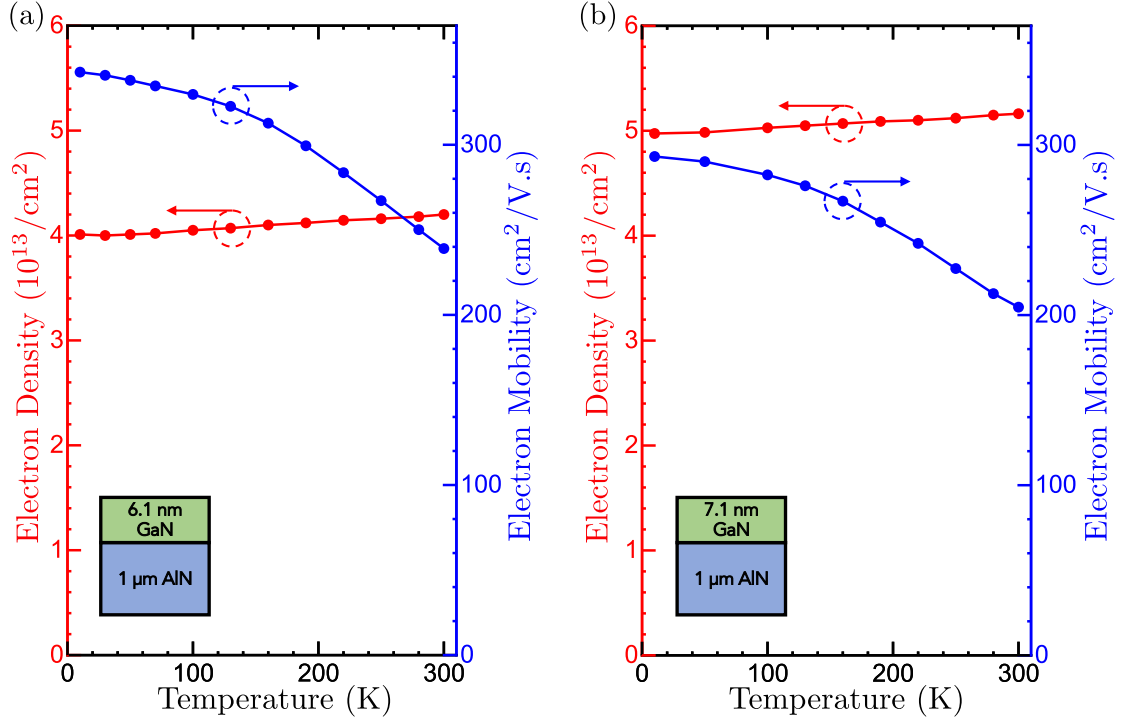


Figure 5.7: Temperature-dependent measured electron densities (red circles) and electron mobilities (blue circles) for two samples with varying GaN channel thicknesses of (a) 6.1 nm and (b) 7.1 nm.

show a gradual increase with decreasing temperature owing to the freeze-out of polar optical phonon scattering as the temperature is lowered. In these heterostructures, there simply are no other carriers such as parallel electrons or hole channels that can mask the direct and unambiguous measurement of the properties of the 2D electron gas.

In summary, we report the observation of the unexplored polarization-induced 2DEGs in undoped pseudomorphic N-polar GaN/AlN heterostructures on N-polar single-crystal AlN substrates with smooth surface morphology and sharp hetero-interfaces by plasma-assisted MBE. The presence of high-density polarization-induced 2DEGs, which maintain down to cryogenic temperatures, was confirmed by temperature-dependent Hall-effect measurements on multiple samples with varying

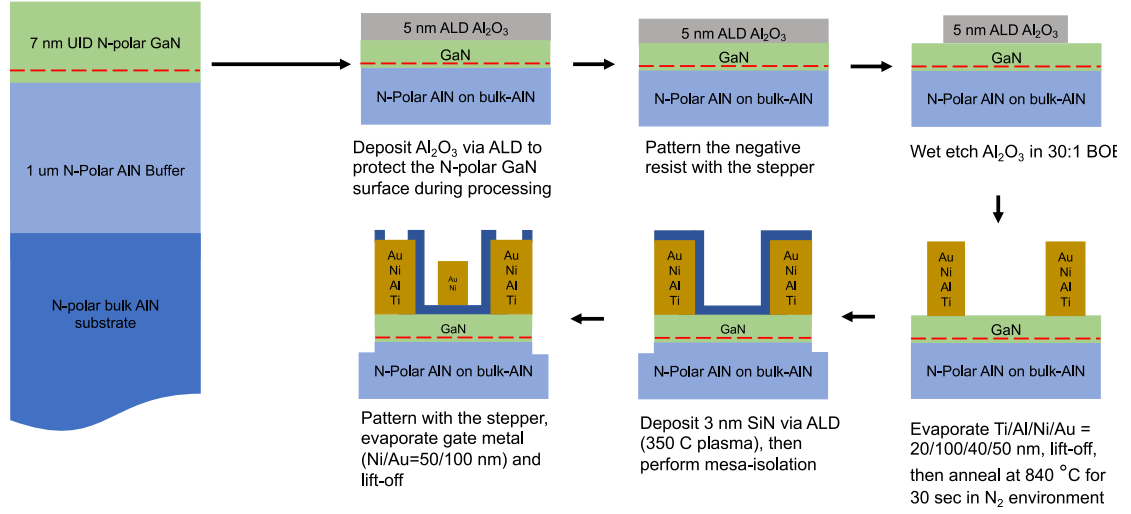


Figure 5.8: Fabrication process flow of N-polar GaN/AlN HEMT

GaN thicknesses.

5.2.2 N-polar GaN/AlN HEMTs: 1st generation

In this section, we introduce the N-polar HEMTs on single-crystal aluminum nitride (AlN) substrates with the GaN/AlN heterostructure. As shown in the previous section, a thin N-polar GaN layer grown over N-polar AlN hosts a 2DEG, and this high electron density 2DEG can then be utilized to fabricate HEMT devices. The epitaxial structure used for the 1st generation of HEMT devices consisted of a 7 nm-thick GaN channel grown over a 1- μm thick AlN buffer layer on bulk AlN substrate similar to the sample shown in 5.7(b).

The fabrication flow as shown in Figure 5.8 began with the deposition of a thin Al_2O_3 layer via atomic layer deposition to protect the reactive N-polar GaN surface during processing. The ohmic contacts were then defined by photolithography, and

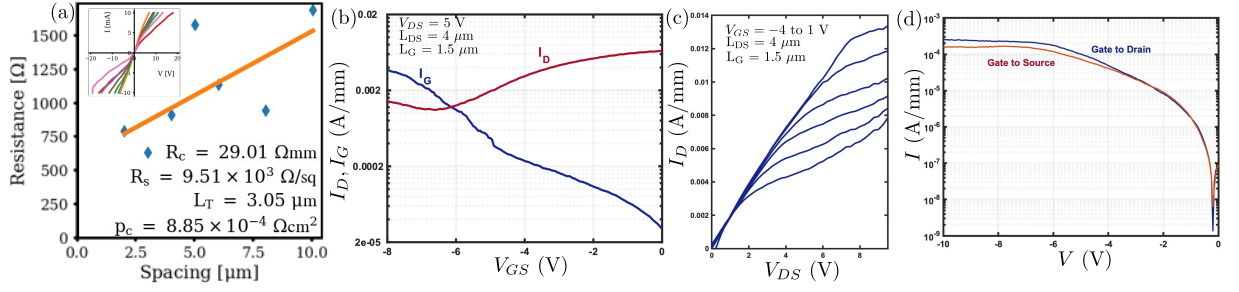


Figure 5.9: DC device characteristics of 1st generation N-polar GaN/AlN HEMT

Ti/Al/Ni/Au metal stack was deposited via electron beam evaporation and annealed at 780 °C for 30 seconds in N₂ environment. The HEMTs were then isolated via chlorine-based ICP dry etch, and a 10-nm silicon nitride gate dielectric layer was deposited via high-density plasma chemical vapor deposition. Finally, the gate contacts (Ni/Au) were defined by photolithography.

Following the device fabrication, contacts contact resistance $R_C = 29 \Omega\cdot\text{mm}$ was measured using transfer-length method (TLM) patterns as shown in Figure 5.9(a). This high contact resistance could possibly be due to the 2DEG being damaged during processing. Figure 5.9(b,c) shows DC characteristics of the fabricated HEMT with a gate length of $L_G = 1.5 \mu\text{m}$, a gate-to-source distance and a source-to-drain distance $L_{DS} = 4 \mu\text{m}$. Transfer I-V characteristics shown in Figure 5.9(b) reveal an on/off ratio of ~ 7 . This on/off ratio is small compared to that of many other reported N-polar HEMTs as well as metal-polar HEMTs and it is limited by high gate leakage current resulting from a non-optimized gate dielectric layer. The devices show a maximum on-current density of $\sim 13 \text{ mA/mm}$ as shown in Figure 5.9(c) which is considerably low, mainly because of the high contact resistance. As expected, fabricated devices exhibited very low leakage current through the AlN buffer layer as shown in Figure 5.9(d).

5.3 The Undoped N-polar $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}$ 2DEGs

This section is adapted from the paper "Polarization-induced 2d electron gases in N-polar AlGaN/AlN heterostructures on single-crystal AlN substrates" with an equal contribution authorship with Zexuan Zhang.

Unlike in metal-polar AlGaN [2, 123, 173, 44, 94], reports on polarization-induced electrons in N-polar AlGaN, however, have been limited [110, 214]. Analogous to the polarization-induced two-dimensional electron gases (2DEGs) observed at metal-polar $\text{Al}_y\text{Ga}_{1-y}\text{N}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ heterointerfaces ($y > x$), [2, 123, 173] the positive polarization charge and conduction band offset at the heterointerface should also generate a 2DEG in a N-polar AlGaN/AlN heterostructure. Such 2DEGs, despite being largely unstudied, can be used as the channels for N-polar AlGaN channel HEMTs on AlN where the absence of top barriers can potentially mitigate the issue of poor electrical contacts faced by their metal-polar counterparts while simultaneously taking advantage of the large breakdown fields of the wide bandgap AlGaN channel and AlN barrier [110, 214].

In addition to the energy bandgap of the channel, the properties of 2DEGs in N-polar AlGaN/AlN heterostructures are also expected to be tunable by varying the Al composition in AlGaN [173]. Besides a significant scientific interest in understanding carrier transport in N-polar AlGaN, a systematic study of the compositional dependence of the structural, electrical, and optical properties of N-polar AlGaN/AlN heterostructures is of technological importance as these properties translate directly to the device performance. Moreover, since structural defects are known to affect the properties of a material and degrade device performance [88, 82, 25, 114], it is desirable to explore how N-polar AlGaN/AlN structures on lattice-matched, structurally-pure single-crystal AlN substrates with dislocation densities $< 10^4/\text{cm}^2$ compare with the commonly-used

foreign substrates such as SiC or sapphire where the large lattice mismatch between AlN and the substrates leads to high density of dislocations ($\sim 10^9/\text{cm}^2$) [220, 110, 214].

In this section, we investigated the formation and properties of polarization-induced 2DEGs in N-polar $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ heterostructures ($x = 0$ to $x = 0.6$) on single-crystal AlN. The thicknesses of the top $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and bottom $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ layers are ~ 8 and 40 nm, respectively. Optical bandgaps of the top AlGa_N layers extracted from photoluminescence (PL) spectra span from 3.56 eV to 4.77 eV. In addition to a charge control from $n_s = 3.8 \times 10^{13}/\text{cm}^2$ at $x = 0$ to $n_s = 7.6 \times 10^{12}/\text{cm}^2$ at $x = 0.49$ and eventually not measurable when $x = 0.6$, a decrease of electron mobility is observed upon increasing Al content x , from $\sim 650 \text{ cm}^2/\text{V}\cdot\text{s}$ ($x = 0$) to $\sim 40 \text{ cm}^2/\text{V}\cdot\text{s}$ ($x = 0.49$) at 300 K, as expected from alloy scattering.

The epitaxial heterostructures shown in Fig. 5.10(a) were grown using plasma-assisted molecular beam epitaxy (MBE) in a Veeco GEN10 system equipped with standard effusion cells for Ga and Al and a radio frequency plasma source for active N species. Two Al cells were used for the growth of abrupt heterojunctions. Free-standing N-polar single-crystal AlN substrates from Asahi-Kasei Corporation were used [221, 218, 219]. Before the growth of epi-layers, 100 cycles of *in-situ* Al-assisted surface cleaning were performed in the MBE growth chamber to remove the native oxides and other chemical impurities from the N-polar AlN substrate surface and to ensure that the overgrown layers by MBE maintain N-polarity and not flip to metal-polarity [220]. Details about the Al-assisted cleaning process can be found in our previous work [219, 220, 174].

After the Al-assisted cleaning, a 500 nm homoepitaxial AlN layer was grown under optimized Al-rich growth condition [219, 174]. The excess Al droplets were *in-situ* desorbed at an elevated temperature of ~ 1200 °C before cooling down the substrate to $\sim$

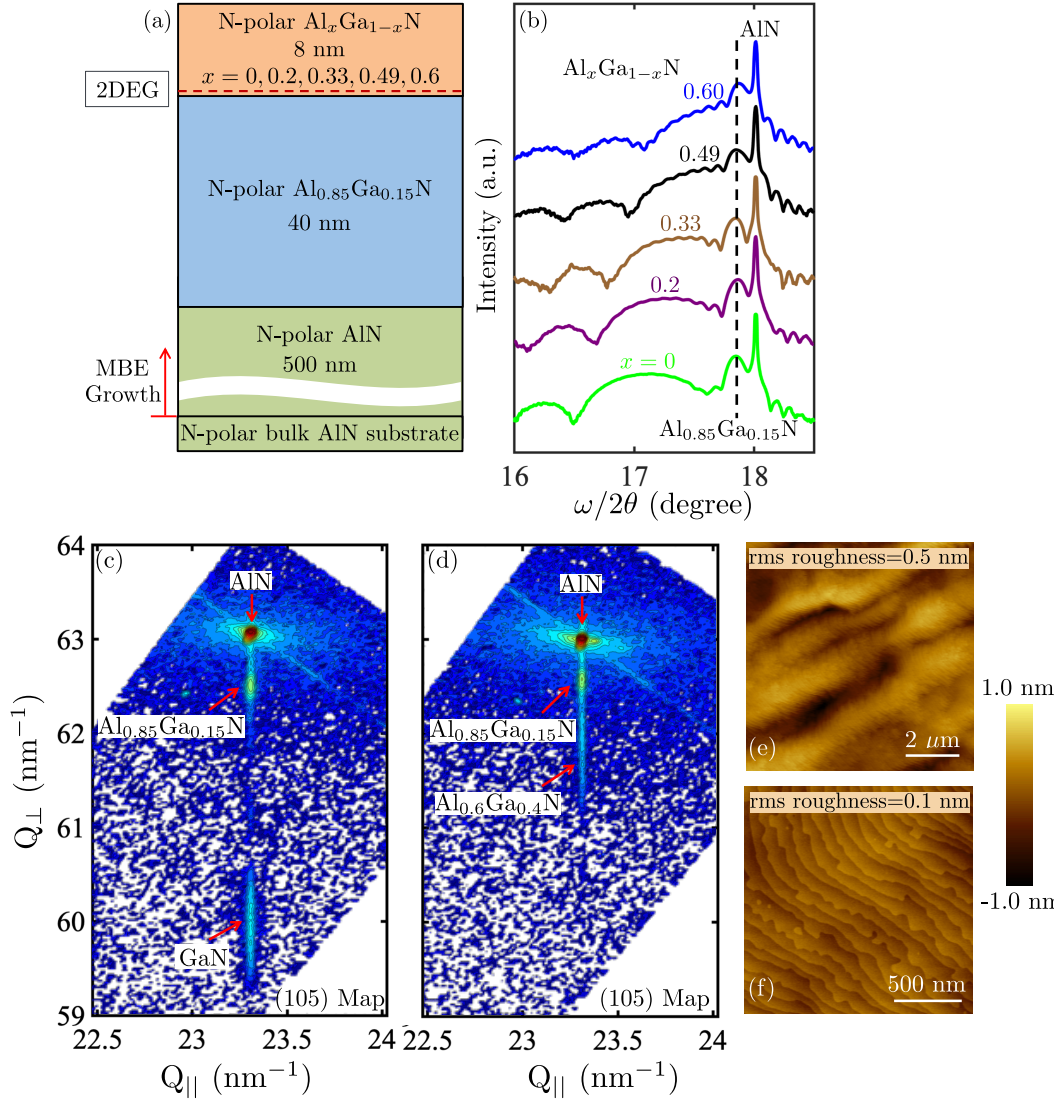


Figure 5.10: (a) Schematic of the epitaxial layer structures in this study. (b) Symmetric $2\theta/\omega$ XRD scans across the (002) diffractions with various Al content. [(c) and (d)] RSMs across the asymmetric (105) diffractions taken from the samples with (c) $x = 0$ and (d) $x = 0.6$. The green, blue, and red circles mark the expected reciprocal lattice points of pseudomorphic GaN, $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ and $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$, respectively. (e) $10 \times 10 \mu\text{m}^2$ and (f) $2 \times 2 \mu\text{m}^2$ AFM micrographs of the as-grown surface with $x = 0.49$, showing smooth surface with parallel atomic steps.

900 °C for the deposition of a 40 nm undoped $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ layer. After that, for the GaN channel sample ($x = 0$), an 8 nm GaN layer was deposited at a lower substrate temperature of ~ 810 °C. A similar growth condition has been used in our previous report [219]. In contrast, for all the AlGaN channel samples ($x > 0$), the 8 nm $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel layers were grown at the same growth temperature as the $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ layers without growth interruption at the heterojunctions. The Al compositions in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers were controlled via Al cell temperature. All the AlGaN (and GaN) layers were grown under metal-rich growth conditions and the substrates were held at the growth temperatures for long enough after growth to *in-situ* desorb excess Ga droplets before cooling down to room temperature.

The purpose of inserting an $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ “impurity blocking” layer between AlN and the top $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers is to boost 2DEG mobility by blocking unwanted impurities such as silicon “floating” on the growth front of the AlN under the Al-rich growth condition from reaching the top heterojunction where the 2DEG is desired [218, 219, 33, 35].

Fig. 5.10(b) shows the symmetric $2\theta/\omega$ XRD scans of the five samples shown in Fig. 5.10(a) measured using a PANalytical Empyrean setup at 45 kV and 40 mA with Cu $K\alpha 1$ radiation ($1.5406 \text{ \AA}$). The observation of clearly resolved thickness fringes indicates abrupt hetero-interfaces. Moreover, good agreement between the measured XRD spectra and the simulations (not shown) based on the layer structures in Fig. 5.10(a) confirm the realization of the targeted structures. Reciprocal space maps (RSMs) around the asymmetric (105) diffraction peaks of GaN, AlGaN and AlN were performed to extract the in-plane lattice constants and quantify the strain of the AlGaN (and GaN) layers. All the AlGaN and GaN layers in this study are found to be fully strained to the underlying AlN. Figs. 5.10(c) and (d) show the representative RSM scans from the samples with

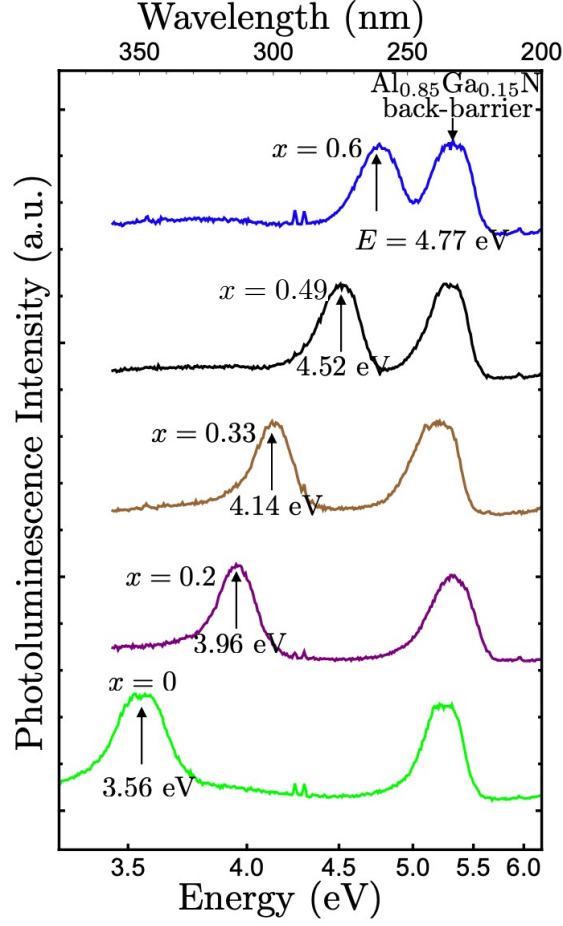


Figure 5.11: Photoluminescence spectra of N-polar $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ heterostructures with varying Al composition x of the top AlGa N channel layer at $T = 300$ K, showing photon emission from all the samples.

$x = 0$ and $x = 0.6$, respectively. Quantification of strain in the Ga N and AlGa N layers is important for understanding the transport properties since strain affects the piezoelectric polarization and hence the 2DEG density.

The surface morphologies of the samples were examined using atomic force microscopy (AFM) in an Asylum Research Cypher ES setup. Figs. 5.10(e) and (f) show the as-grown surface with $x = 0.49$ as an example. Smooth surface free of spiral hillocks with a low root-mean-square (rms) roughness of 0.5 nm was measured in a $10 \times 10 \mu\text{m}^2$

area [Fig. 5.10(e)]. The zoomed-in $2 \times 2 \mu\text{m}^2$ scan shown in Fig. 5.10(f) reveals parallel atomic steps, suggesting a step-flow growth mode. Similar surface morphologies with sub-nm rms roughness in a $10 \times 10 \mu\text{m}^2$ scan and parallel atomic steps were also observed from the other samples. No clear correlation between the surface roughness and Al composition was observed.

Figure 5.11 shows the 300 K photoluminescence (PL) spectra of the five samples. All the samples were excited by a 193 nm ArF excimer laser from the top. Band-to-band PL emission from the top AlGaIn channel layer is observed for all five samples. The top AlGaIn layer PL peaks at 348 nm (3.56 eV), 312 nm (3.96 eV), 300 nm (4.14 eV), 274 nm (4.52 eV) and 260 nm (4.77 eV) for the GaN, $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$, $\text{Al}_{0.33}\text{Ga}_{0.67}\text{N}$, $\text{Al}_{0.49}\text{Ga}_{0.51}\text{N}$ and $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ channel samples, respectively. The interband transition PL peak blue-shifts when the Al composition x of the channel increases, providing a direct signature of the increasing bandgap of the channel. It is noted that the apparent optical bandgap of the AlGaIn channel measured by PL could differ from the bulk bandgap due to energy quantization, quantum-confined Stark effect (QCSE) and strain. It is interesting to note that photon emission is also observed from the wider bandgap $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ back-barrier at ~ 234 nm (5.3 eV) from all the samples. A detailed analysis of the PL spectra is not attempted here, and is proposed for future work.

Hall-effect measurements were performed on the samples using soldered corner indium contacts to the N-polar AlGaIn channel 2DEGs. The results are summarized in Table 5.1, together with the energy bandgap obtained from PL. All samples, with the exception of the one with an $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ channel, displayed measurable 2DEGs down to cryogenic temperatures as expected due to their polarization-induced origin. Fig. 5.12(a) shows the simulated energy band diagrams using a self-consistent Schrödinger-Poisson solver for the channel Al content $x = 0, 0.33, 0.6$ with a surface barrier height

Table 5.1: Structural details of the N-polar $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ HEMT heterostructures studied in this work, with the corresponding bandgap of the AlGaN channel measured via PL and their 2DEG densities n_s , mobilities μ measured via Hall-effect at 300 and 77 K. Sheet resistance R_s of $> 10^3$ k Ω per sq. indicates resistive samples in which the transport could not be extracted using Hall effect measurements. The surface barrier heights $q\phi_b$ are extracted by fitting the simulation with the measured 2DEG densities.

Channel	Energy bandgap	n_s^{300K}	μ^{300K}	R_s^{300K}	n_s^{77K}	μ^{77K}	R_s^{77K}	$q\phi_b$
Layer	from PL (eV)	($10^{13}/\text{cm}^2$)	($\text{cm}^2/(\text{V.s})$)	(k Ω per sq.)	($10^{13}/\text{cm}^2$)	($\text{cm}^2/(\text{V.s})$)	(k Ω per sq.)	(eV)
GaN	3.56	3.8	653	0.25	3.3	1430	0.13	0.4
$\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$	3.96	3.0	156	1.33	2.8	192	1.16	0.5
$\text{Al}_{0.33}\text{Ga}_{0.67}\text{N}$	4.14	2.0	101	3.09	1.7	105	3.5	1.0
$\text{Al}_{0.49}\text{Ga}_{0.51}\text{N}$	4.52	0.76	43	19.12	0.69	39	23.22	1.7
$\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$	4.77	-	-	$> 10^3$	-	-	$> 10^3$	-

$q\phi_B$ of 0.3 eV, as has been reported for N-polar GaN [219, 76]. As shown in Fig. 5.12(b), high-density 2DEGs are induced at the top $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ interfaces. The secondary channel at the bottom interface has been found to show no measurable conductivity [219]. The reason behind the high resistivity of the secondary channel is still under investigation at this point. One possible explanation is the localization in deep levels. The following discussion will focus only on the 2DEGs at the top heterointerface.

With increasing Al content in the channel, the conduction band edge E_c at the top heterointerface moves up towards the Fermi level [Fig. 5.12(a)] and the 2DEG density decreases [Fig. 5.12(b)]. While the energy band diagram simulation with a fixed surface barrier height of 0.3 eV *qualitatively* explains the diminishing trend of 2DEG density with increasing Al content in the channel, it predicts a high density ($n_s > 1 \times 10^{13}/\text{cm}^2$) 2DEG at $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$, which contrasts the absence of any measurable conductivity in that sample. Meanwhile, it also predicts a 2DEG density of $n_s > 1.7 \times 10^{13}/\text{cm}^2$ for $x = 0.49$, which is more than a factor of 2 overestimate of the measured 2DEG density of $0.76 \times 10^{13}/\text{cm}^2$. This is further illustrated in Fig. 5.13 (a): although the measured 300 K 2DEG density for $x \leq 0.2$ agrees reasonably well with the simulation with $q\phi_B = 0.3$ eV, the measured 2DEG density drops much faster than is predicted for $x \geq 0.33$, which indicates a substantial deviation of fixed surface barrier height $q\phi_B = 0.3$ eV for high Al content AlGaN channel. For example, a surface barrier height of ~ 2 eV is expected for $x = 0.49$ from Fig. 5.13(a). The surface barrier height $q\phi_B$ that matches the simulated 2DEG density at $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ interface with the measured value at 300 K for each sample is listed in the last column of Table. 5.1. The increase of surface barrier height with increasing Al composition has been reported for metal-polar AlGaN using X-ray photoelectron spectroscopy (XPS) technique [156]. It is interesting that a similar trend is also observed for N-polar AlGaN.

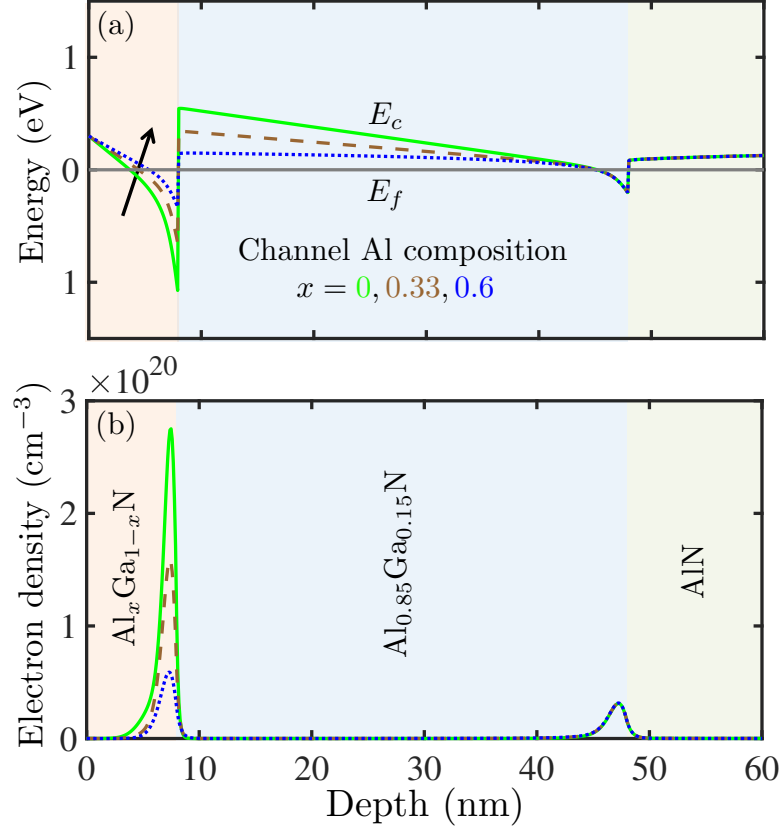


Figure 5.12: (a) Simulated energy band diagrams for three different Al compositions $x = 0$ (green), 0.33 (brown), 0.6 (blue) with a surface barrier height $q\phi_B \sim 0.3$ eV. (b) Simulated electron densities confirm the presence of high-density 2DEGs at $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ interfaces. The secondary channel at the bottom interface does not show measurable conductivity [219].

Figure 5.13(b) shows the measured 77 K (filled symbols) and 300 K (hollow symbols) Hall effect mobilities as a function of Al composition x . The 2DEG mobility degrades monotonically with increasing Al composition x , from $\mu > 1400 \text{ cm}^2/\text{V}\cdot\text{s}$ for $x = 0$ to $\mu < 50 \text{ cm}^2/\text{V}\cdot\text{s}$ for $x = 0.49$ at 77 K. It is apparent that the 77 K mobility shows $> 2\times$ increase compared to its 300 K value for the GaN channel ($x = 0$) as expected due to freeze-out of phonon scattering. A slight increase in low-temperature mobility is also observed for $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ channel compared to its room-temperature value, whereas the change is almost negligible for $\text{Al}_{0.33}\text{Ga}_{0.67}\text{N}$ and $\text{Al}_{0.49}\text{Ga}_{0.51}\text{N}$ 2DEG channels. Both

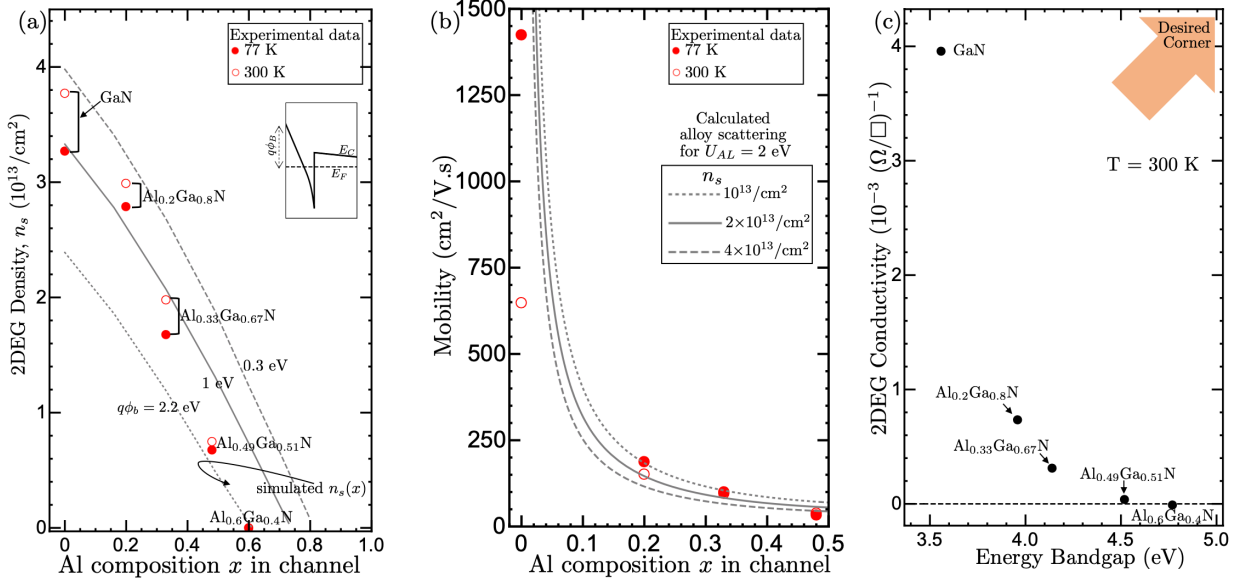


Figure 5.13: (a) Measured 2DEG Hall densities at 77 K (filled circles) and 300 K (hollow circles) as a function of Al composition x in the AlGaN channel layer for different samples. The simulated 2DEG densities (gray lines) are also plotted as a function of Al composition for different surface barrier heights $q\phi_B$ (inset) and show good agreement with the experimental data. (b) 77 K (filled circles) and 300 K (hollow circles) electron mobilities as a function of Al composition x in the AlGaN 2DEG channel. The gray curves show the calculated alloy scattering mobilities for different carrier densities n_s for the same alloy scattering potential $U_{AL} = 2$ eV which confirms that the major scattering mechanism in high Al composition AlGaN channel 2DEGs is alloy scattering. (c) Sheet conductivity versus energy bandgap from PL for various Al compositions. High conductivity is desired for high current whereas large energy bandgap is preferred for high breakdown voltage.

the degradation of 2DEG mobility with increasing Al content and the negligible temperature dependence in high Al content AlGaN channels are explained by alloy disorder scattering, which is temperature independent [23]. The alloy scattering limited mobility is known to follow a U-shaped curve as a function of alloy composition x due to the $1/\{x(1-x)\}$ dependence [131]. As a result, within the alloy composition range studied in this work, an increase in Al content x should lead to a decrease in 2DEG mobility.

The lines in Fig. 5.13(b) plot the alloy scattering limited 2DEG mobility as a function of Al content for given 2DEG densities ranging from $1 \times 10^{13}/\text{cm}^2$ to $4 \times 10^{13}/\text{cm}^2$. An alloy scattering potential $U_{AL} = 2$ eV gives a good fit to the experimental data and falls in the typical range of U_{AL} (between 1.3 and 2.2 eV) reported for metal-polar AlGaIn [85, 172, 146, 173]. Indeed, a good agreement between the calculation and measurement is observed, especially for high Al composition ($x > 0.3$). The nearly temperature-independent 2DEG mobilities in high Al content AlGaIn channels are attractive for applications that require stable operation at high and variable temperatures.

As mentioned earlier, the N-polar AlGaIn/AlN 2DEGs observed here can be the enablers for N-polar AlGaIn channel HEMTs on AlN. These devices are expected to bring compelling advantages over their GaN channel counterparts, which have been demonstrated recently with promising DC and RF characteristics such as an on-current of 2.6 A/mm and a maximum oscillation frequency (f_{max}) of 100 GHz [96, 97]. In addition, thanks to the absence of top barriers, exploiting AlGaIn channel in an N-polar structure has the potential to overcome the issue with poor electrical contacts, which has remained one of the major challenges faced by metal-polar AlGaIn transistors [123, 89, 2]. For RF HEMTs, sheet conductivity σ and energy bandgap of the channel E_g are key predictors of their performances. This is because a high σ is desired to achieve large on-currents and low access resistances, whereas a large E_g is also desired for a high critical electric field in the 2DEG channel.

To better illustrate the potential of these 2DEGs for RF and power applications, the experimentally measured room temperature Hall sheet conductivity σ as a function of the experimentally measured energy bandgap from PL for the five samples in the present study are plotted in Figure 5.13(c). σ drops rapidly as the E_g of the channel increases. This presents a trade-off between σ and E_g for use in AlGaIn channel HEMTs.

On the other hand, the absence of as-grown 2DEG in $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ heterostructure can be advantageous for applications where normally-off operation is desired such as power switching and energy conversion,[19] although clever strategies such as selective-area ion implantation of Si need to be employed to lower the access resistance in such devices. Therefore, this study provides useful experimental data for heterostructure design and device engineering towards N-polar AlGaN channel HEMTs for next-generation RF and power electronics.

In summary, a systematic study of the structural, optical, and electronic transport properties of N-polar $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ heterostructures with AlGaN channel composition ranging from $x = 0$ to $x = 0.6$, grown using MBE, is reported in this work. Photoluminescence spectra show that the bandgap of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel increases with x , ranging from 3.56 eV to 4.77 eV. Polarization-induced 2DEGs are observed with 2DEG densities varying from $\sim 3.8 \times 10^{13}/\text{cm}^2$ in the GaN channel to no measurable 2DEG in an $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ channel of thickness 8 nm. Temperature-independent alloy scattering is found to be the major scattering mechanism for high Al content ($x > 0.3$) AlGaN channel 2DEGs. These results lay the groundwork for the design of N-polar AlGaN channel HEMTs on AlN for high-frequency, high-power and high-temperature performance.

5.4 The Undoped N-polar graded AlGaN/AlN 3DEGs

In the previous two sections, we discussed sharp heterojunctions on the N-polar AlN buffer platform generating 2DEGs via polarization doping in the GaN and AlGaN channels. Instead of abrupt heterojunctions, we can spread out the fixed polarization charges at the heterointerfaces in a three-dimensional way by gradually increasing or decreasing

the Al composition in AlGaN alloys along the growth direction. The bound charge profiles are determined by the divergence of polarization fields following the relationship $\rho(z) = \nabla \cdot \vec{P}(z) = \partial P / \partial z$, where $\rho(z)$ is the charge density along the growth direction z , and $\vec{P}(z)$ is the total polarization field of the graded AlGaN alloy [83, 155]. This imbalanced background charge attracts free carriers from remote dopant-like states to satisfy charge neutrality giving rise to a 3D carrier gas. Moreover, this type of carrier concentration and profile can easily be modulated by specially designing the grading scheme of AlGaN alloys.

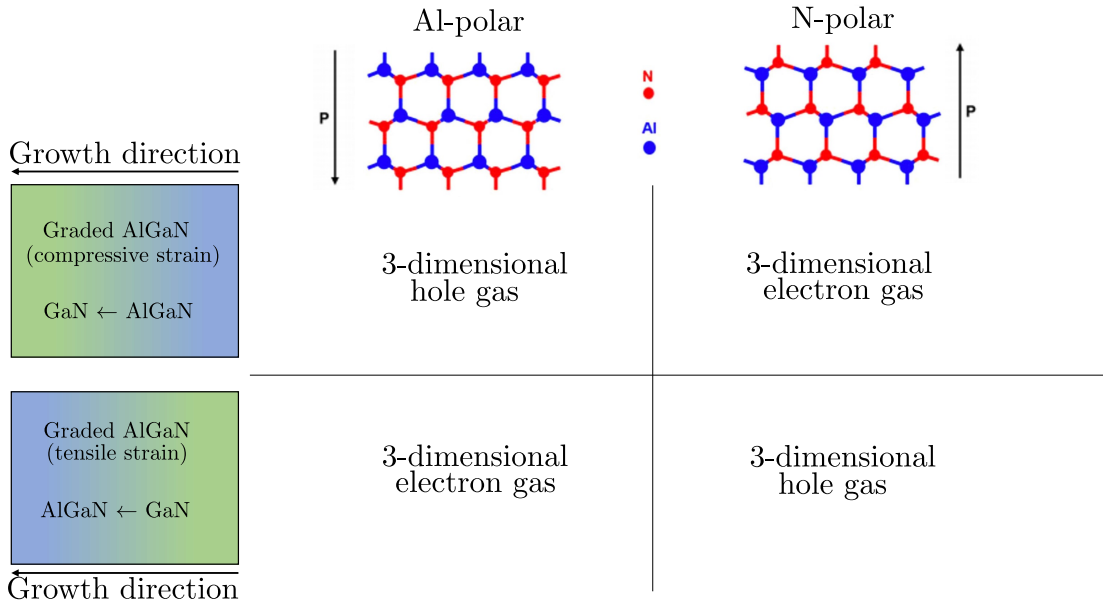


Figure 5.14: Different ways of generating 3-dimensional carriers in graded Al-GaN by various grading schemes.

The generative mechanism of 3d carriers, 3DEG or 3DHG strongly depends on the polarity of AlGaN films and whether the AlGaN grading is done from higher Al composition to lower composition or vice versa. These 2 degrees of freedom allow for 4 possible cases for realizing 3DEG or 3DHG as shown in Figure 5.14. A polarization-induced three-dimensional electron slab in graded AlGaN alloys was first reported by

Jena and Mishra *et al.* in the early 2000s [83, 155]. They achieved a $10^{18}/\text{cm}^3$ 3DEG concentration in an AlGa_N alloy that was linearly graded from GaN to AlGa_N in the [0001] growth direction. Similarly, Zhang *et al.* confirmed that a 3DHG of density $10^{18}/\text{cm}^3$ could also be induced by polarization by linearly decreasing the Al composition in the metal-polar direction from Al_{0.3}Ga_{0.7}N to GaN [217].

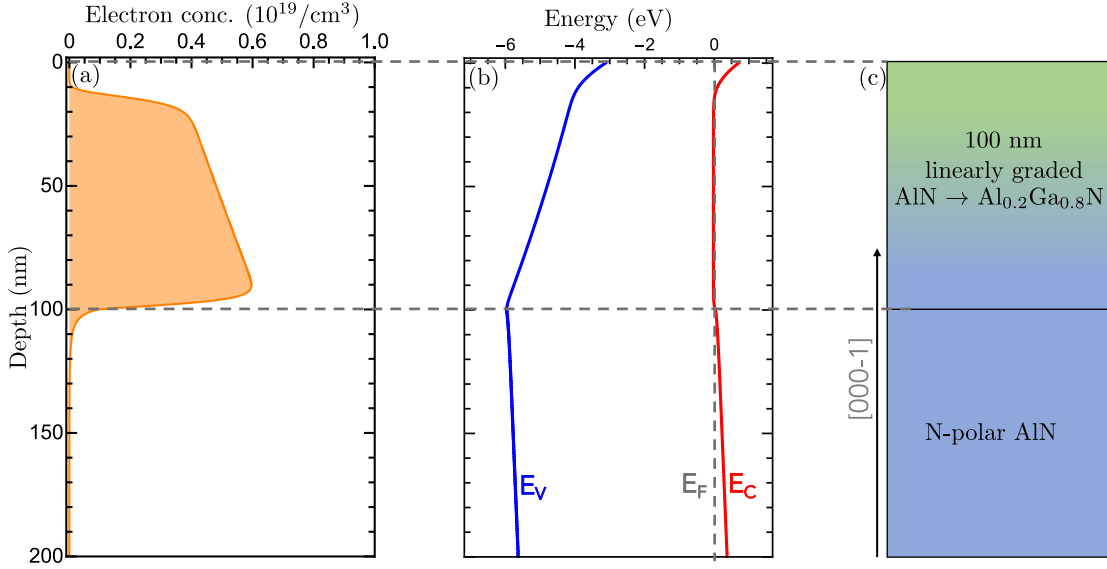


Figure 5.15: (a) The 3DEG carrier profile and (b) energy band diagram of the N-polar AlGa_N alloy on AlN with decreasing Al composition along the growth direction for the (c) layer structure with AlN $\rightarrow$ Al_{0.2}Ga_{0.8}N 3DEG channel.

On the flipped polarity i.e. the N-polar orientation of AlGa_N, there are again two possibilities to obtain 3d carriers. Simon *et al.* successfully demonstrated polarization-induced 3DHG in N-polar graded AlGa_N alloys grown on semi-insulating N-face [000 $\bar{1}$] GaN substrates [171]. A 3DEG can also be generated in an N-polar downward-graded AlGa_N alloy (from Al_xGa_{1-x}N to a GaN surface). Recently, Lemettinen *et al.* demonstrated an N-polar 3DEG on SiC substrate with a graded AlN $\rightarrow$ Al_{0.8}Ga_{0.2}N channel for the first time, with an electron density of $1.3 \times 10^{18}/\text{cm}^3$ [110]. However, single crystal N-polar AlN is a more attractive choice of substrate for realizing such a

graded AlGa_N 3DEG heterostructure as it provides a suitable lattice match to high composition Al_xGa_{1-x}N at the bottom. The band diagrams and charge distributions calculated by a self-consistent Schrodinger–Poisson solution for a representative N-polar AlN → Al_{0.2}Ga_{0.8}N 3DEG channel are shown in Figure 5.15. Since these carriers are polarization-induced, their carrier densities are nearly temperature-independent. On the contrary, the carrier concentration of conventional Si-doped n-AlGa_N and Mg-doped p-AlGa_N alloys decreases exponentially at low temperatures, due to the freeze-out effect of thermally activated electrons and holes.

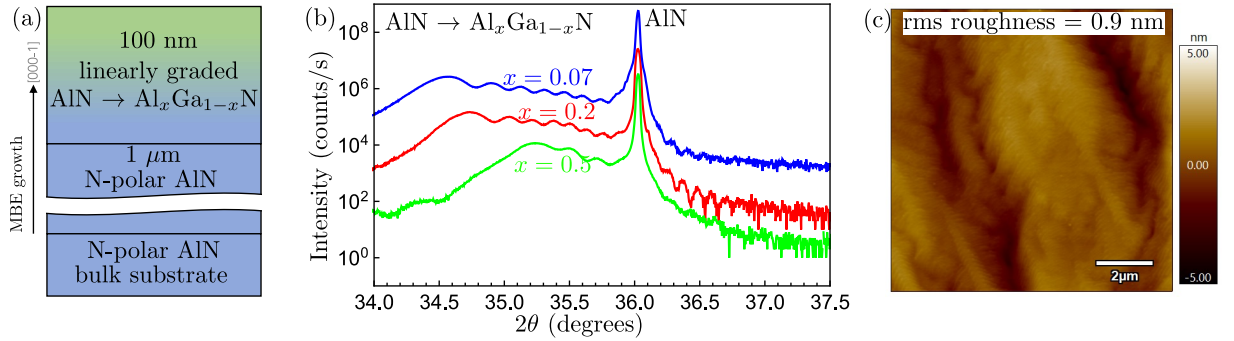


Figure 5.16: (a) Schematic of the epitaxial layer structures in this study. (b) Symmetric $2\theta/\omega$ XRD scans across the (002) diffractions with various Al content. (c) $10\ \mu\text{m} \times 10\ \mu\text{m}$ AFM micrograph of the linearly graded AlN → Al_{0.2}Ga_{0.8}N sample showing smooth surface morphology with sub-nm rms roughness.

In this work, we investigated the formation and properties of polarization-induced 3DEGs in N-polar linearly graded Al_xGa_{1-x}N ← AlN/AlN heterostructures ($x = 0.07, 0.2$ and 0.5) on single-crystal AlN. The epitaxial heterostructures shown in Figure 5.16(a) were grown using plasma-assisted MBE in a Veeco GEN10 system equipped with standard effusion cells for Ga and Al and a radio frequency plasma source for active N species. Free-standing N-polar single-crystal AlN substrates from Asahi-Kasei Corporation were used. [174]

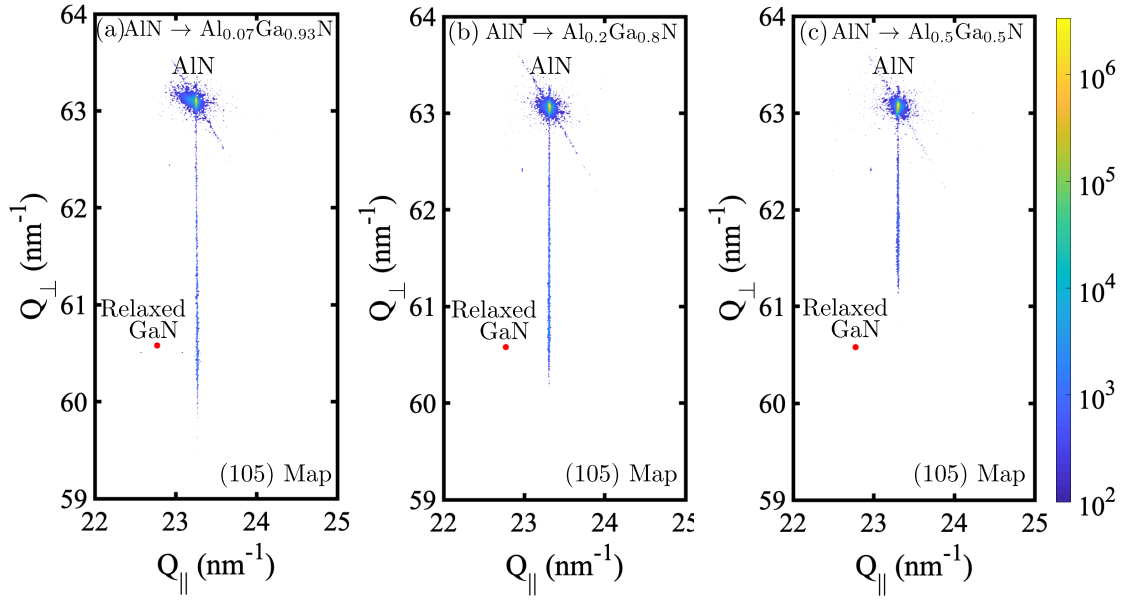


Figure 5.17: RSMs across the asymmetric (105) diffractions taken from the samples with linearly graded $\text{AlN} \rightarrow \text{Al}_x\text{Ga}_{1-x}\text{N}$ layer with (a) $x = 0.07$, (b) $x = 0.2$ and (c) $x = 0.5$

After the Al-assisted cleaning, a $1\ \mu\text{m}$ homoepitaxial AlN layer was grown under optimized Al-rich growth conditions. [174] The excess Al droplets were *in-situ* desorbed at an elevated temperature of $\sim 1200\ ^\circ\text{C}$ before cooling down the substrate to $\sim 900\ ^\circ\text{C}$. Next, a 100 nm thick compositionally graded AlGaN layer was grown. The Al-mole fraction was decreased linearly from 1 to x . The top Al composition $x = 0.07, 0.2$, and 0.5 was systematically varied across three samples (calibrated by XRD as discussed later). All the graded AlGaN layers were grown under metal-rich growth conditions, and the substrates were held at the growth temperatures for long enough after growth to *in-situ* desorb excess Ga droplets before cooling down to room temperature.

Figure 5.16(b) shows the symmetric $2\theta/\omega$ XRD scans of the three samples shown in Figure 5.16(a). Simulation of the XRD scans yielded a good fit (not shown) to the experimental data for a linearly graded layer, coherently grown on AlN, with the composition

varying from $x = 1.0$ to $x = 0.07$, 0.2 , and 0.5 , for the three samples respectively, and a thickness of 100 nm . All the samples exhibit similar smooth surface morphologies measured by AFM with rms roughness $< 1\text{ nm}$ over a $10\text{ }\mu\text{m} \times 10\text{ }\mu\text{m}$ area. Figure 5.16(c) shows a representative AFM scan from the sample with grading from $\text{AlN} \rightarrow \text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$.

The RSM of the grazing exit (105) asymmetrical reflection, Figure 5.17, indicates that all three graded layers were grown coherently to the AlN substrate, as the AlGaIn reciprocal lattice points (RLPs) lie on a vertical line passing through the substrate RLP. All the graded AlGaIn layers in this study are thus fully strained to the underlying AlN .

Figure 5.18 shows the temperature-dependent photoluminescence spectra of two graded N-polar AlGaIn samples with the top Al composition being $x = 0.07$ and $x = 0.2$. Both the samples were excited by a 193 nm ArF excimer laser from the top. A broad PL emission is observed from the graded AlGaIn layers. This further confirms the presence of a range of Al compositions in the samples while also suggesting the high crystalline quality of the epitaxial layers.

Thus, the graded N-polar $\text{AlN} \rightarrow \text{Al}_x\text{Ga}_{1-x}\text{N}$ samples have the desired structures in which the electrical transport properties of 3DEGs can be studied systematically as a function of Al composition x . On the N-face $[000\bar{1}]$, when the composition of the layer is graded with decreasing Al mole fraction, the net unbalanced charge is positive approximately given by $\rho \sim 5 \times 10^{13} \times (x_2 - x_1)/d\text{ /cm}^3$, where x_1 and x_2 are the Al compositions at the ends of the graded layer of thickness d (in centimeters). To neutralize this bound, positive charge, free electron carriers from remote donor-like states form a high-density 3D electron gas with approximately the same density as ρ . The concentration of the 3D electron gas should then exhibit a weak temperature dependence and resist freezeout at low temperatures. Since the bottom Al composition

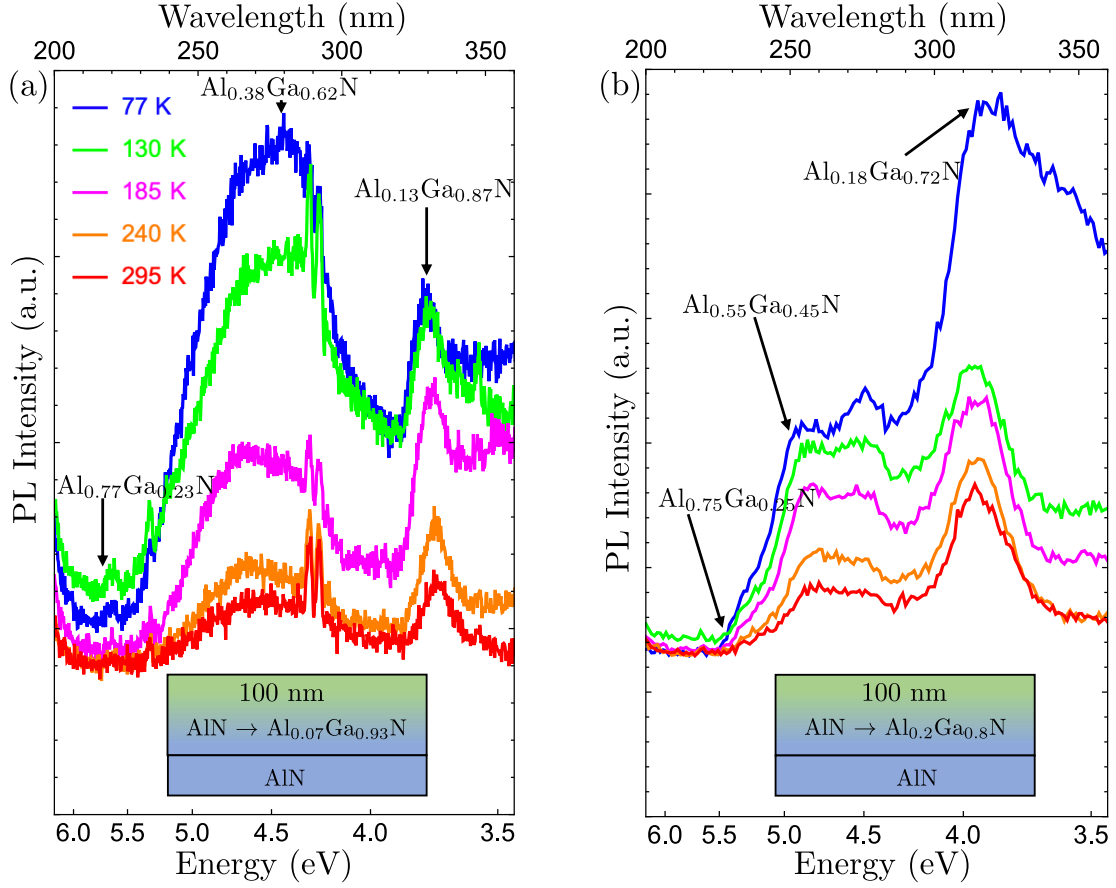


Figure 5.18: Temperature-dependent photoluminescence spectra of the graded N-polar $\text{AlN} \rightarrow \text{Al}_x\text{Ga}_{1-x}\text{N}$ heterostructures (a) $x = 0.07$ and (b) $x = 0.2$

($x_2 = 1$) and thickness ($d = 10^{-5}$ cm) are constant across the three samples in this study, the 3DEG density should decrease with increasing top Al composition (x_1) given by $\sim 5 \times 10^{18} \times (1 - x_1)/\text{cm}^3$.

Hall-effect measurements were performed on the samples using soldered corner indium contacts to the graded AlGa_N 3DEGs. The results are shown in Figure 5.19. As the top Al mole fraction x_1 of the graded AlGa_N layer increases, the measured Hall density decreases from $3.8 \times 10^{13}/\text{cm}^2$ for $x_1 = 0.07$ to $3 \times 10^{13}/\text{cm}^2$ for $x_1 = 0.2$ to eventually $1.8 \times 10^{13}/\text{cm}^2$ for $x_1 = 0.5$, following the expected trend.

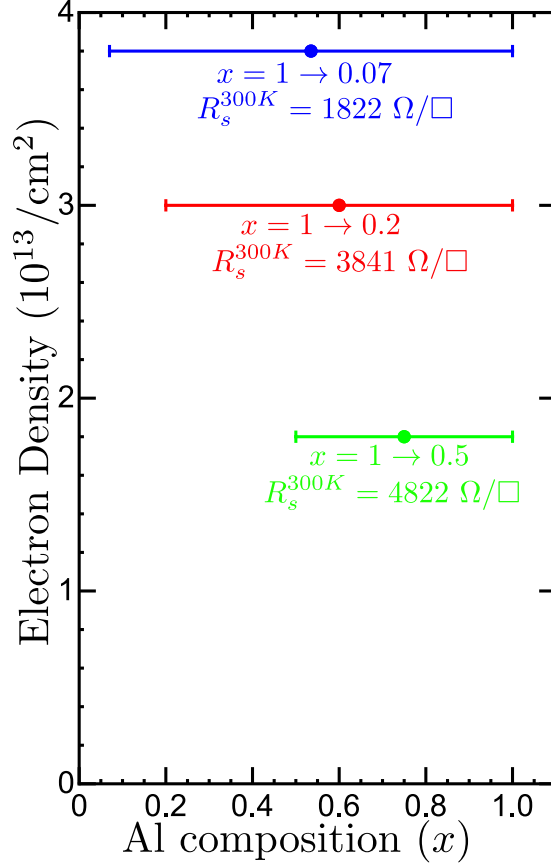


Figure 5.19: Measured sheet densities at 300 K as a function of Al composition x in the graded AlGaIn channel for different samples. The spread on the x-axis for each data point signifies the spread in grading.

Next, a temperature-dependent electron transport study was performed for two graded N-polar AlGaIn samples with the top Al composition being $x = 0.07$ and $x = 0.2$. Figures 5.20(a) and 5.20(b) show the temperature-dependent Hall-effect measurement results from 300 K down to 10 K. In both the samples, the electron density does not show significant variation with temperature. This robustness of the electron densities with temperature confirms their polarization-induced origin.

Even though the conventional HEMTs based on abrupt AlGaIn/GaN heterostructures have demonstrated extraordinary levels of performance in the microwave frequency range and for power electronics, the pursuit of such devices for higher-frequency and

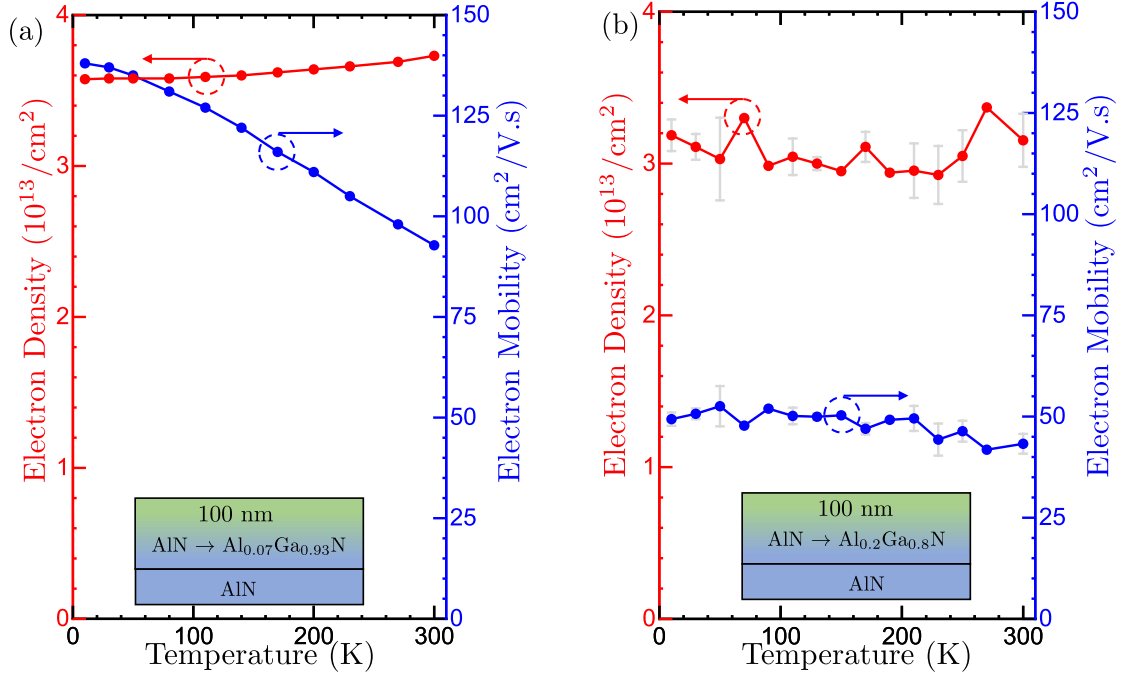


Figure 5.20: Temperature-dependent carrier sheet densities and mobility for the graded N-polar $\text{AlN} \rightarrow \text{Al}_x\text{Ga}_{1-x}\text{N}$ heterostructures (a) $x = 0.07$ and (b) $x = 0.2$. Electrons in polarization-doped layers are resistant to freezeout at low temperatures, and their mobility and concentration can be measured down to cryogenic temperatures. For the heterostructure with top Al composition $x = 0.5$, the sheet electron density is $1.8 \times 10^{13}/\text{cm}^2$ and the electron mobility is $72 \text{ cm}^2/\text{V.s}$ at 300 K.

higher-voltage operation requires more precise control over carrier behavior, in most cases, electron behavior in the conductive channels. Graded AlGaN alloys can provide an efficient way of tailoring the charge profile of the carrier and the resulting transport characteristics. Graded AlGaN channels with high-density 3DEGs have been used to improve the linearity of the RF transistor or to enable highly conductive Al-rich Al-GaN channels for high-voltage applications [20, 185, 9, 8]. Furthermore, graded Al-GaN structures can function as ohmic contact layers, which facilitate electron transport through metal-semiconductor contacts, or as back-barrier layers, which confine electrons in conductive channels sufficiently to decrease undesirable leakage current.

5.5 Future Directions

1. Advanced channel grading in N-polar AlGaN

The work presented in this chapter described the linearly graded N-polar AlGaN

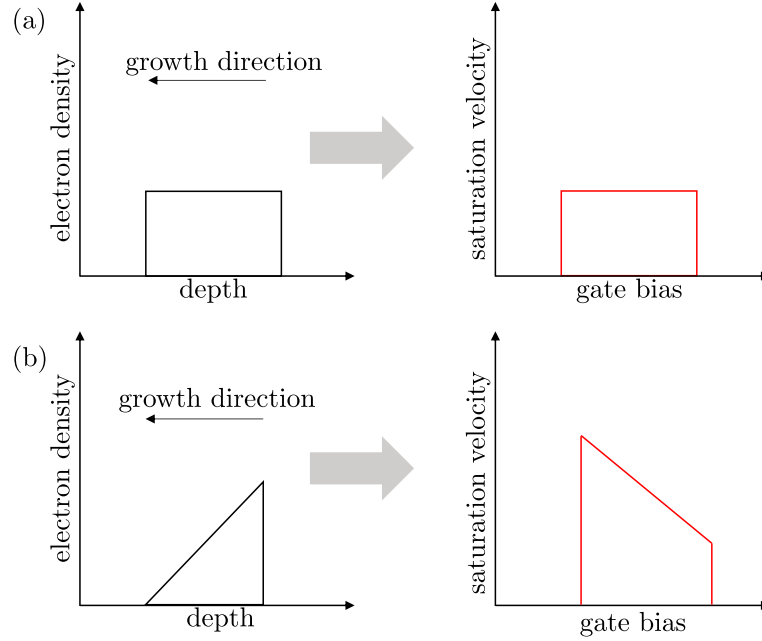


Figure 5.21: Schematic illustration of the charge profile and the corresponding velocity profile for two cases: (a) linearly graded AlGaN with constant charge profile as a function of depth; and (b) decreasing charge profile.

channels to obtain 3d electron gas, which can be used to make transistors that have a constant transconductance g_m over a wide range of bias gate voltages, for linearity improvement as shown in Figure 5.21(a). Polarization grading provides much more flexibility in device design. For example, charge profiles can be altered such that the desired velocity profiles are achieved as shown in Figure 5.21(b). These designs can help achieve the appropriate $g_m/f_T/f_{max}$ profiles for large-signal linearity, which may not be constant.

2. Composite 2D-3D channel on N-polar AlN platform

Graded channel transistors with a 3-D electron channel have demonstrated strong potential for achieving high linearity RF performance. Nonetheless, in order to achieve high values of transconductance and gain, the gate-to-channel distance must be reduced. Unfortunately, obtaining a scaled gate-to-channel distance in a 3D electron channel alone is challenging. To simultaneously get the benefits from a scaled gate-to-channel distance and a 3-D channel, a composite 2D-3D channel such as the one demonstrated in Figure 5.22 could be useful. The charge profile consists of a 2D (from N-polar GaN/AlN) as well as a 3D (from polarization graded N-polar AlGa_{0.5}N) electron gas. These composite 2D-3D channel HEMTs combine the advantages of HEMTs and MESFETs by offering high transconductance g_m and tailored flat g_m - V_{gs} profile.

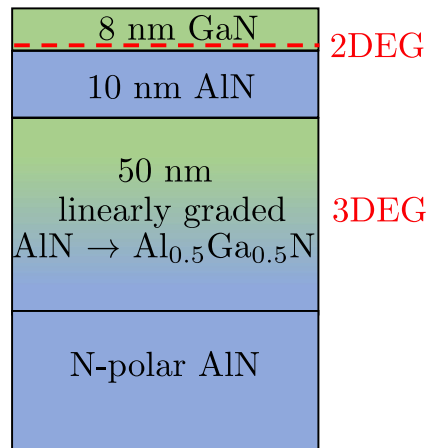


Figure 5.22: Schematic layer structure for N-polar GaN channel HEMT with graded AlGa_{0.5}N subchannel on N-polar AlN.

CHAPTER 6

A UNIFIED BALLISTIC TRANSPORT RELATION FOR ANISOTROPIC DISPERSIONS AND GENERALIZED DIMENSIONS: MODELING HIGH-FIELD TRANSPORT IN SEMICONDUCTORS

This chapter is divided into two sections. In the first section, an analytical formula is derived for particle and energy densities of fermions and bosons, and their ballistic momentum and energy currents for anisotropic energy dispersions in generalized dimensions. The formulation considerably simplifies the comparison of the statistical properties and ballistic particle and energy transport currents of electrons, acoustic phonons, and photons in various dimensions in a unified manner. Assorted examples of its utility are discussed, ranging from blackbody radiation to Schottky diodes and ballistic transistors, quantized electrical and thermal conductance, generalized ballistic Seebeck and Peltier coefficients, their Onsager relations, the generalized Wiedemann-Franz law and the robustness of the Lorenz number, and ballistic thermoelectric power factors, all of which are obtained from the single formula. The new formulation predicts a thermoelectric power factor behavior of three-dimensional Dirac bands which has not been observed yet.

In the second section, we employ this unified ballistic transport formulation to model high-field transport in polar semiconductors. A generalized analytical formulation is obtained for the phonon-limited electron velocity saturation in semiconducting structures in the high field regime. The resulting electron velocity degradation and carrier density-dependent transport have been investigated both theoretically and experimentally for specific cases in the past, here we provide a unified solution to the fundamental intrinsic limit of phonon-limited current carrying capacity for a wide range of electronic materials and devices of varying bandstructures and dimensionality.

6.1 Unified transport

6.1.1 Introduction

The need for analytical expressions for particle, energy, and current densities arises frequently in various branches of science and engineering. They are typically handled separately for each case of interest. This is because the densities depend on the quantum statistics of the type of particle or field of interest (i.e., whether they are fermions or bosons), on their specific energy dispersions (e.g. $E = \hbar^2 |\mathbf{k}|^2 / 2m$ or $E = \hbar v_F |\mathbf{k}|$), or the specific dimensionality under consideration (e.g. $d = 1, 2, 3$). A single unified analytical expression is found in this work for all the above densities and their ballistic momentum and energy currents for anisotropic dispersions in the non-interacting ballistic transport regime. This enables particle and energy densities, and ballistic particle and energy transport currents of electrons, phonons and photons to be treated in a unified manner amplifying their similarities and differences, the need for which has been advocated [36]. Though the discussion in this work is limited to electrons, phonons and photons, the results apply to ballistic transport in general, such as that of ultra-cold atoms and molecular gases (e.g. [90]).

6.1.2 Setup

For particles in a box of dimension $d = 1, 2, 3$ and volume L^d , wave-particle duality allows discrete wavevectors $k_i = p_i(2\pi/L)$ where $p_i = 0, \pm 1, \dots$ are integers. The resulting energy dispersion is written as $E = [\sum_{i=1}^d (\alpha_i k_i)^2]^{\frac{t}{2}}$. Here the *type* $t = 1$ represents linear (or conical) dispersion with $\alpha_i = \hbar v_i$ and $t = 2$ represents parabolic dispersion with $\alpha_i = \hbar / \sqrt{2m_i}$, where $\hbar = h/2\pi$ is the reduced Planck's constant. Table 6.1 shows

Table 6.1: Generalized energy dispersion in d –dimensions

$$E = [\sum_{i=1}^d (\alpha_i k_i)^2]^{\frac{t}{2}}$$

	t	α_i	$d = 1$	$d = 2$	$d = 3$
Conical	1	$\hbar v_i$	$\hbar v_F k_1$	$\hbar \sqrt{(v_1 k_1)^2 + (v_2 k_2)^2}$	$\hbar \sqrt{(v_1 k_1)^2 + (v_2 k_2)^2 + (v_3 k_3)^2}$
Parabolic	2	$\frac{\hbar}{\sqrt{2m_i}}$	$\frac{\hbar^2 k_1^2}{2m_1}$	$\frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2}$	$\frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2} + \frac{\hbar^2 k_3^2}{2m_3}$

that this formulation captures anisotropic dispersions via direction-dependent wave velocities v_i (e.g. anisotropic, non-dispersive and transparent optical or acoustic media) or effective masses m_i (e.g. the electron energy bandstructure of the semiconductor Silicon). Though the table and the following discussion is restricted to massless Dirac-like and massive parabolic dispersions, the formulation holds for other t . Extensions to other dispersions ought to be feasible along similar lines.

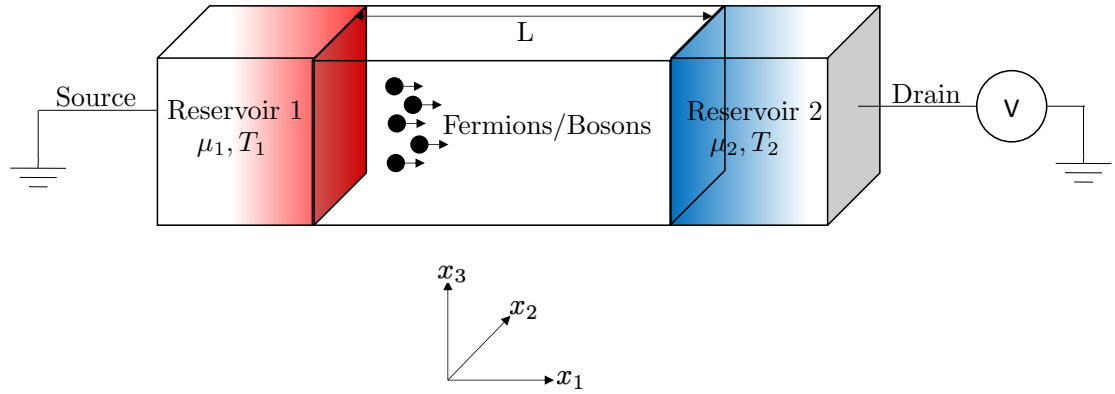


Figure 6.1: Fermionic or Bosonic systems whose ballistic transport is explored in this work. The ‘particles’ may be electrons, photons, phonons, or atoms or molecules, in a potential that produces either a parabolic or conical energy eigenvalue dispersion with momentum.

‘Source’ (1) and ‘drain’ (2) reservoirs, characterized by dimensionless parameters

$\eta_1 = \beta_1 \mu_1$ and $\eta_2 = \beta_2 \mu_2$ are connected to the box of particles of dimension d on opposite faces of dimension $d - 1$ as shown in Fig. 6.1. Here $\beta = (k_b T)^{-1}$ where k_b is the Boltzmann constant. The chemical potentials μ_1 and μ_2 and temperatures T_1 and T_2 of the source and drain may in general be different. The particles in the source and drain reservoirs follow the equilibrium distribution functions $f_{\pm}(E) = 1/(\exp[\beta(E - \mu)] \pm 1)$ with + for fermions and - for bosons with the corresponding chemical potential and temperature.

The particles in the box are in quasi-equilibrium with two reservoirs via ballistic transport: for example, particles injected from the source share the same distribution as the source. Let x_1 denote the coordinate along which the potential difference is applied across the source and drain reservoirs. The generalized current injected from reservoir 1 flowing in the positive x_1 direction is given by $J_1 = g L^{-d} \sum (v_{g1}(\mathbf{k}))^a E^b f_{\pm}(E)$ in each valley of the dispersion. Here $v_{g1}(\mathbf{k}) = (\hbar^{-1} \nabla_{\mathbf{k}} E) \cdot \hat{x}_1$ is the group velocity projected along the x_1 coordinate, a and b may be fractions or integers, and g combines degeneracies (e.g. valley, spin, polarization) and physical constants (e.g. electron charge, mass). The sum runs over all $\mathbf{k}$ states in the dispersion such that $k_1 > 0$. Choice of exponents a and b of 0 or 1 describe scalar particle densities or vector current densities. The subscript in J_i denotes the reservoir from which the current is injected. The net current flowing from reservoir 1 to reservoir 2 along the positive x_1 direction is $J_{net} = J_1 + J_2$ for scalar densities (e.g. particle density or energy density) and $J_{net} = J_1 - J_2$ for vector current densities (e.g. particle current densities or energy current densities). The parameters β and μ in $f_{\pm}$ are dictated by the respective reservoirs, and the group velocity neglects Berry-phase contributions.

6.1.3 Main Result

The generalized current J_1 can be recast as linear combination of sums of the type $I_{d,t}^{u,s} = \sum_{\Omega_{k_1}} k_1^u E^s f_{\pm}(E)$ that run over grid points in the d -dimensional hemisphere Ω_{k_1} for $k_1 \geq 0$. This converts to the integral

$$I_{d,t}^{u,s} = \int_{k_1=0}^{\infty} \int_{k_2=-\infty}^{\infty} \dots \int_{k_d=-\infty}^{\infty} \frac{dk_1 dk_2 \dots dk_d}{\left(\frac{2\pi}{L}\right)^d} k_1^u E^s f_{\pm}(E). \quad (6.1)$$

Substituting $\alpha_i k_i \rightarrow k_i$ and splitting off k_1 using $k_0^2 = k_1^2 + \tilde{k}^2$ where $\tilde{k}^2 = k_2^2 + \dots + k_d^2$, then passing into spherical coordinates $d^{d-1}\tilde{k} = S_{d-2}\tilde{k}^{d-2}d\tilde{k}$ where $S_{d-1} = 2\pi^{d/2}/\Gamma(d/2)$ and $\Gamma(\dots)$ is the Gamma function, this becomes

$$I_{d,t}^{u,s} = \frac{S_{d-2}}{\frac{(2\pi)^d \alpha_1^u (\prod_{i=1}^d \alpha_i)}{L^d}} \int_0^{\infty} dk_1 k_1^u \int_{k_1}^{\infty} dk_0 k_0 (k_0^2 - k_1^2)^{\frac{d-3}{2}} E^s f_{\pm}(E), \quad (6.2)$$

which upon switching the order of integration evaluates to the exact closed form

$$I_{d,t}^{u,s} = \left(\frac{L}{\lambda_{dB}}\right)^d \cdot \frac{1}{\beta^s \left(\frac{\lambda_{dB_1}}{2\sqrt{\pi}}\right)^u} \cdot \frac{\Gamma(\frac{u+1}{2})\Gamma(s + \frac{d+u}{t})}{t \sqrt{\pi}\Gamma(\frac{d+u}{2})} \cdot F_{s+\frac{d+u}{t}-1}^{\pm}(\eta), \quad (6.3)$$

where $\lambda_{dB}^d = \lambda_{dB_1} \dots \lambda_{dB_d} = (4\pi)^{d/2} (\alpha_1 \alpha_2 \dots \alpha_d) \beta^{d/t}$, and $\lambda_{dB_i} = \sqrt{4\pi} \alpha_i \beta^{1/t}$ is the generalized anisotropic thermal de-Broglie wavelength in the direction i that characterizes the spatial spread of the wavepacket carrying the current. For example, $\lambda_{dB_i} = h / \sqrt{2\pi m_i k_b T}$ for parabolic ($t = 2$) and $\lambda_{dB_i} = h v_i / \sqrt{\pi} k_b T$ for Dirac-like ($t = 1$) dispersion. $F_j^{\pm}(\eta) = \frac{1}{\Gamma(j+1)} \int_0^{\infty} dx \frac{x^j}{\exp[x-\eta] \pm 1}$ is the Fermi-Dirac or Bose-Einstein integral [1]. Though Equation 6.2 is not defined for $d = 1$, Equation 6.3 holds for all d .

The generalized current in terms of Equation 6.3 therefore is $J_1 = g L^{-d} \sum (v_{g1}(\mathbf{k}))^a E^b f_{\pm}(E) =$

$g/L^d(t\alpha_1^2/\hbar)^a I_{d,t}^{a,b+a-\frac{2a}{t}}$, which takes the compact form

$$J_{d,t}^{a,b} = g \cdot \frac{1}{\lambda_{dB}^d \beta^b} \cdot \left(\frac{\lambda_{dB_1}}{h\beta} \right)^a \cdot C_{d,t}^{a,b} \cdot F_j^\pm(\eta), \quad (6.4)$$

which is the main result of this work. $J_{d,t}^{a,b}$ is an explicit closed formula for J_1 . Physically, this is the desired single expression for the density and current of particles, momentum, or heat, carried by both Fermions and Bosons flowing in the x_1 direction and injected from reservoir 1. Here a and b are the exponents of the velocity and energy. $j = a + b + r - 1$, $r = \frac{d-a}{t}$, and $C_{d,t}^{a,b} = \frac{\Gamma(\frac{1+a}{2})\Gamma(j+1)}{(t\sqrt{\pi})^{1-a}\Gamma(\frac{a+d}{2})}$ are constants that depend in a simple and compact way on the dimension d , bandstructure type t , and type of current (e.g. particle, momentum, heat, etc) via the whole numbers (a,b) . The four numbers (d,t,a,b) via Equation 6.4 thus yield all currents.

The interpretation of Equation 6.4 as a generalized current density becomes transparent by identifying it as a product of the following quantities: g , which represents physical constants and/or degeneracies, $1/(\lambda_{dB}^d \beta^b)$ which is dimensionally the (energy) ^{b} /volume, $(\lambda_{dB_1}/h\beta)^a$ which is dimensionally the (velocity) ^{a} , $C_{d,t}^{a,b}$ which is a dimensionless constant of order 1 for choices of $\{d,t,a,b\}$, and the dimensionless Fermi-Dirac or the Bose-Einstein integral $F_j^\pm(\eta)$. Since this is a new general formulation for ballistic transport, we expect it to both unify previously known transport phenomena in new light, and also predict new phenomena. We highlight both aspects in the rest of this work.

6.1.4 Low Temperature Asymptotics

To highlight the utility of the unified formalism, we first explore the low temperature limits of generalized Fermion and Boson currents. For example, the ballistic

charge current ($a = 1, b = 0$) in parabolic bands ($t = 2$) in d -dimensions for Fermions is obtained by choosing F^+ in Equation 6.4 as $J_{d,2}^{1,0} = q(\frac{k_b T}{h})(\frac{2\pi m k_b T}{h^2})^{\frac{d-1}{2}} F_{\frac{d-1}{2}}^+(\frac{\mu}{k_b T})$, which in the limit of a highly degenerate Fermion distribution is $J_{d,2}^{1,0}(T \ll \mu/k_b) = \frac{q}{h^d}(2\pi m)^{\frac{d-1}{2}} \frac{\mu^{\frac{d+1}{2}}}{\Gamma(\frac{d+1}{2})} \left[1 + \frac{\pi^2}{6} \frac{\Gamma(\frac{d+1}{2})}{\Gamma(\frac{d-1}{2})} \left(\frac{k_b T}{\mu} \right)^2 \right]$, indicating a T^2 dependence. While yielding the transport coefficients explicitly for different dimensions d , the above low temperature limit of ballistic charge current shows that this T^2 dependence is independent of the dimensions. The independence of the $J \sim T^2$ dependence actually is seen to extend beyond the dimensionality, to other ballistic currents, which include heat or energy currents with a general (a, b) and also to other dispersions (all t), because when expanded at low temperatures for fermions for $\mu > 0$ up to $\mathcal{O}(T^2)$, Equation 6.4 gives:

$$J_{d,t}^{a,b}(T \ll \frac{\mu}{k_b}) = \frac{g(4\pi)^{\frac{a-d}{2}} \alpha_1^a C_{d,t}^{a,b}}{(\alpha_1 \alpha_2 \dots \alpha_d) h^a} \frac{\mu^{j+1}}{\Gamma(j+1)} \left[1 + \frac{\pi^2}{6} j \left(\frac{k_b T}{\mu} \right)^2 \right] \quad (6.5)$$

which guarantees the same temperature dependence for all dimensions d , as well as for all currents (a, b) and types of bandstructures.

Unlike the ‘universal’ T^2 dependence that results from the Sommerfeld expansion for all Fermion currents in the degenerate limit, that of Bosons depends on the dimensions, bandstructure, and the type of current. Bose-Einstein statistics enforces $\eta \rightarrow 0$ as $T \rightarrow 0$ for all dimensions [40]. In the degenerate limit the generalized Bosonic current obtained from Equation 6.4 is

$$J_{d,t}^{a,b}(T \rightarrow 0) = \frac{g(4\pi)^{\frac{a-d}{2}} \alpha_1^a C_{d,t}^{a,b}}{(\alpha_1 \alpha_2 \dots \alpha_d) h^a} (k_b T)^{j+1} \zeta(j+1), \quad (6.6)$$

where $\zeta(\dots)$ is the zeta-function. As an example the thermal energy density ($a = 0, b = 1$) stored in long-wavelength acoustic phonons with a linear dispersion ($t = 1$) in a d -dimensional crystal is $J_{d,1}^{0,1}(T \rightarrow 0) \propto T^{d+1}$, the specific case of $J_{d,t}^{a,b}(T \rightarrow 0) \propto T^{a+b+\frac{d-a}{t}}$, which leads to a heat capacity $\sim T^d$.

6.1.5 Assorted Applications

We now remove the low temperature restriction to systematically illustrate with assorted examples the versatility of the new formulation in unifying the treatment of several disparate physical phenomena across dispersions and dimensions, and in predicting new phenomena.

I: Particle Densities ($a = 0, b = 0$)

From Equation 6.4 the generalized particle density for various statistics, dispersions, and dimensions is obtained with $a = 0, b = 0$:

$$n_{d,t} = 2J_{d,t}^{0,0} = \frac{2g}{\lambda_{dB}^d} \cdot \frac{\Gamma(\frac{d}{t})}{t\Gamma(\frac{d}{2})} \cdot F_{\frac{d}{t}-1}^{\pm}(\eta). \quad (6.7)$$

The number density of photons of $g = 2$ polarizations in thermal equilibrium with a radiation source at temperature T is obtained using $F_{\frac{d}{t}-1}^{-}(0)$ in Equation 6.7. The chemical potential $\mu = 0$ for photons which are bosons whose particle number is not conserved in thermodynamic equilibrium with matter at temperature T . In $d = 3$ it is $2J_{3,1}^{0,0} = 16\pi\zeta(3)(\frac{k_b T}{hc})^3$ where c is the speed of light, and in $d = 2$ is $2J_{2,1}^{0,0} = 2\pi^2(\frac{k_b T}{hc})^2$. Because the photon has a positive branch dispersion, no energy gap, and Bose-Einstein statistics, no mass action law exists unlike for electrons and holes in semiconductors.

For a $t = 2$ parabolic conduction band energy dispersion with $E = E_c + \sum_{i=1}^d (\alpha_{ci} k_i)^2$ with spin degeneracy $g_s = 2$, valley degeneracy g_c and the +ve sign for fermions, Equation 6.7 gives the generalized volume density of electrons in d -dimensions $n_d = 2J_{d,2}^{0,0} = N_c^d F_{(d/2)-1}^{+}[(\mu - E_c)/k_b T]$ where the band-edge density of states $N_c^d = 2g_c/\lambda_{dBc}^d$ is twice the inverse of the conduction band edge thermal de Broglie volume [11, 66]. The

equivalent d -dimensional distribution for the valence band $E = E_v - \sum_{i=1}^d (\alpha_{vi} k_i)^2$ is $p_d = N_v^d F_{(d/2)-1}^+[(E_v - \mu)/k_b T]$. For an energy gap $E_c - E_v = E_g$, the d -dimensional mass-action law governing equilibrium carrier statistics is $n_d p_d = n_{id}^2$ which is obtained with $n_{id} \approx \sqrt{N_c^d N_v^d} \exp[-E_g/2k_b T]$.

For $t = 1$ with a conical energy dispersion $E = \hbar v_F |\mathbf{k}|$, the fermion density per valley is $n_d(\mu) = 2J_{d,1}^{0,0} = (4/\lambda_{dB}^d)(\Gamma(d)/\Gamma(d/2))F_{d-1}^+(\mu/k_b T)$. If the Fermi level is at the Dirac point $\mu = 0$ for metallic carbon nanotubes ($d = 1$), monolayer graphene ($d = 2$), and HgCdTe ($d = 3$), the intrinsic thermally generated electron density in each valley is $n_{di} = \frac{4}{(2\sqrt{\pi})^d} (\frac{k_b T}{\hbar v_F})^d (\frac{\Gamma(d)}{\Gamma(d/2)}) \cdot F_{d-1}^+(0)$, varying with temperature as $n_i \sim T^d$ in d -dimensions. This sets the lowest carrier density (and hence highest electrical resistivity) that may be reached in such materials at any temperature. For $E = \pm \hbar v_F |\mathbf{k}|$ where two cones touch, the sum of electron and hole densities is $n_d(+\mu) + n_d(-\mu)$, resulting in a corresponding mass-action law for Dirac dispersions. The temperature dependence of the intrinsic electron/hole densities for conical bandstructure is therefore identical to the density of photons.

II: Energy Densities ($a = 0, b = 1$)

The volume density of energy stored in a photon field in equilibrium with a radiation source of temperature T is $2J_{d,1}^{0,1}$, which for $d = 3$ is $\frac{4\pi^5 (k_b T)^4}{(hc)^3}$, with corresponding results for other dimensions. For long-wavelength acoustic phonons, the thermal energy stored in a solid is similarly obtained by choosing $g = 1$ for each branch of sound velocity v_s via $\alpha_i = \hbar v_s$, with $t = 1$ and $a = 0, b = 1$. This gives the thermal energy density $2J_{3,1}^{0,1} = (\frac{4\pi^5 k_b^4}{15h^3 v_s^3}) T^4$, and a heat capacity per atomic density n of $\frac{C_v}{n} = 2\partial J_{3,1}^{0,1}/\partial T = (\frac{16\pi^5 k_b^4}{15h^3 v_s^3}) T^3$, the $T \rightarrow 0$ limit of the Debye- T^3 law [48, 11].

Because $J_{d,t}^{0,0}$ is the particle density and $J_{d,t}^{0,1}$ is the energy density, their ratio

$$u_{d,t} = \frac{J_{d,t}^{0,1}}{J_{d,t}^{0,0}} = \frac{d}{t} k_b T \frac{F_{\frac{d}{t}}^{\pm}(\eta)}{F_{\frac{d}{t}-1}^{\pm}(\eta)} \approx d \times \frac{k_b T}{t} \quad (6.8)$$

is the generalized law of the equipartition of energy. For $-\eta \gg 1$, the Boltzmann approximation is valid for both Fermions and Bosons. For particles in d -dimensions with mass and $t = 2$, there is $k_b T/2$ energy per each dimension. For linear dispersion ($t = 1$) on the other hand, there is $k_b T$ energy per each dimension as identified by Tolman [193] in the relativistic limit and investigated further for other dispersions [196, 28].

For degenerate fermions characterized by $\eta \gg +1$, the equilibrium average energy is $u_d \approx \mu d/(d+t)$ and the resulting electronic specific heat $c_v = \partial J_{d,t}^{0,1}/\partial T = \frac{g\pi^2 d}{3t^2} \frac{k_b T}{\mu} n_d k_b$ if $d/t \neq 1$ and $c_v = \frac{g\pi^2}{3} \frac{k_b T}{\mu} n_d k_b$ if $d/t = 1$ [193, 106]. For example, for electrons in metals with $d = 3$, $g = 2$, and $t = 2$, $c_v = \frac{\pi^2}{2} \frac{k_b T}{\mu} n_{3d} k_b$, and for degenerately doped graphene with $d = 2$, $g = 4$ and $t = 1$ is $c_v = \frac{8\pi^2}{3} \frac{k_b T}{\mu} n_{2d} k_b$.

III: Ballistic Charge Currents ($a = 1, b = 0$)

Suppose a solid with electronic bandstructure valleys of the types of Table 6.1 is connected to two reservoirs held at the dimensionless potentials η_1 and η_2 . By setting $g = 2q$ where q is the electron charge of spin degeneracy $= 2$, $a = 1, b = 0$, while using f^+ for Fermions, Equation 4 yields the charge current density for each valley in quasi-equilibrium with the source reservoir:

$$J_1 = J_{d,t}^{1,0} = \underbrace{\frac{2q^2}{h} \frac{\lambda_{dB1}}{\lambda_{dB}^d} \frac{\Gamma(1+r)}{\Gamma(\frac{d+1}{2})}}_{J_0} \frac{k_b T}{q} F_r^+(\eta_1), \quad (6.9)$$

where $r = (d - 1)/t$. The difference $J_{\text{net}} = J_1 - J_2 = J_0[F_r^+(\eta_1) - F_r^+(\eta_2)]$ is the net macroscopic current, where the characteristic J_0 depends on t, d and λ_{dB} , and is independent of the potential difference across the terminals.

The generalized form enables direct computation of ballistic currents in diodes and transistors of various dimensions and bandstructures. Applying Equation 6.9 to a Schottky diode of electron barrier height $q\phi_b$ between a metal and a semiconductor with anisotropic bandstructure of dispersion type $t = 2$ yields a generalized current density $\propto [F_{\frac{d-1}{t}}^+(\eta_1) - F_{\frac{d-1}{t}}^+(\eta_2)]$:

$$J_{\text{schottky}} \approx \underbrace{\frac{2q(2\pi m_e)^{\frac{d-1}{2}} k_b^{\frac{d+1}{2}}}{h^d}}_{A_{d,2}} f_d T^{\frac{d+1}{2}} e^{-\frac{q\phi_b}{k_b T}} (e^{\frac{qV}{k_b T}} - 1) \quad (6.10)$$

for $\beta(\eta_1 - \eta_2) = qV$ in the limit of $-\eta_1, -\eta_2 \gg 1$ as is typically the case in experiments. The case for $d = 3$ was first derived by bethe1942radiation [26]; $A_{d,2}$ is the d -dimensional Richardson coefficient, and the dimensionless form factor $f_d = \prod_{i \neq 1} \sqrt{m_i/m_e}$ accounts for bandstructure anisotropy by excluding the mass component in the direction of transport. For 3D Silicon which has 6 valleys of the type $E = E_c + \frac{\hbar^2}{2} (\frac{k_x^2}{m_l} + \frac{k_y^2}{m_t} + \frac{k_z^2}{m_t})$ along the 100 axis in k -space, the form factor for $d = 3$ current along the 100 axis is $f_3 = \frac{2m_t + 4\sqrt{m_l m_t}}{m_e}$ [186, 43] where the form factor is obtained from the 100 projections for each of the 6 valleys. The characteristic J_0 of Equation 6.9 is the reverse saturation current density in d -dimensions for the diode relation given by Equation 6.10. The formulation presented here therefore generalizes and extends the recent work of Schottkyuniversal [6] which found that the lateral 2D Schottky reverse saturation current scales universally with temperature as $\ln(J_0/T^{3/2}) \propto -1/T$. This result is extended to d -dimensional ballistic Schottky diodes using our formulation for J_0

in the generalized Richardson formula:

$$\ln\left(\frac{J_0}{T^{\frac{d+1}{2}}}\right) = \ln(A_{d,2}f) - \frac{q\phi_b}{k_bT}, \quad (6.11)$$

yielding for $d = 2$ the $\ln(J_0/T^{3/2}) \propto -1/T$ dependence of 2D lateral Schottky heterojunctions. For example, a lateral monolayer NbSe₂/WSe₂ junction forms a 2D-2D ballistic Schottky diode for which the current is $J_{\text{schottky}} \approx A_{2,2} \sqrt{\frac{m^*}{m_e}} T^{\frac{3}{2}} e^{-\frac{q\phi_b}{k_bT}} \cdot (e^{\frac{qV}{k_bT}} - 1)$ for an isotropic 2D bandstructure. The ballistic current-voltage characteristics of Schottky diodes in d -dimensions calculated from the unified formula is shown in Fig. 6.2 at 300K. The formulation indicates the ranges of barrier heights and voltages in which the signature of the dimensionality should be imprinted in the variation of the ballistic current with temperature, and therefore experimentally measurable.

Equation 6.9 also applies for ballistic electron transport in 2-terminal resistors, or 3-terminal field-effect transistors (FETs). For example, for a 2D electron gas channel with $d = 2$ and bandstructure type $t = 2$, the current per unit width per each valley is $J = \frac{2q^2}{h} \frac{1}{\lambda_{dB}} \frac{k_bT}{q} [F_{1/2}^+(\eta_1) - F_{1/2}^+(\eta_2)]$, in Natori's form [138]. For bandstructure type $t = 1$ and $d = 2$ encountered in monolayer graphene or surface-bands of topological insulators, the current is $J = \frac{2q^2}{h} \frac{2}{\sqrt{\pi}\lambda_{dB}} \frac{k_bT}{q} [F_1^+(\eta_1) - F_1^+(\eta_2)]$. The 1D ballistic current per valley for $d = 1$ is $J = \frac{2q^2}{h} \frac{k_bT}{q} \ln\left(\frac{1+e^{\eta_1}}{1+e^{\eta_2}}\right)$, which in the limit $\eta_1, \eta_2 \gg +1$ typically encountered in experiments reduces to the Landauer limit [107] given by $J = \frac{2q^2}{h} V$, indicating the conductance J/V is quantized to $2q^2/h$ regardless of the type of bandstructure. For ballistic currents for $t = 2$, simultaneously fixing the total d -dimensional fermionic density $n_d = J_{d,t}^{0,0}(\eta_1) + J_{d,t}^{0,0}(\eta_2)$ (say via capacitive gate control) requires a self-consistent solution for η_1 and η_2 for charge and current, resulting in the saturation of the ballistic current beyond a certain voltage difference between the source and drain. This is the hallmark of ballistic transistors that provide electronic gain for signal amplification, and switching for digital logic.

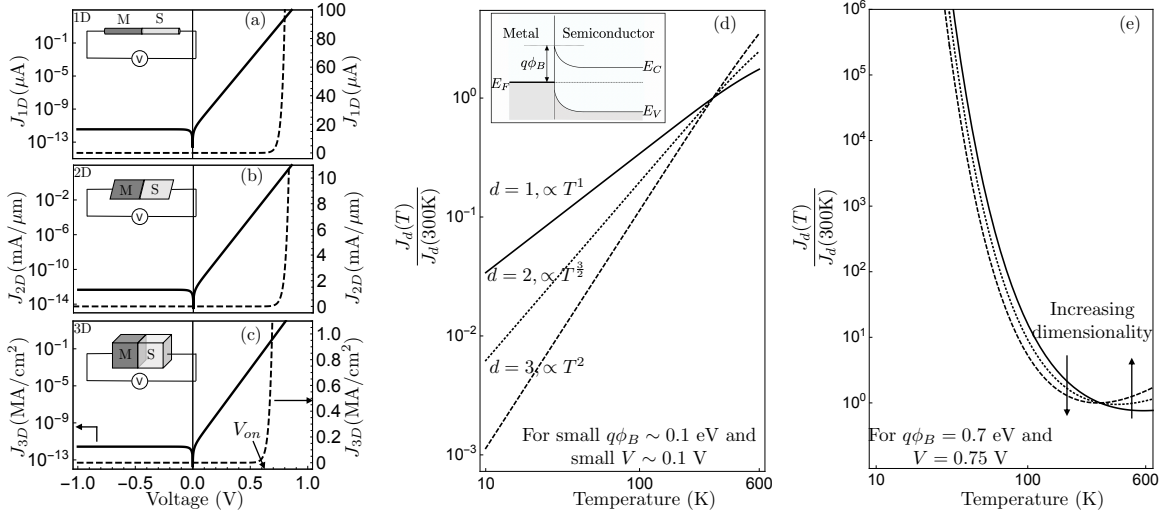


Figure 6.2: (a), (b) and (c) are representative 300 K $J - V$ characteristics of Metal (M) - Semiconductor (S) Schottky junctions in 1D, 2D and 3D respectively with $q\phi_B = 0.7$ eV where the semiconductor has parabolic dispersion ($t = 2$). The solid curve is the logarithmic scale plot with axis on the left and the dashed curve is the linear scale plot with axis on the right. (d) $J_d(T)/J_d(300\text{ K})$ vs. temperature for a small barrier ($q\phi_B \sim 0.1$ eV) and small positive bias (~ 0.1 V) showing a $T^{\frac{d+1}{2}}$ dependence for $T < 300$ K. (e) Temperature dependence of $J_d(T)/J_d(300\text{ K})$ converges for different dimensions for appreciable barrier heights and voltages.

IV: Ballistic Heat Currents (a=1, b=1)

The heat current density is obtained directly from the entropy in the ballistic case using a Landauer approach (see for example [176]) or in the scattering-limited diffusive case using the Boltzmann approach in the relaxation-time approximation (see for example [179]). The ballistic heat current from an electrode is $Q = gL^{-d} \sum v_{g1}(k)(E - \mu)f_{\pm}(E)$, where μ is the chemical potential and T the temperature of that electrode. The generalized ballistic heat current density in quasi-equilibrium with the source reservoir is then obtained from Equation 6.4 as $Q_1 = J_{d,t}^{1,1} - \mu_1 J_{d,t}^{1,0}$:

$$Q_1 = \frac{gk_b^2}{h} \cdot \frac{\Gamma(r+1)}{\Gamma(\frac{d+1}{2})} \cdot \frac{\lambda_{dB_1}}{\lambda_{dB}^d} \cdot T^2 [(1+r)F_{r+1}^\pm(\eta_1) - \eta_1 F_r^\pm(\eta_1)], \quad (6.12)$$

and the net heat current density is $Q = Q_1 - Q_2$.

Since $\mu = 0$ for bosons whose particle number is not conserved, for $t = 1$ and $v_i = c$ the net heat current with f_- becomes

$$Q_1 - Q_2 = \frac{g\pi^{\frac{d-1}{2}}k_b^{d+1}}{h^d c^{d-1}} \cdot \frac{\Gamma(d+1)}{\Gamma(\frac{d+1}{2})} \cdot F_d^-(0) \cdot [T_1^{d+1} - T_2^{d+1}], \quad (6.13)$$

which is a generalized d -dimensional radiative cooling law. For a blackbody source at temperature $T_1 = T$ radiating in $d = 3$ dimensions and $g = 2$ polarizations, Equation 6.13 yields $Q = (\frac{2\pi^5 k_b^4}{15c^2 h^3})T^4$. This is the Stefan-Boltzmann radiation law [27, 150], a spectral integral over the Planck blackbody radiation density in the photon field. The corresponding currents for blackbody radiators in $d = 2$ is $J_{2,1}^{1,1} = (\frac{8\zeta(3)k_b^3}{ch^2})T^3$ and $d = 1$ is $J_{1,1}^{1,1} = (\frac{\pi^2 k_b^2}{3h})T^2$. The case of $d = 1$ is special since it does not depend on the speed of light; indeed it is independent of the energy dispersion altogether because the velocity cancels the density of states. Identical behavior exists for phonons and electrons, as discussed next.

For each branch of acoustic phonons, Equation 6.13 also gives the ballistic heat current between electrodes, with the speed of light replaced by the corresponding sound velocity. When the drain electrode is at $T_2 = 0$ K, the $d = 1$ heat current by an acoustic phonon branch of polarization $g = 1$ is $J_{1,1}^{1,1} = (\pi^2 k_b^2 / 6h)T^2$, identical to the photon current per polarization. Though the ballistic phonon heat currents depend on temperature non-linearly, for $T_2 = T_0$ and a slightly hotter source at $T_1 = T_0 + \Delta T$, the heat current is

$$Q \approx \frac{g\pi^{\frac{d-1}{2}}k_b^{d+1}}{h^d v^{d-1}} \cdot \frac{\Gamma(d+2)}{\Gamma(\frac{d+1}{2})} \cdot F_d^-(0) \cdot T_0^d \cdot \Delta T, \quad (6.14)$$

which is linear in temperature difference $Q = G\Delta T$. For $d = 1$ the thermal conductance quantum $G_0 = \pi^2 k_b^2 T / (3h)$ is obtained. This was theoretically anticipated [157, 7] and subsequently experimentally observed [162].

Because for electrons $\mu \neq 0$, Equation 6.12 gives a heat current dependent nonlinearly on both μ and T of the source and drain reservoirs. For small differences, for $t = 2$ dispersion and $d = 1$ to leading order in $\eta = \beta\mu \gg 1$ it is

$$Q \approx \frac{gk_b^2\pi^2}{6h}(T_1^2 - T_2^2) - \frac{g}{2h}(\mu_1^2 - \mu_2^2), \quad (6.15)$$

which when linearized around a temperature T and $\mu_1 = \mu_2$ gives the same heat conductance quantum $\pi^2 k_b^2 T / (3h)$ per spin channel as for photons and phonons. In spite of the cancellation of the group velocity and the density of states in $d = 1$, the heat conductance quantum due to electrons derives from its Fermionic statistics, yet is identical to the heat conductance quantum of phonons *and* photons that follow Bosonic statistics. This strange similarity was recognized in [59, 158, 60], and Haldane's fractional exclusion statistics [64, 206] was invoked to explain its possible origin [159]. The similarity of the 1d energy conductance quantum as a physical quantity independent of bosonic or fermionic statistics arising in the formulation here is traced to the following identities connecting the Fermi-Dirac and Bose-Einstein integrals:

$$\begin{aligned} F_1^-(0) = \frac{\pi^2}{6} &= \lim_{\eta \rightarrow \infty} \left[F_1^+(\eta) - \frac{(F_0^+(\eta))^2}{2F_{-1}^+(\eta)} \right], \\ &= \lim_{\eta \rightarrow \infty} \left[F_1^+(\eta) - \eta F_0^+(\eta) + \frac{\eta^2}{2} F_{-1}^+(\eta) \right]. \end{aligned} \quad (6.16)$$

Unlike photons and phonons though, the electron chemical potential difference also

drives an energy current, which is captured well in the generalized linear transport coefficients.

V: Linear Response Coefficients

Linearizing the above exact generalized formulations for ballistic transport for small differences in the reservoir chemical potentials $\mu_1 - \mu_2 = \Delta\mu$ and temperatures $\beta_1 - \beta_2 = \Delta\beta$ brings correlations between particle and energy currents into sharper focus. Instead of linearizing the distribution function (e.g. see [121] for ballistic and diffusive thermoelectric coefficients), here the unified generalized currents embodied by various choices of (a, b) in Equation 6.4 are expanded to linear order $J_{d,t}^{a,b} \approx g_\mu^{a,b} \Delta\mu + g_\beta^{a,b} \Delta\beta$ around the average chemical potential $\mu_0 = (\mu_1 + \mu_2)/2$ and the average temperature T_0 given by $\beta_0 = 1/k_b T_0 = (\beta_1 + \beta_2)/2$. The linear coefficients are directly obtained as $g_\mu^{a,b} = (\partial J_{d,t}^{a,b} / \partial \mu)|_{\mu=\mu_0}$ and $g_\beta^{a,b} = (\partial J_{d,t}^{a,b} / \partial \beta)|_{\beta=\beta_0}$ and mapped to the traditional forms $J = L_{11} \Delta V + L_{12} \Delta T$ and $Q = L_{21} \Delta V + L_{22} \Delta T$, where $J = J_{d,t}^{1,0}$ is the charge current density and $Q = J_{d,t}^{1,1} - \mu_0 J_{d,t}^{1,0}$ is the heat current density in the linear response regime. Instead of the coefficients L_{ij} , the generalized linear coefficients obtained in experiments are the resistivity $\rho = \sigma^{-1} = L_{11}^{-1}$, the Seebeck coefficient $S = L_{12}/L_{11}$, the Peltier coefficient $\Pi = L_{21}/L_{11}$ and the electronic thermal conductivity $\kappa = L_{22} - L_{12}L_{21}/L_{11}$. The ballistic linear response coefficients obtained from Equation 6.4 are

$$\begin{aligned}
\rho &= \sigma^{-1} = \left(\frac{g_0 q^2}{h} \cdot \frac{\lambda_{dB_1}}{\lambda_{dB}^d} \cdot \frac{\Gamma(r+1)}{\Gamma(\frac{d+1}{2})} \cdot F_{r-1}^+(\eta) \right)^{-1}, \\
S &= -\frac{k_b}{q} \left[\eta - (r+1) \frac{F_r^+(\eta)}{F_{r-1}^+(\eta)} \right], \\
\Pi &= S \cdot T_0, \text{ and} \\
\kappa &= \frac{g_0 k_b^2 T_0}{h} \cdot \frac{\lambda_{dB_1}}{\lambda_{dB}^d} \cdot \frac{\Gamma(r+1)}{\Gamma(\frac{d+1}{2})} \cdot \\
&\quad [(r+1)(r+2)F_{r+1}^+(\eta) - (r+1)^2 \frac{(F_r^+(\eta))^2}{F_{r-1}^+(\eta)}]. \tag{6.17}
\end{aligned}$$

where g_0 is the product of spin and valley degeneracies, $\eta = \mu_0 \beta_0$, and $r = (d-1)/t$ generalizes the expressions for the several bandstructure types and dimensions. A conceptual difference of the ballistic coefficients is that the diffusive coefficients represent local properties, whereas the ballistic ones represent terminal (or system) properties as discussed lucidly for $d = 1$ by Butcher in [29]. The quantization of both σ and κ in $d = 1$ for $\eta \gg +1$ is explicit for all t in Equation 6.17. The Onsager symmetry relation $\Pi = ST_0$ is seen to remain valid for the ballistic situation for all d, t . The generalized Lorenz number $\mathcal{L}_{d,t} = \kappa/(\sigma T_0)$ obtained from Equations 6.17 goes to $\mathcal{L}_{d,t} \rightarrow \frac{\pi^2}{3} (\frac{k_b}{q})^2$ in the degenerate fermion limit of $\beta\mu \gg 1$ for all d and t , highlighting the robustness of the Wiedemann-Franz law in the ballistic limit [222, 29]. In the non-degenerate limit of $-\beta\mu \gg 1$ relevant for semiconductors, $\mathcal{L}_{d,t} \rightarrow (\frac{d-1}{t} + 1) (\frac{k_b}{q})^2$.

The generalized formulation of Equation 6.17 brings a novel feature of the dependence of the ballistic power factor ($S^2\sigma$) on dimensions and band-structures into sharp focus, as highlighted in Figure 6.3. Because the Seebeck coefficient $S \sim -\frac{k_b}{q} \cdot \frac{E_F - E_c}{k_b T}$ decreases with increasing E_F , whereas σ increases with increasing E_F , conventional wisdom states that the power factor product $S^2\sigma$ should exhibit a maximum somewhere near $E_F = E_c$. As Figure 6.3 shows, for all d, t the ballistic thermoelectric power factor $S^2\sigma$ indeed shows a maximum near $\mu = 0$, *except* for the $d = 3, t = 1$ conical elec-

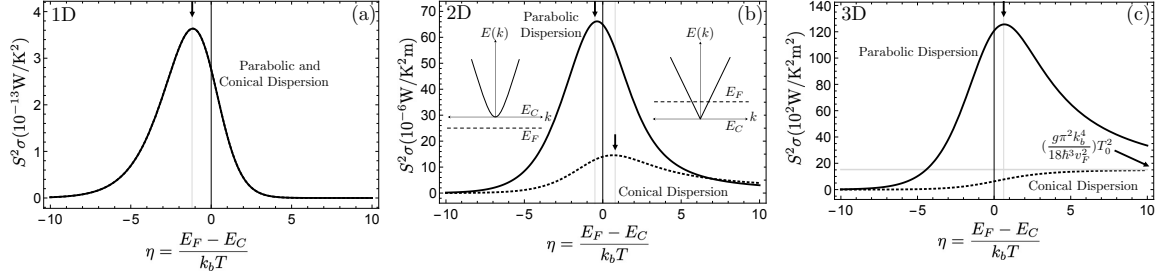


Figure 6.3: Ballistic Power factor in different dimensions plotted as a function of the Fermi level location via the dimensionless parameter $\eta = (E_F - E_C)/k_b T$ at 300 K. The dotted curve is the power factor for materials with conical dispersion $E = \hbar v_F |k|$ with $v_F = 10^6$ m/s and solid curve is the power factor for parabolic dispersion with $E = \hbar^2 k^2/2m$ with $m = 0.2m_e$. The arrows on the top show the η where the power factor shows maximum for both dispersions. Inset of Fig. 6.3(b) shows the conical and parabolic $E - k$ band-structures with the position of E_F for maximum power factor.

tron energy dispersion. For this case, it increases monotonically with μ and saturates to $S^2\sigma \rightarrow (\frac{g\pi^2 k_b^4}{18\hbar^3 v_F^2})T_0^2$. This behavior has neither been identified theoretically, nor observed experimentally in the past. This dependence of the power factor on the dimensionality warrants an experimental search for the monotonic increase with the Fermi level. Such behavior could potentially be observed in the bulk states of 3D topological Dirac semimetals such as Na_3Bi [118] and Cd_3As_2 [140]. This prediction emerged from the ballistic transport study and highlights an example of the value of the generalized d -dimensional formulation for various bandstructures that is achieved in this work.

6.1.6 Conclusions and Future Directions

The generalized ballistic current expression obtained in Equation 6.4 is found to be a versatile tool to compute and compare in a unified manner the particle and energy densities, charge and energy currents, thermoelectric coefficients and more for fermions

and bosons of various energy dispersions. Such a compact formulation is well suited for optimization problems, in which the extrema of one or more densities, currents, transport coefficients, or their combinations need to be determined as a function of the dimensionality, type of dispersion, effective masses, wave velocities etc. To facilitate such studies, the generalized ballistic currents $J_{d,t}^{a,b}$ for various a, b are summarized in Table 6.2, and Table 6.3 shows the linear response coefficients.

The energy dispersion types are not restricted to the specific cases of $t = 1, 2$ discussed, or to integers. The ballistic current expression may be extended for mixed dispersions of the tight-binding type $E = E_0 + 2t \cos ka \approx E_0 + 2t[1 - (ka)^2/2 + (ka)^4/24 \dots]$ near band edges, and to those that involve $k_i k_j$ and $k_i^a + k_j^b$, as present in some realistic systems, and topologically non-trivial terms may be introduced. Extending the formulation to multi-terminal cases in the spirit of the Landauer–Büttiker formalism [30, 47], and especially for generalized nonlinear response in a magnetic field for various dimensions and dispersions is of high interest. So is exploring the various non-linear response predictions for ballistic electronic and thermoelectric transport phenomena. Extension of this approach to ballistic particle and energy transport in hetero-dimensional situations (mixed d), and for mixed dispersions and statistics (e.g. plasmons or phonon-polaritons) is also suggested as future work. The formulation is not limited to electrons, photons and phonons as discussed here, and is applicable to molecular systems that undergo ballistic motion. Ballistic electron transport in condensed matter systems is seen primarily in nanoscale structures, which also have small numbers of particles, sometimes on the verge of failing the large number requirements on which traditional thermodynamic relations rest. The implications of recently revealed non-equilibrium thermodynamics equalities in nanoscale systems and on fluctuations of the densities, energies, and currents discussed here are therefore of significant theoretical and practical interest [77, 42].

Table 6.2: Generalized ballistic currents in d -dimensions for Fermions (+) and Bosons (−)

$J_{d,t}^{a,b}$, with $\eta = \frac{\mu}{k_b T}$. $[t = 1: E = \hbar v_F k] \ \& \ [t = 2: E = \frac{\hbar^2 k ^2}{2m}]$. $F_j^\pm(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty dx \frac{x^j}{\exp [x-\eta] \pm 1}$, and $F_0^\pm(\eta) = \pm \ln [1 \pm e^\eta]$.					
Particle Density		Energy Density	Particle Current	Heat Current	
$(d, t) \downarrow$	$(a, b) \rightarrow$	$(2)J_{d,t}^{0,0}$	$J_{d,t}^{1,0}$	$J_{d,t}^{1,1} - \mu J_{d,t}^{1,0}$	
$(1, 1)$	$2g(\frac{k_b T}{\hbar v_F}) F_0^\pm(\eta)$	$2g\frac{(k_b T)^2}{\hbar v_F} F_1^\pm(\eta)$	$g\frac{k_b T}{h} F_0^\pm(\eta)$	$g\frac{(k_b T)^2}{h} (F_1^\pm(\eta) - \eta F_0^\pm(\eta))$	
$(2, 1)$	$2\pi g(\frac{k_b T}{\hbar v_F})^2 F_1^\pm(\eta)$	$4\pi g\frac{(k_b T)^3}{(\hbar v_F)^2} F_2^\pm(\eta)$	$2g v_F (\frac{k_b T}{\hbar v_F})^2 F_1^\pm(\eta)$	$2g\frac{(k_b T)^3}{\hbar^2 v_F} (2F_2^\pm(\eta) - \eta F_1^\pm(\eta))$	
$(3, 1)$	$8\pi g(\frac{k_b T}{\hbar v_F})^3 F_2^\pm(\eta)$	$24\pi g\frac{(k_b T)^4}{(\hbar v_F)^3} F_3^\pm(\eta)$	$2\pi g v_F (\frac{k_b T}{\hbar v_F})^3 F_2^\pm(\eta)$	$2\pi g\frac{(k_b T)^4}{\hbar^3 v_F^2} (3F_3^\pm(\eta) - \eta F_2^\pm(\eta))$	
$(1, 2)$	$g(\frac{2\pi m k_b T}{\hbar^2})^{\frac{1}{2}} F_{-\frac{1}{2}}^\pm(\eta)$	$g\frac{k_b T}{2} (\frac{2\pi m k_b T}{\hbar^2})^{\frac{1}{2}} F_{\frac{1}{2}}^\pm(\eta)$	$g\frac{k_b T}{h} F_0^\pm(\eta)$	$g\frac{(k_b T)^2}{h} (F_1^\pm(\eta) - \eta F_0^\pm(\eta))$	
$(2, 2)$	$g(\frac{2\pi m k_b T}{\hbar^2}) F_0^\pm(\eta)$	$g\frac{k_b T}{2} (\frac{2\pi m k_b T}{\hbar^2}) F_1^\pm(\eta)$	$g\frac{k_b T}{h} (\frac{2\pi m k_b T}{\hbar^2})^{\frac{1}{2}} F_{\frac{1}{2}}^\pm(\eta)$	$g\frac{(k_b T)^2}{h} (\frac{2\pi m k_b T}{\hbar^2})^{\frac{1}{2}} \left(\frac{3}{2} F_{\frac{3}{2}}^\pm(\eta) - \eta F_{\frac{1}{2}}^\pm(\eta) \right)$	
$(3, 2)$	$g(\frac{2\pi m k_b T}{\hbar^2})^{\frac{3}{2}} F_{\frac{1}{2}}^\pm(\eta)$	$g\frac{3k_b T}{2} (\frac{2\pi m k_b T}{\hbar^2})^{\frac{3}{2}} F_{\frac{3}{2}}^\pm(\eta)$	$g\frac{k_b T}{h} (\frac{2\pi m k_b T}{\hbar^2}) F_1^\pm(\eta)$	$g\frac{(k_b T)^2}{h} (\frac{2\pi m k_b T}{\hbar^2}) (2F_2^\pm(\eta) - \eta F_1^\pm(\eta))$	

Table 6.3: Generalized ballistic linear response coefficients in d -dimensions

$\eta = \frac{\mu_0}{k_b T_0}$ and $g_0 = (\text{spin degeneracy}) \times (\text{valley degeneracy})$. Note: The Peltier Coefficient $\Pi = S \cdot T_0$ by the Onsager relation.			
$(d, t) \downarrow$	Resistivity $\rho = \sigma^{-1}$	Seebeck Coefficient S	Thermal Conductivity κ
$(1, 1)$	$\left(\frac{g_0 q^2}{h} \frac{1}{1+e^{-\eta}} \right)^{-1}$	$-\frac{k_b}{q} (\eta - (1 + e^{-\eta}) \ln[1 + e^{\eta}])$	$\frac{g_0 k_b^2 T_0}{h} (2F_1^+(\eta) - (1 + e^{-\eta}) \ln^2[1 + e^{\eta}])$
$(2, 1)$	$\left(\frac{2g_0 q^2}{h} \left(\frac{k_b T_0}{h\nu_F} \right) \ln[1 + e^{\eta}] \right)^{-1}$	$-\frac{k_b}{q} \left(\eta - \frac{2F_1^+(\eta)}{\ln[1+e^{\eta}]} \right)$	$4g_0 k_b \frac{(k_b T_0)^2}{h^2 \nu_F} \left(3F_2^+(\eta) - \frac{2(F_1^+(\eta))^2}{\ln[1+e^{\eta}]} \right)$
$(3, 1)$	$\left(\frac{2\pi g_0 q^2}{h} \left(\frac{k_b T_0}{h\nu_F} \right) {}^2F_1^+(\eta) \right)^{-1}$	$-\frac{k_b}{q} \left(\eta - \frac{3F_2^+(\eta)}{F_1^+(\eta)} \right)$	$6\pi g_0 k_b \frac{(k_b T_0)^3}{h^3 \nu_F^2} \left(4F_3^+(\eta) - 3 \frac{(F_2^+(\eta))^2}{F_1^+(\eta)} \right)$
$(1, 2)$	$\left(\frac{g_0 q^2}{h} \frac{1}{1+e^{-\eta}} \right)^{-1}$	$-\frac{k_b}{q} (\eta - (1 + e^{-\eta}) \ln[1 + e^{\eta}])$	$\frac{g_0 k_b^2 T_0}{h} (2F_1^+(\eta) - (1 + e^{-\eta}) \ln^2[1 + e^{\eta}])$
$(2, 2)$	$\left(\frac{g_0 q^2}{h} \left(\frac{2\pi m k_b T_0}{h^2} \right)^{\frac{1}{2}} F_{-\frac{3}{2}}^+(\eta) \right)^{-1}$	$-\frac{k_b}{q} \left(\eta - \frac{3}{2} \frac{F_{\frac{1}{2}}^+(\eta)}{F_{-\frac{3}{2}}^+(\eta)} \right)$	$\frac{3g_0}{4} \frac{k_b^2 T_0}{h} \left(\frac{2\pi m k_b T_0}{h^2} \right)^{\frac{1}{2}} \left(5F_{\frac{3}{2}}^+(\eta) - 3 \frac{(F_{\frac{1}{2}}^+(\eta))^2}{F_{-\frac{3}{2}}^+(\eta)} \right)$
$(3, 2)$	$\left(\frac{g_0 q^2}{h} \left(\frac{2\pi m k_b T_0}{h^2} \right) \ln[1 + e^{\eta}] \right)^{-1}$	$-\frac{k_b}{q} \left(\eta - \frac{2F_1^+(\eta)}{\ln[1+e^{\eta}]} \right)$	$2g_0 \frac{k_b^2 T_0}{h} \left(\frac{2\pi m k_b T_0}{h^2} \right) \left(3F_2^+(\eta) - 2 \frac{(F_1^+(\eta))^2}{\ln[1+e^{\eta}]} \right)$

6.2 Intrinsic limit of optical phonon limited electronic currents in parabolic and conical bandstructures in d -dimensions

6.2.1 Introduction

With the rise of nanoscale transistor technologies, as the lateral electric fields in a field-effect transistor (FET) increase, the average injection velocities (v_{inj}) of charge carriers approach the saturation values (v_{sat}) due to the increase in the scattering rate with phonons. While the low-field transport properties such as mobility are essential in understanding and optimizing the material properties for various electronic applications, the performance of electronic devices such as RF amplifiers and highly scaled transistors depend strongly on high-field transport where the carrier velocity is no longer proportional to the electric field but rather saturates. Back in the early 1950s, in his pioneering work, Shockley [167] showed that the high-field saturation velocity in 3D bulk semiconductors such as Germanium was limited by optical phonon scattering. Consequently, from rule-of-thumb considerations, the saturation velocity in a non-degenerate semiconductor is given by $v_{sat} = \sqrt{\hbar\omega_{op}/m^*}$, where ω_{op} is the optical phonon frequency and m^* is the effective electronic mass in the material. This saturation velocity has no dependence on carrier density and it is an intrinsic property of the bulk material but at high carrier densities and for materials with strong electron-phonon interaction, this simplified picture of velocity saturation breaks down.

In order to characterize the nature of high-field transport i.e. to effectively obtain v_{sat} , the study of velocity field curves is necessary. While the experimental measurement of velocity field curves presents its own possible challenges such as sample self-heating, spurious substrate effects etc., the theoretical modeling isn't straightforward either with

the Monte Carlo method being the norm for such simulations since the 1970s. Monte Carlo simulations are time intensive and require a large number of input parameters, and since it is a statistical way to solve the Boltzmann transport equation, often times it falls short of providing a physical insight behind the observed effects. Through this work, we aim to provide a simple, unified physical model to accurately estimate the saturation velocity and its charge carrier density dependence over a wide range of material systems across various dimensions.

To accurately model the electron-phonon scattering, a close examination of the strength of electron-optical phonon interactions in the material of interest is critical. In the past few decades, the consensus has been that in materials with strong electron-optical phonon coupling, the accumulation of hot phonons increases the momentum relaxation time of electrons while not changing the energy relaxation time which leads to velocity saturation at a high field. In general, if the lifetime of optical phonons τ_{ph} in the electron channel is much longer than their generation time τ_{e-ph} , the resulting accumulation of nonequilibrium phonons would eventually manifest itself as the drift velocity getting clamped, i.e. not changing with the field.

Strength of electron-optical phonon interaction: The generation rate of LO phonons by electrons heated by an external electric field in any material is given by the polar Fröhlich interaction

$$\frac{1}{\tau_{e-ph}} = \frac{q^2}{4\pi\hbar} \sqrt{\frac{2m^*\hbar\omega_{LO}}{\hbar^2}} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right), \quad (6.18)$$

where q is the electron charge, $\hbar$ is the reduced Planck's constant, $\hbar\omega_{LO}$ is the LO phonon energy, m^* is the electron effective mass, and ϵ_∞ and ϵ_0 are the high-frequency and dc dielectric constants in the material under investigation. Table 6.4 lists this generation rate and compares it with phonon lifetimes for various polar semiconductors.

Table 6.4: Material parameters and theoretical electron-phonon scattering time

Material parameters used in calculation						
	GaN	AlN	InN	GaAs	β -Ga ₂ O ₃	h-BN
Effective Mass m^*	0.21	0.4	0.1	0.063	0.28	0.26
Band gap E_g / eV	3.39	6.026	0.7	1.42	4.6-4.9	5.9
Static permittivity ϵ_0	9.7	8.5	15.3	12.9	10.2	7.04
High-frequency permittivity ϵ_∞	5.28	5.35	8.4	10.89	3.57	4.95
Optical phonon energy $\hbar\omega_{LO}$ / meV	92	99.2	73	35	44	169.5
Timescales						
τ_{e-ph} / fs (theoretical from Equation 1)	7.47	6.50	19.5	133.4	4.43	7.11
τ_{ph} / fs (experimental at 300K)	3000	580	660	-	-	-

6.2.2 Description of the optical phonon-induced scattering model

In typical nanoscale transistors, carriers injected from the source and moving along the channel have little probability of being backscattered because the mean free path can exceed the channel length. However, this is not the case in materials with high carrier density, strong electron-phonon interaction, and long phonon lifetime where it is absolutely necessary to take into account optical phonon-induced carrier backscattering. When an electron accelerates a length $l_T = \hbar\omega_{op}/qE_{ext} = (\hbar\omega_{LO}/qV_{ds}) \cdot L$ in the electric field E_{ext} it attains sufficient excess energy to emit an optical phonon. Once this energy is attained by the electron, the energetic electrons emit optical phonons on a length scale given by the mean free path $\lambda_{op} \sim a_B^* \epsilon_\infty / (\epsilon_0 - \epsilon_\infty)$ [51]. Here a_B^* is the effective Bohr

radius. The total length that the electron traverses before an optical phonon scattering event occurs is on the order of $l_T + \lambda_{op}$, which can be approximated as λ_{op} in devices with sufficiently small channel lengths. For materials with strong electron-phonon interaction such as GaN, β -Ga₂O₃, h-BN etc. λ_{op} approximately evaluates to 3.5 nm, 9 nm and 3.4 nm respectively. These length scales are much shorter than most other semiconductors such as Si and GaAs, the mean free paths in which are 20 nm and 100 nm respectively.

The onset of optical phonon emission can be understood more clearly near the limit of zero temperature when as soon as the applied voltage is large enough for the electrons to emit a single phonon, $V_{ds} \geq \hbar\omega_{op}/q$, the carrier instantaneously loses an energy $\hbar\omega_{op}$ to the lattice while the electron relaxes to the bottom of its band after the inelastic phonon emission event. So, at a sufficiently high field, it is energetically favorable for the high energy carriers injected from the source to emit optical phonons and backscatter into the source, thus leading to a back-current of the carriers and thereby clamping the net forward current. This model is illustrated in Figure 6.4. The seeds of this simple yet novel model of optical phonon scattering limited electronic transport were first laid down by Jena *et al.* [79] in one-dimensional semiconductors such as CNTs, this model was later extended to explain the high field transport in Graphene [52] and finally it was used to explain the velocity saturation in GaN HEMTs [51]. The crux of the model is that the energy difference between injected and back-scattered electrons ($E_{FS} - E_{FD}$) is fixed by the optical phonon energy $\hbar\omega_{op}$ due to ultra-fast optical emission, meaning at saturation ($qV_{ds} \geq \hbar\omega_{op}$): $E_{FS} - E_{FD} = \hbar\omega_{op}$ and hence, $\eta_S - \eta_D = \hbar\omega_{op}/k_bT$. It is important to note that below the saturation i.e. at low-field, the difference in quasi-Fermi levels $E_{FS} - E_{FD}$ is still given by the applied bias ($qV_{ds} < \hbar\omega_{op}$): $E_{FS} - E_{FD} = qV_{ds}$. This model has also been applied to study optical-phonon-limited high-field transport in layered materials [32]. We can extend the same model to a more general scenario

in order to find the limit of current density in such an optical phonon scattering limited transport regime for d -dimensional material with polynomial band structure of order t . Employing the generalized ballistic transport formulation presented in the previous section, we can write the current density J_d and carrier concentration n_d as:

$$J_d = J_0 \cdot \left[F_{\frac{d-1}{t}}(\eta_S) - F_{\frac{d-1}{t}}\left(\eta_S - \frac{\hbar\omega_{op}}{k_b T}\right) \right], \quad (6.19)$$

$$n_d = g_s g_v \cdot \frac{1}{(\lambda_{dB})^d} \cdot \frac{\Gamma\left(\frac{d}{t}\right)}{t \Gamma\left(\frac{d}{2}\right)} \cdot \left[F_{\frac{d-t}{t}}(\eta_S) + F_{\frac{d-t}{t}}\left(\eta_S - \frac{\hbar\omega_{op}}{k_b T}\right) \right]. \quad (6.20)$$

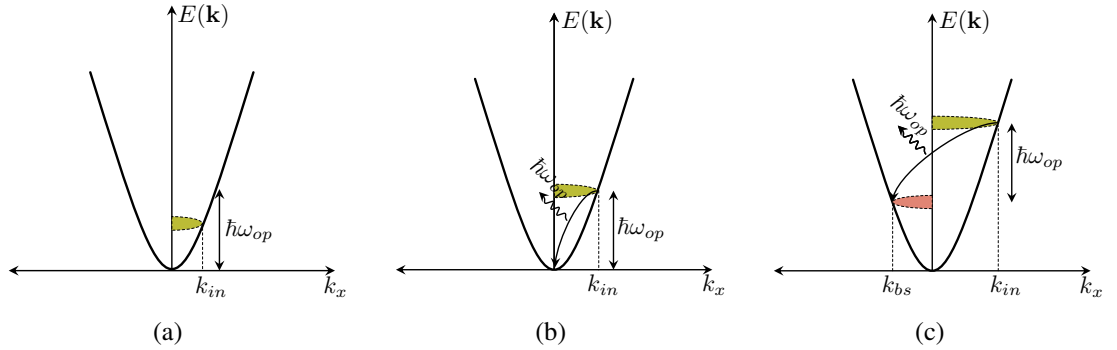


Figure 6.4: Arbitrary energy band diagram with increasing carrier densities from (a) to (c), at the top of the barrier, in the optical phonon scattering model. The momentum states of injected and back-scattered electrons are indicated by k_{in} and k_{bs} respectively. Optical phonon scattering takes place once the energy of injected electrons gets higher than $\hbar\omega_{op}$ and then the difference in the energies of injected and backscattered electrons is locked to $\hbar\omega_{op}$.

Injection velocity: To connect with the classical notion of current being a product of charge and velocity, one can define an ensemble injection velocity v_{inj} as simply the net current divided by the net sheet charge qn_d at the source injection point via the relation

$v_{inj} = J_d / qn_d$:

$$v_{inj} = \underbrace{\lambda_{dB_1} \cdot \frac{k_b T}{h}}_{\text{Thermal velocity}=v_{th}} \cdot \underbrace{\frac{\gamma_I}{\gamma_n}}_{\text{Numerical Factor}=\gamma_v} \cdot \left[\frac{F_{\frac{d-1}{t}}(\eta_S) - F_{\frac{d-1}{t}}(\eta_D)}{F_{\frac{d-t}{t}}(\eta_S) + F_{\frac{d-t}{t}}(\eta_D)} \right]. \quad (6.21)$$

We observe from Eq. (6.21) that the injection velocity v_{inj} is simply the thermal velocity times a numerical factor (γ_v) dependent on d and t times a voltage-dependent ratio of Fermi-Dirac integrals. The numerical factor γ_v is given by:

$$\gamma_v = \begin{cases} \frac{\pi^{\frac{1}{2}} t}{\Gamma(\frac{1}{t})} & d = 1 \\ 2 \frac{\Gamma(\frac{d-1}{t}) \cdot \Gamma(\frac{d}{2})}{\Gamma(\frac{d-1}{2}) \cdot \Gamma(\frac{d}{t})} & d > 1 \end{cases} \quad (6.22)$$

We can estimate the thermal velocity (v_{th}) at 300K for two cases.

1. Conical band-structure $E = \hbar v_F |k|$, $t = 1$, $v_F = 10^8$ cm/s: $v_{th} = 5.64 \times 10^7$ cm/s.
2. Parabolic band-structure $E = \frac{\hbar^2 k^2}{2m^*}$, $t = 2$, $m^* = 0.2 \cdot m_e$: $v_{th} = 6.01 \times 10^6$ cm/s.

Eq. (6.21) gives us a compact expression for the injection velocity in ballistic conduction, but the expression in such a form is not always easy to solve analytically, so we consider two extreme limits: non-degenerate and degenerate, of Eq. (6.21) to see how v_{inj} behaves. Degenerate limit $\eta_S \gg 1$ is the physical limit of the system at very high carrier density or at very low temperature. Similarly, the non-degenerate limit $\eta_S \ll -1$ is the limit at very low carrier density or very high temperature. Using the approximations for Fermi-Dirac integrals, we find:

$$v_{inj} = \begin{cases} v_{th} \cdot \gamma_v \cdot \tanh\left(\frac{qV_{ds}}{2k_b T}\right) & \eta_S \ll -1 \\ v_{th} \cdot \gamma_v \cdot \frac{1 - \left(1 - \frac{v_d}{\eta_S}\right)^{\frac{d-1}{t} + 1}}{1 - \left(1 + \frac{v_d}{\eta_S}\right)^{\frac{d-1}{t} + 1}} & \eta_S \gg 1 \end{cases} \quad (6.23)$$

For small V_{ds} such that $v_d = \frac{qV_{ds}}{k_bT} \ll \eta_S$, we can simplify the degenerate limit ($\eta_S \gg 1$) even further:

$$v_{inj} = v_{th} \cdot \gamma_v \cdot \frac{(d+t-1) \frac{v_d}{\eta_S}}{2t - (d+t-1) \frac{v_d}{\eta_S}}. \quad (6.24)$$

It is interesting to note that $\gamma_v \leq 2$ for $d \in \{1, 2, 3\}$ and $t \in \{1, 2\}$. So, in the non-degenerate limit (very high temperature or very low carrier concentration), $\forall V_{ds}$ $v_{inj} \leq 2v_{th}$ if $d \in \{1, 2, 3\}$ and $t \in \{1, 2\}$.

6.2.3 Results in the optical phonon scattering limit

Injection current as a function of carrier density

We will now try to solve Equations (6.19) and (6.20) in the high-density (and high-current) regime to get a dependence of J_d on n_d . Since it is difficult to solve this system of equations analytically, we can use the degenerate approximation for Fermi-Dirac integrals $F_j(\eta) \approx \eta^{j+1}/\Gamma(j+2)$. This degenerate approximation is valid for $\eta \gg 1$ which in our case would correspond to either very high carrier concentration or very low temperature. Using the approximation we get,

$$J_d \approx J_0 \cdot \left[\frac{\eta_S^{\frac{d-1}{t}+1}}{\Gamma(\frac{d-1}{t}+2)} - \frac{\left(\eta_S - \frac{\hbar\omega_{op}}{k_bT}\right)^{\frac{d-1}{t}+1}}{\Gamma(\frac{d-1}{t}+2)} \right], \quad (6.25)$$

$$n_d \approx \frac{g_s g_v}{\lambda_{dB}^d} \cdot \frac{\Gamma(\frac{d}{t})}{t\Gamma(\frac{d}{2})} \cdot \left[\frac{\eta_S^{\frac{d}{t}}}{\Gamma(\frac{d}{t}+1)} + \frac{\left(\eta_S - \frac{\hbar\omega_{op}}{k_bT}\right)^{\frac{d}{t}}}{\Gamma(\frac{d}{t}+1)} \right]. \quad (6.26)$$

On solving equations (6.25) and (6.26), while making the approximation $\hbar\omega_{op}/k_B T \ll$

η_S , we get the following relationship between J_d and n_d :

$$J_d \approx \underbrace{\frac{(g_s g_v)^{\frac{1}{d}} q}{2\pi \Gamma(\frac{d+1}{2})} \cdot \left(\frac{d \cdot \Gamma(\frac{d}{2})}{2} \right)^{\frac{d-1}{d}}}_{\text{characteristic property of } d} \cdot \omega_{op} \cdot n_d^{\frac{d-1}{d}} \quad (6.27)$$

The above relationship between J_d and n_d is plotted in Fig. 6.5 for different dimensions. From Eq. (6.27), clearly $J_d \propto n_d^{\frac{d-1}{d}}$. What is interesting to note is that in the optical phonon saturation limit, the saturation current does not depend on the type of band-structure (no t or α dependence) and is only dependent on the number of dimensions d . Fig. 6.5 shows this d -dependence of J_d . Note that the above expressions are approximately true when $n > n_{op}$ where n_{op} is the degenerate limit of carrier concentration when the Fermi-energy is equal to the optical phonon energy: $E_F = \hbar\omega_{op}$.

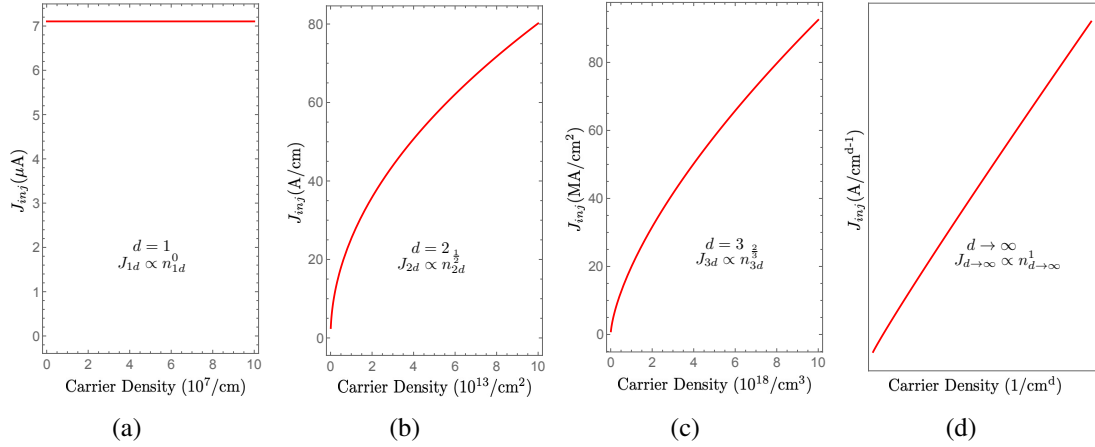


Figure 6.5: The saturation current versus carrier concentration in various dimensions.

Injection velocity as a function of carrier density

We can evaluate v_{inj} in the optical phonon limited regime as

$$v_{inj} = v_{th} \cdot \gamma_v \cdot \left[\frac{F_{\frac{d-1}{t}}(\eta_S) - F_{\frac{d-1}{t}}\left(\eta_S - \frac{\hbar\omega_{op}}{k_b T}\right)}{F_{\frac{d-t}{t}}(\eta_S) + F_{\frac{d-t}{t}}\left(\eta_S - \frac{\hbar\omega_{op}}{k_b T}\right)} \right]. \quad (6.28)$$

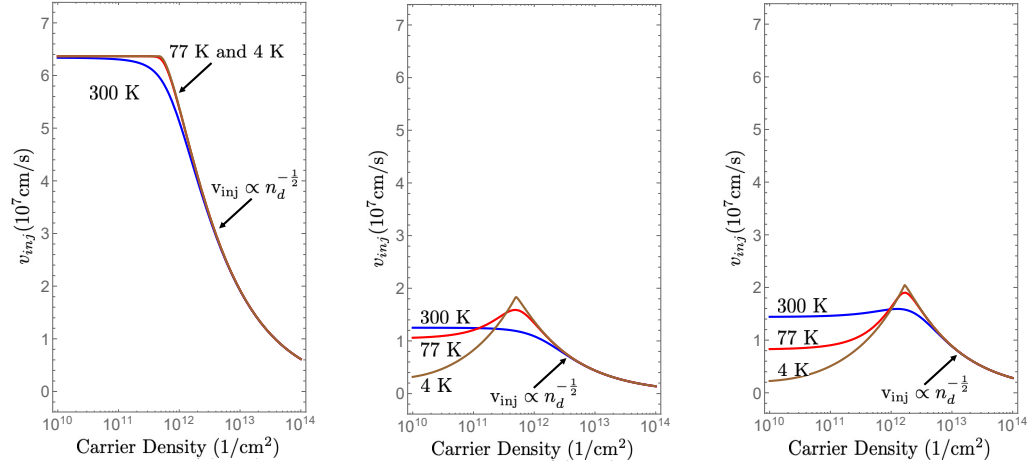
Using Eq. 6.28, we can plot the optical phonon limited injection velocity in 2D for both conical and parabolic bands for different material systems as shown in Fig. 6.6. In Fig. 6.6(a), injection velocity varies with carrier concentration and is not constant for graphene. The injection velocity in graphene approaches a magnitude that is proportional to the Fermi velocity in it, $v_{inj} \rightarrow \frac{2}{\pi} v_F \sim 6.3 \times 10^7 \text{cm/s}$ as $n_d \rightarrow 0$, and falls to $\sim 10^7 \text{cm/s}$ as $n_d \sim 10^{13} / \text{cm}^2$. The fall-off follows the square-root relation as proposed in Ref.[52]. In Fig. 6.6(e), for GaN 2DEG, just like graphene we observe that the injection velocity is not constant, and in fact, has a peak at carrier concentration $n_d = 3 \sim 4 \times 10^{12} / \text{cm}^2$ depending on temperature, and falls off as $n_d^{-\frac{1}{2}}$ at higher carrier density. Recently, Romanczyk *et al.* [160] experimentally confirmed this "peaky" behavior of injection velocity as a function of gate bias (which in turn controls the carrier density in the channel) in N-polar GaN HEMTs, thus highlighting the utility of this simple model.

To understand how v_{inj} behaves as a function of n_d , we can take the two asymptotic limits of v_{inj} as done previously. To find the injection velocity v_{inj} dependence on carrier concentration n_d for the limit $n_d \gg n_{op}$ ($n_d \ll n_{op}$), we take the degenerate (non-degenerate) limit of Eq. 6.28 to obtain:

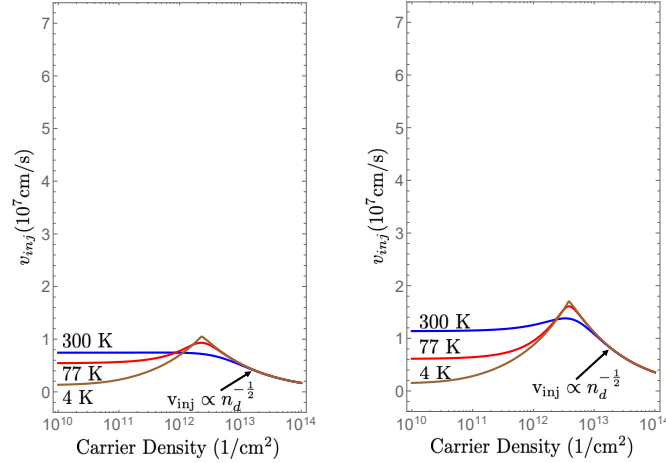
$$v_{inj}(n_d) = \begin{cases} v_{th} \cdot \gamma_v \cdot \tanh\left(\frac{\hbar \omega_{op}}{2k_b T}\right) & n_d \ll n_{op} \\ \frac{(g_s g_v)^{\frac{1}{d}} q}{2\pi \Gamma\left(\frac{d+1}{2}\right)} \cdot \left(\frac{d \cdot \Gamma\left(\frac{d}{2}\right)}{2}\right)^{\frac{d-1}{d}} \cdot \omega_{op} \cdot n_d^{-\frac{1}{d}} & n_d \gg n_{op}. \end{cases} \quad (6.29)$$

6.2.4 Discussion

The optical phonon model presented in this section can be used to extract useful device parameters such as its transconductance and cut-off frequency. The intrinsic transconductance of a FET is given by



(a) For conical band ($E = \hbar v_F |k|$), with $v_F = 10^8$ cm/s and $E_{op} = 160$ meV (for Graphene).
 (b) For parabolic band ($E = \frac{\hbar^2 k^2}{2m^*}$), with $m^* = 0.067 * m_e$ and $E_{op} = 36$ meV (for GaAs).
 (c) For parabolic band ($E = \frac{\hbar^2 k^2}{2m^*}$), with $m^* = 0.11 * m_e$ and $E_{op} = 73$ meV (for InN).



(d) For parabolic band ($E = \frac{\hbar^2 k^2}{2m^*}$), with $m^* = 0.25 * m_e$ and $E_{op} = 44$ meV (for Ga_2O_3).
 (e) For parabolic band ($E = \frac{\hbar^2 k^2}{2m^*}$), with $m^* = 0.2 * m_e$ and $E_{op} = 92$ meV (for GaN).

Figure 6.6: Injection velocity as a function of carrier density in 2D for various material systems.

$$g_m = \frac{\partial J_d}{\partial V_g} = C_{gs} (v_{sat} + n_d \frac{\partial v_{sat}}{\partial n_d}), \quad (6.30)$$

where C_{gs} is the intrinsic capacitance per unit area between the gate metal and the source injection point and n_d is the carrier concentration at that point. The second term

is negligible for a transistor working in the saturation region. C_{gs} can be solved as a function of V_{gs} using a self-consistent Poisson-Schrodinger solver for a given FET device, to get a quantitative dependence of g_m on V_{gs} .

Similarly, the cut-off frequency f_T of a transistor follows the same trend as transconductance as the gate voltage changes. The cut-off frequency of a transistor is given by

$$2\pi f_T = \frac{1}{\frac{C_{gs}+C_{gd}}{g_m} + C_{gd}(R_s + R_d)}, \quad (6.31)$$

where C_{gd} , R_s , and R_d are parasitic capacitance and resistances and g_m is the intrinsic transconductance. Without any parasitic effects, the intrinsic delay of the transistor is $\tau_c = C_{gs}/g_m$. The intrinsic delay can also be written as the ratio of gate length and electron velocity, that is $\tau_c = L_g/v_{in}$, which only depends on the device geometry (L_g) and the material property (v_{in}).

This phonon model can help obtain current drive, g_m , and f_T for a wide variety of transistors ranging across material systems and dimensions. In our model, the optical phonon scattering is considered alone. We ignore other scattering mechanisms, like acoustic phonon and interface roughness scattering. In systems where other scattering mechanisms start dominating, this simple model will break down. Optical phonon scattering sets the velocity limit of the carrier injected from source to channel. Although the model is based on an assumed electron distribution in k -space, its simplicity makes it a useful analytical design tool.

APPENDIX A

GENERALIZED KINETIC COEFFICIENTS IN BOLTZMANN TRANSPORT REGIME FOR ISOTROPIC DISPERSIONS IN GENERALIZED DIMENSIONS

An analytical formula is derived for particle and energy densities, and their momentum and energy currents for isotropic energy dispersions in generalized dimensions in the diffusive regime. The formulation considerably simplifies the comparison of the statistical properties and particle and energy transport currents of electrons, in various dimensions in a unified manner.

The electric current density j and heat current density w_q for isotropic bandstructure $E(k) = \alpha_t |k|^t$ in d -dimensions and $f = f_0 - (\partial f_0 / \partial E) \delta \phi$ are given by:

$$\begin{aligned} j &= -\frac{e}{\hbar} \int d^d k \nabla_k E(k) \left(-\frac{\partial f_0}{\partial E} \right) \delta \phi g(k), \\ w_q &= \frac{1}{\hbar} \int d^d k \nabla_k E(k) \left(-\frac{\partial f_0}{\partial E} \right) (E(k) - \mu) \delta \phi g(k). \end{aligned} \quad (\text{A.1})$$

Following Madelung's notations we can write down j and w_q as functions of fields E and B , and of the temperature gradient $\frac{\nabla T}{T}$ as:

$$\begin{aligned} j &= M_{00}E + M_{10}B \times E + M_{20}B(B \cdot E) \\ &\quad + M_{01}\frac{\nabla T}{T} + M_{11}B \times \frac{\nabla T}{T} + M_{21}B(\mathbf{B} \cdot \frac{\nabla T}{T}), \\ -w_q &= M_{01}E + M_{11}B \times E + M_{21}B(B \cdot E) \\ &\quad + M_{02}\frac{\nabla T}{T} + M_{12}B \times \frac{\nabla T}{T} + M_{22}B(\mathbf{B} \cdot \frac{\nabla T}{T}). \end{aligned} \quad (\text{A.2})$$

We then find for the M_{ik} in d -dimensions and type t bandstructure as $M_{ik}^{d,t}$ given by:

$$M_{ik}^{d,t} = \mathcal{C}_{ik}^{d,t} \int_0^\infty \frac{E^{1+\frac{d-2}{t}+(1-\frac{2}{t})i}}{1+E^{2-\frac{4}{t}}(\tau(E))^2 s^2} \cdot (\tau(E))^{i+1} \cdot (E-\mu)^k \left(-\frac{\partial f_0}{\partial E} \right) dE \quad (\text{A.3})$$

where $\mathcal{C}_{ik}^{d,t} = \frac{ge^{2+i-k}t^{i+1}\alpha_t^{\frac{2i+2-d}{t}}}{(2\sqrt{\pi})^d\Gamma(\frac{d}{2}+1)\hbar^{2i+2}}$ and $s = et\alpha_t^{\frac{2}{t}}B/\hbar^2$. It is also important to note that $\{i, k\} \in \{0, 1, 2\}$.

A.1 Thermo-electric effects

While dealing with thermo-electric coefficients we can effectively consider $B = 0$. To first explore the validity of the Wiedemann-Franz Law, the Equation A.2 becomes

$$\begin{aligned} j &= M_{00}^{d,t} E + M_{01}^{d,t} \frac{\nabla T}{T}, \\ -w_q &= M_{01}^{d,t} E + M_{02}^{d,t} \frac{\nabla T}{T}. \end{aligned} \quad (\text{A.4})$$

The electronic thermal conductivity $\kappa = 1/T [M_{02}^{d,t} - ((M_{01}^{d,t})^2 / M_{00}^{d,t})]$ and electrical conductivity $\sigma = M_{00}^{d,t}$. To check the validity of Wiedemann-Franz Law, we evaluate $\kappa / \sigma T$

$$\begin{aligned} \frac{\kappa}{\sigma T} &= \frac{1}{T^2} \left(\frac{M_{02}^{d,t}}{M_{00}^{d,t}} - \left(\frac{M_{01}^{d,t}}{M_{00}^{d,t}} \right)^2 \right) \\ &= \frac{1}{e^2 T^2} \left(\frac{\mathcal{J}_{3+\frac{d-2}{t}}}{\mathcal{J}_{1+\frac{d-2}{t}}} - \left(\frac{\mathcal{J}_{2+\frac{d-2}{t}}}{\mathcal{J}_{1+\frac{d-2}{t}}} \right)^2 \right). \end{aligned} \quad (\text{A.5})$$

Here we define the integral $\mathcal{J}_a = \int_0^\infty E^a \tau(E) (-\partial f_0 / \partial E) dE$. The whole question reduces to finding the expression for $\mathcal{J}_a$ which can be done under various approximations.

A.1.1 Degenerate condition

Using Sommerfeld Expansion, we can easily write

$$\begin{aligned} \mathcal{J}_a &= \mu^a \tau(\mu) + \frac{\pi^2}{6} (k_b T)^2 [a(a-1) \mu^{a-2} \tau(\mu) \\ &\quad + 2a \mu^{a-1} \tau'(\mu) + \mu^a \tau''(\mu)]. \end{aligned} \quad (\text{A.6})$$

When we substitute this in Equation A.5, we get the Wiedemann-Franz law: $\mathcal{L}_{d,t} = \frac{\kappa}{\sigma T} \rightarrow \frac{\pi^2}{3} \left(\frac{k_b}{e} \right)^2$ where $\mathcal{L}_{d,t}$ is often called Lorenz number.

A.1.2 Non-degenerate conditions

If we know the exact form of $\tau(E)$ depending upon the various scattering processes involved, the integral $\mathcal{J}_a$ should be fairly easy to evaluate as in the degenerate limit $\mathcal{J}_a \propto \int_0^\infty E^a \tau(E) e^{-\frac{E}{k_b T}} dE$. Let us take the specific case when we describe the relaxation time τ by a power law $\tau(E) = \tau_0 (\frac{E}{k_b T})^r$. We get $\mathcal{J}_a = \tau_0 (k_b T)^a \Gamma(a+r+1) F_{a+r-1}(\eta)$ where $F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty dx \frac{x^j}{\exp[x-\eta]+1}$ is the Fermi-Dirac integral and $\eta = \mu/k_b T$. In the non-degenerate limit $\mathcal{J}_a$ then becomes $\tau_0 (k_b T)^a \Gamma(a+r+1) e^\eta$. When we substitute this in Equation A.5, we get the Wiedemann-Franz law: $\mathcal{L}_{d,t} \rightarrow (\frac{d-2}{t} + r + 2) (\frac{k_b}{e})^2$.

A.2 Non-Zero Magnetic Field

A.2.1 Weak magnetic fields

In order to simplify Equation A.3, let us consider $|B| \ll 1$ such that Equation A.3 can be expanded in increasing powers of the magnetic field. We can reduce all integrals to the form

$$\int_0^\infty E^a (\tau(E))^b \left(-\frac{\partial f_0}{\partial E} \right) dE \quad (\text{A.7})$$

which again simply converts to $\tau_0^b \Gamma(a+rb+1) F_{a+rb-1}(\eta)$ for power law scattering $\tau(E) = \tau_0 E^r$.

A.2.2 Strong magnetic fields

In order to simplify Equation A.3, let us consider $|B| \gg 1$ such that Equation A.3 can be written as

$$M_{ik}^{d,t} = \mathcal{D}_{ik}^{d,t}(B) \int_0^\infty E^{\frac{d+2}{t} + (1-\frac{2}{t})i-1} \cdot (\tau(E))^{i-1} \cdot (E-\mu)^k \left(-\frac{\partial f_0}{\partial E} \right) dE$$

where $\mathcal{D}_{ik}^{d,t} = \mathcal{C}_{ik}^{d,t} \cdot \frac{\hbar^4}{e^2 t^2 \alpha_t^{\frac{4}{t}} |B|^2}$. For power law scattering $\tau(E) = \tau_0 E^r$, we can further simplify to

$$M_{ik}^{d,t} = \mathcal{D}_{ik}^{d,t}(B) \int_0^\infty E^{\frac{d+2}{t} + (1-\frac{2}{t}+r)i-1-r} \cdot (E-\mu)^k \left(-\frac{\partial f_0}{\partial E} \right) dE. \quad (\text{A.8})$$

The kinetic coefficients then become

$$\begin{aligned} M_{i0}^{d,t} &= \mathcal{D}_{i0}^{d,t} \Gamma(u+1) F_{u-1}(\eta) \\ M_{i1}^{d,t} &= \mathcal{D}_{i1}^{d,t} [\Gamma(u+2) F_u(\eta) - \mu \Gamma(u+1) F_{u-1}(\eta)] \\ M_{i2}^{d,t} &= \mathcal{D}_{i2}^{d,t} [\Gamma(u+3) F_{u+1}(\eta) - 2\mu \Gamma(u+2) F_u(\eta) + \\ &\quad \mu^2 \Gamma(u+1) F_{u-1}(\eta)]. \end{aligned} \quad (\text{A.9})$$

$$\text{Here } u = \frac{d+2}{t} + (1 - \frac{2}{t} + r)i - 1 - r.$$

A.3 Conductivity and mobility

We can write the generalized conductivity as:

$$\sigma_{d,t} = M_{00}^{d,t} = \frac{g e^2 t \alpha_t^{\frac{2-d}{t}}}{(4\pi)^{\frac{d}{2}} \Gamma(\frac{d}{2} + 1) \hbar^2} \int_0^\infty E^{1+\frac{d-2}{t}} \tau(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \quad (\text{A.10})$$

We can write the generalized mobility as:

$$\mu_{d,t} = \frac{\sigma_{d,t}}{en_{d,t}} = \frac{2e\alpha_t^{2/t} (k_b T)^{1-\frac{2}{t}}}{\hbar^2} \underbrace{\frac{\int_0^\infty \frac{u^{1+\frac{d-2}{t}} \tau(u) du}{\cosh^2(\frac{u-\eta}{2})}}{\frac{8d}{t^2} \Gamma(\frac{d}{t}) F_{\frac{d}{t}-1}(\eta)}}_{\tau_{d,t}} \quad (\text{A.11})$$

For power law $\tau(E) = \tau_0(\frac{E}{k_b T})^r$, $\sigma_{d,t}$ simplifies to:

$$\sigma_{d,t} = \frac{ge^2 t \alpha_t^{\frac{2-d}{t}}}{(4\pi)^{\frac{d}{2}} \Gamma(\frac{d}{2} + 1) \hbar^2} \tau_0 (k_b T)^{1+\frac{d-2}{t}} \Gamma(2 + \frac{d-2}{t} + r) F_{\frac{d-2}{t}+r}(\eta) \quad (\text{A.12})$$

So we can generalize the mobility as:

$$\mu_{d,t} = \frac{2e\alpha_t^{2/t} (k_b T)^{1-\frac{2}{t}}}{\hbar^2} \cdot \tau_0 \cdot \frac{\Gamma(2 + \frac{d-2}{t} + r)}{\frac{2}{t} \Gamma(\frac{d}{t} + 1)} \frac{F_{\frac{d-2}{t}+r}(\eta)}{F_{\frac{d}{t}-1}(\eta)} \quad (\text{A.13})$$

For non-degenerate case,

$$\mu_{d,t} = \frac{2e\alpha_t^{2/t} (k_b T)^{1-\frac{2}{t}}}{\hbar^2} \cdot \tau_0 \cdot \frac{\Gamma(2 + \frac{d-2}{t} + r)}{\frac{2}{t} \Gamma(\frac{d}{t} + 1)} \quad (\text{A.14})$$

For degenerate case,

$$\mu_{d,t} = \frac{2e\alpha_t^{2/t} (k_b T)^{1-\frac{2}{t}}}{\hbar^2} \cdot \tau_0 \cdot \frac{\mu^{1+r-\frac{2}{t}}}{(k_b T)^r} \quad (\text{A.15})$$

A.4 Seebeck Coefficient and Power Factor

We can write the Seebeck Coefficient $S_{d,t} = -M_{01}^{d,t}/M_{00}^{d,t}T$ which simplifies to

$$S_{d,t} = -\frac{k_b}{e} \left(\frac{1}{k_b T} \frac{\int_0^\infty E^{1+\frac{d-2}{t}} \tau(E) \left(-\frac{\partial f_0}{\partial E}\right) dE}{\int_0^\infty E^{2+\frac{d-2}{t}} \tau(E) \left(-\frac{\partial f_0}{\partial E}\right) dE} - \frac{\mu}{k_b T} \right) \quad (\text{A.16})$$

For power law $\tau(E) = \tau_0(\frac{E}{k_b T})^r$, $S_{d,t}$ simplifies to:

$$S_{d,t} = -\frac{k_b}{e} \left(\left(2 + \frac{d-2}{t} + r\right) \frac{F_{1+\frac{d-2}{t}+r}(\eta)}{F_{\frac{d-2}{t}+r}(\eta)} - \eta \right) \quad (\text{A.17})$$

And,

$$S_{d,t} \underset{\eta \ll -1}{=} -\frac{k_b}{e} \left(2 + \frac{d-2}{t} + r - \eta \right) \quad (\text{A.18})$$

$$S_{d,t} \underset{\eta \gg 1}{=} -\frac{k_b}{e} \left(1 + \frac{d-2}{t} + r \right) \frac{\pi^2}{3\eta} \quad (\text{A.19})$$

A.5 All Thermoelectric Coefficients

$$\begin{aligned}
\rho &= \sigma^{-1} = \left(\frac{ge^2 t \alpha_t^{\frac{2-d}{t}}}{(4\pi)^{\frac{d}{2}} \Gamma(\frac{d}{2} + 1) \hbar^2} \tau_0 (k_b T)^{1+\frac{d-2}{t}} \Gamma(2 + \frac{d-2}{t} + r) F_{\frac{d-2}{t}+r}(\eta) \right)^{-1}, \\
S &= -\frac{k_b}{e} \left(\left(2 + \frac{d-2}{t} + r \right) \frac{F_{1+\frac{d-2}{t}+r}(\eta)}{F_{\frac{d-2}{t}+r}(\eta)} - \eta \right) \\
\Pi &= S \cdot T, \text{ and} \\
\kappa &= \frac{gt \alpha_t^{\frac{2-d}{t}}}{T (4\pi)^{\frac{d}{2}} \Gamma(\frac{d}{2} + 1) \hbar^2} \tau_0 (k_b T)^{3+\frac{d-2}{t}} \Gamma(4 + \frac{d-2}{t} + r) \\
&\quad \times \left(F_{2+\frac{d-2}{t}+r}(\eta) - \left(\frac{2 + \frac{d-2}{t} + r}{3 + \frac{d-2}{t} + r} \right) \frac{(F_{1+\frac{d-2}{t}+r}(\eta))^2}{F_{\frac{d-2}{t}+r}(\eta)} \right). \tag{A.20}
\end{aligned}$$

BIBLIOGRAPHY

- [1] The asymptotic approximations of the Fermi-Dirac Integral are: for $\eta \ll -1$, $F_j^+(\eta) \approx e^\eta$ and for $\eta \gg 1$, $F_j^+(\eta) \approx \eta^{j+1}/\Gamma(j+2)$. The $\eta = 0$ value of the Bose-Einstein Integral is $F_j^-(0) = \zeta(j+1)$, where $\zeta(\dots)$ is the Zeta-function.
- [2] Idriss Abid, Jash Mehta, Yvon Cordier, Joff Derluyn, Stefan Degroote, Hideto Miyake, and Farid Medjdoub. AlGa_N Channel High Electron Mobility Transistors with Regrown Ohmic Contacts. *Electronics*, 10(6), 2021.
- [3] AA Allerman, AM Armstrong, AJ Fischer, JR Dickerson, MH Crawford, MP King, MW Moseley, JJ Wierer, and RJ Kaplar. Al_{0.3}Ga_{0.7}N pn diode with breakdown voltage > 1600 V. *Electronics Letters*, 52(15):1319–1321, 2016.
- [4] Gustavo Alvarez-Escalante, Ryan Page, Renjiu Hu, Huili Grace Xing, Debdeep Jena, and Zhiting Tian. High thermal conductivity and ultrahigh thermal boundary conductance of homoepitaxial AlN thin films. *APL Materials*, 10(1):011115, 2022.
- [5] O. Ambacher, J. Smart, J. R. Shealy, N. G. Weimann, K. Chu, M. Murphy, W. J. Schaff, L. F. Eastman, R. Dimitrov, L. Wittmer, M. Stutzmann, W. Rieger, and J. Hilsenbeck. Two-dimensional electron gases induced by spontaneous and piezoelectric polarization charges in N- and Ga-face AlGa_N/Ga_N heterostructures. *Journal of Applied Physics*, 85(6):3222–3233, 1999.
- [6] Yee Sin Ang, Hui Ying Yang, and L. K. Ang. Universal Scaling Laws in Schottky Heterostructures Based on Two-Dimensional Materials. *Phys. Rev. Lett.*, 121:056802, Aug 2018.
- [7] DE Angelescu, MC Cross, and ML Roukes. Heat transport in mesoscopic systems. *Superlattices Microstruct.*, 23(3-4):673–689, 1998.
- [8] Andrew M Armstrong, Brianna A Klein, Albert G Baca, Andrew A Allerman, Erica A Douglas, Albert Colon, Vincent M Abate, and Torben R Fortune. Al_{0.6}Ga_{0.4}N polarization-doped field effect transistor with compositionally graded channel from Al_{0.6}Ga_{0.4}N to AlN. *Applied Physics Letters*, 114(5):052103, 2019.
- [9] Andrew M Armstrong, Brianna A Klein, Albert Colon, Andrew A Allerman, Erica A Douglas, Albert G Baca, Torben R Fortune, Vincent M Abate, Sanyam Bajaj, and Siddharth Rajan. Ultra-wide band gap Al_{0.6}Ga_{0.4}N polarization-doped field effect transistor. *Japanese Journal of Applied Physics*, 57(7):074103, 2018.

- [10] Robert G Arns. The other transistor: early history of the metal-oxide semiconductor field-effect transistor. *Engineering Science & Education Journal*, 7(5):233–240, 1998.
- [11] N.W. Ashcroft and N.D. Mermin. *Solid State Physics*. Cengage Learning, 1976.
- [12] M Asif Khan, A Bhattarai, JN Kuznia, and DT Olson. High electron mobility transistor based on a gan-al x gal- x n heterojunction. *Applied Physics Letters*, 63(9):1214–1215, 1993.
- [13] Albert G. Baca, Andrew M. Armstrong, Andrew A. Allerman, Erica A. Douglas, Carlos A. Sanchez, Michael P. King, Michael E. Coltrin, Torben R. Fortune, and Robert J. Kaplar. An $\text{AlN/Al}_{0.85}\text{Ga}_{0.15}\text{N}$ high electron mobility transistor. *Applied Physics Letters*, 109(3):033509, 2016.
- [14] Albert G Baca, Andrew M Armstrong, Brianna A Klein, Andrew A Allerman, Erica A Douglas, and Robert J Kaplar. Al-rich AlGaN based transistors. *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, 38(2):020803, 2020.
- [15] Albert G. Baca, Brianna A. Klein, Joel R. Wendt, Stefan M. Lepkowski, Christopher D. Nordquist, Andrew M. Armstrong, Andrew A. Allerman, Erica A. Douglas, and Robert J. Kaplar. RF Performance of $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N/Al}_{0.70}\text{Ga}_{0.30}\text{N}$ High Electron Mobility Transistors With 80-nm Gates. *IEEE Electron Device Letters*, 40(1):17–20, 2019.
- [16] Samuel James Bader. *GaN-on-AlN as a Platform for High-Voltage Complementary Electronics*. Cornell University, 2020.
- [17] Sanyam Bajaj. *Design and engineering of AlGaN channel-based transistors*. PhD thesis, The Ohio State University, 2018.
- [18] Sanyam Bajaj, Fatih Akyol, Sriram Krishnamoorthy, Yuewei Zhang, and Siddharth Rajan. AlGaN channel field effect transistors with graded heterostructure ohmic contacts. *Applied Physics Letters*, 109(13):133508, 2016.
- [19] Sanyam Bajaj, Ting-Hsiang Hung, Fatih Akyol, Digbijoy Nath, and Siddharth Rajan. Modeling of high composition AlGaN channel high electron mobility transistors with large threshold voltage. *Applied Physics Letters*, 105(26):263503, 2014.
- [20] Sanyam Bajaj, Zhichao Yang, Fatih Akyol, Pil Sung Park, Yuewei Zhang,

- Aimee L Price, Sriram Krishnamoorthy, David J Meyer, and Siddharth Rajan. Graded algan channel transistors for improved current and power gain linearity. *IEEE Transactions on Electron Devices*, 64(8):3114–3119, 2017.
- [21] B Jayant Baliga. *Power semiconductor devices*. Brooks/Cole, 1996.
 - [22] John Bardeen and Walter Hauser Brattain. The transistor, a semi-conductor triode. *Physical Review*, 74(2):230, 1948.
 - [23] G Bastard. *Wave Mechanics Applied to Semiconductor Heterostructures*. Wiley-Interscience, Hoboken, NJ, 1 1988.
 - [24] Enrico Bellotti, Francesco Bertazzi, and Michele Goano. Alloy scattering in AlGa_N and InGa_N: A numerical study. *Journal of Applied Physics*, 101(12):123706, 2007.
 - [25] Sven Besendörfer, Elke Meissner, Farid Medjdoub, Joff Derluyn, Jochen Friedrich, and Tobias Erlbacher. The impact of dislocations on algan/gan schotky diodes and on gate failure of high electron mobility transistors. *Scientific Reports*, 10(1):17252, 2020.
 - [26] HA Bethe. Theory of the boundary layer of crystal rectifiers. *MIT Radiation Laboratory*, 43:12, 1942.
 - [27] Ludwig Boltzmann. Ableitung des stefan’schen gesetzes, betreffend die abhängigkeit der wärmestrahlung von der temperatur aus der electromagnetischen lichttheorie. *Ann. Phys. (Berlin, Ger.)*, 258(6):291–294, 1884.
 - [28] H. A. Buchdahl. Modification of the general theorem of equipartition: Application to the relativistic ideal gas. *Am. J. Phys.*, 52(9):802–804, 1984.
 - [29] PN Butcher. Thermal and electrical transport formalism for electronic microstructures with many terminals. *J. Phys. Condens. Matter*, 2(22):4869, 1990.
 - [30] M. Büttiker. Four-Terminal Phase-Coherent Conductance. *Phys. Rev. Lett.*, 57:1761–1764, Oct 1986.
 - [31] Y. Cai, Y. Zhou, K.M. Lau, and K.J. Chen. Control of threshold voltage of algan/gan hemts by fluoride-based plasma treatment: From depletion mode to enhancement mode. *IEEE Transactions on Electron Devices*, 53(9):2207–2215, 2006.

- [32] H. Chandrasekar, K. L. Ganapathi, S. Bhattacharjee, N. Bhat, and D. N. Nath. Optical-phonon-limited high-field transport in layered materials. *IEEE Transactions on Electron Devices*, 63(2):767–772, 2016.
- [33] Reet Chaudhuri, Zhen Chen, David A Muller, Huili Grace Xing, and Debdeep Jena. High-conductivity polarization-induced 2d hole gases in undoped gan/aln heterojunctions enabled by impurity blocking layers. *Journal of Applied Physics*, 130(2):025703, 2021.
- [34] Reet Chaudhuri, Austin Hickman, Jashan Singhal, Joseph Casamento, Huili Grace Xing, and Debdeep Jena. In Situ Crystalline AlN Passivation for Reduced RF Dispersion in Strained-Channel AlN/GaN/AlN High-Electron-Mobility Transistors. *Physica Status Solidi (a)*, 219(4):2100452, 2022.
- [35] Reet Chaudhuri, Zexuan Zhang, Huili Grace Xing, and Debdeep Jena. Very high density ($> 10^{14} \text{ cm}^{-2}$) polarization-induced 2d hole gases observed in undoped pseudomorphic ingan/aln heterostructures. *Advanced Electronic Materials*, 8(5):2101120, 2022.
- [36] Gang Chen. *Nanoscale Energy Transport and Conversion: A Parallel Treatment of Electrons, Molecules, Phonons, and Photons*. Oxford University Press, 2005.
- [37] YongJin Cho, Celesta S. Chang, Kevin Lee, Mingli Gong, Kazuki Nomoto, Masato Toita, Leo J. Schowalter, David A. Muller, Debdeep Jena, and Huili Grace Xing. Molecular beam homoepitaxy on bulk AlN enabled by aluminum-assisted surface cleaning. *Applied Physics Letters*, 116(17):172106, 2020.
- [38] YongJin Cho, Jimmy Encomendero, Shao-Ting Ho, Huili Grace Xing, and Debdeep Jena. N-polar gan/aln resonant tunneling diodes. *Applied Physics Letters*, 117(14):143501, 2020.
- [39] Michael E. Coltrin, Albert G. Baca, and Robert J. Kaplar. Analysis of 2D Transport and Performance Characteristics for Lateral Power Devices Based on AlGaN Alloys. *ECS Journal of Solid State Science and Technology*, 6(11):S3114–S3118, 2017.
- [40] Brian Cowan. On the chemical potential of ideal fermi and bose gases. *J. Low Temp. Phys.*, 197(5-6):412–444, 2019.
- [41] Scott A Crooker, Menyoun Lee, Ross David McDonald, Jon L Doorn, Ingrid Zimmermann, Y Lai, LE Winter, Y Ren, Y-J Cho, BJ Ramshaw, et al. Gan/algan 2degs in the quantum regime: Magneto-transport and photoluminescence to 60 tesla. *Applied Physics Letters*, 117(26):262105, 2020.

- [42] Gavin E. Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E*, 60:2721–2726, Sep 1999.
- [43] CR Crowell. The Richardson constant for thermionic emission in Schottky barrier diodes. *Solid-State Electron.*, 8(4):395–399, 1965.
- [44] Rafael Dalmau and Baxter Moody. Polarization-induced doping in graded algan epilayers grown on aln single crystal substrates. *ECS Transactions*, 86(12):31, 2018.
- [45] S. Dasgupta, Nidhi, D. F. Brown, F. Wu, S. Keller, J. S. Speck, and U. K. Mishra. Ultralow nonalloyed Ohmic contact resistance to self aligned N-polar GaN high electron mobility transistors by In(Ga)N regrowth. *Applied Physics Letters*, 96(14), 2010.
- [46] Sansaptak Dasgupta, F Wu, JS Speck, and UK Mishra. Growth of high quality N-polar AlN (000 $\bar{1}$) on Si (111) by plasma assisted molecular beam epitaxy. *Applied Physics Letters*, 94(15):151906, 2009.
- [47] Supriyo Datta. *Electronic Transport in Mesoscopic Systems*. Cambridge University Press, 1997.
- [48] P. Debye. Zur theorie der spezifischen wärmen. *Ann. Phys. (Berlin, Ger.)*, 344(14):789–839, 1912.
- [49] Sandra Diez, Subhajit Mohanty, Cagliyan Kurdak, and Elaheh Ahmadi. Record high electron mobility and low sheet resistance on scaled-channel n-polar gan/aln heterostructures grown on on-axis n-polar gan substrates by plasma-assisted molecular beam epitaxy. *Applied Physics Letters*, 117(4):042102, 2020.
- [50] E. A. Douglas, S. Reza, C. Sanchez, D. Koleske, A. Allerman, B. Klein, A. M. Armstrong, R. J. Kaplar, and A. G. Baca. Ohmic contacts to al-rich algan heterostructures. *physica status solidi (a)*, 214(8):1600842, 2017.
- [51] T. Fang, R. Wang, H. Xing, S. Rajan, and D. Jena. Effect of optical phonon scattering on the performance of gan transistors. *IEEE Electron Device Letters*, 33(5):709–711, 2012.
- [52] Tian Fang, Aniruddha Konar, Huili Xing, and Debdeep Jena. High-field transport in two-dimensional graphene. *Phys. Rev. B*, 84:125450, Sep 2011.
- [53] Maziar Farahmand, Carlo Garetto, Enrico Bellotti, Kevin F Brennan, Michele

- Goano, Enrico Ghillino, Giovanni Ghione, John D Albrecht, and P Paul Ruden. Monte carlo simulation of electron transport in the iii-nitride wurtzite phase materials system: binaries and ternaries. *IEEE Transactions on electron devices*, 48(3):535–542, 2001.
- [54] Patrick Fay, Debdeep Jena, and Paul Maki. *High-Frequency GaN Electronic Devices*. Springer, 2019.
- [55] CJ Frosch and L Derick. Surface protection and selective masking during diffusion in silicon. *Journal of The Electrochemical Society*, 104(9):547, 1957.
- [56] Mikhail Gaevski, Shahab Mollah, Kamal Hussain, Joshua Letton, Abdullah Mamun, Mohi Uddin Jewel, MVS Chandrashekhar, Grigory Simin, and Asif Khan. Ultrawide bandgap $\text{Al}_x\text{Ga}_{1-x}\text{N}$ channel heterostructure field transistors with drain currents exceeding 1.3 A mm1. *Applied Physics Express*, 13(9):094002, sep 2020.
- [57] Satyaki Ganguly, Aniruddha Konar, Zongyang Hu, Huili Xing, and Debdeep Jena. Polarization effects on gate leakage in $\text{InAlN}/\text{AlN}/\text{GaN}$ high-electron-mobility transistors. *Applied Physics Letters*, 101(253519):25, 2012.
- [58] S. P. Grabowski, M. Schneider, H. Nienhaus, W. Mönch, R. Dimitrov, O. Ambacher, and M. Stutzmann. Electron affinity of $\text{Al}_x\text{Ga}_{1-x}\text{N}(0001)$ surfaces. *Applied Physics Letters*, 78(17):2503–2505, 2001.
- [59] A. Greiner, L. Reggiani, and T. Kuhn. Comment on “Quantized Thermal Conductance of Dielectric Quantum Wires”. *Phys. Rev. Lett.*, 81:5037–5037, Nov 1998.
- [60] Andreas Greiner, Lino Reggiani, Tilmann Kuhn, and Luca Varani. Thermal Conductivity and Lorenz Number for One-Dimensional Ballistic Transport. *Phys. Rev. Lett.*, 78(6):1114–1117, 1997.
- [61] W Guo, R Kirste, I Bryan, Z Bryan, L Hussey, P Reddy, J Tweedie, R Collazo, and Z Sitar. KOH based selective wet chemical etching of AlN , $\text{Al}_x\text{Ga}_{1-x}\text{N}$, and GaN crystals: A way towards substrate removal in deep ultraviolet-light emitting diode. *Applied Physics Letters*, 106(8):082110, 2015.
- [62] W Guo, J Xie, C Akouala, S Mita, A Rice, J Tweedie, I Bryan, R Collazo, and Z Sitar. Comparative study of etching high crystalline quality AlN and GaN . *Journal of Crystal Growth*, 366:20–25, 2013.

- [63] Herwig Hahn, Ben Reuters, Holger Kalisch, and Andrei Vescan. AlN barrier HFETs with AlGaN channels to shift the threshold voltage to higher positive values: a proposal. *Semiconductor Science and Technology*, 28(7):074017, jun 2013.
- [64] F. D. M. Haldane. “Fractional statistics” in arbitrary dimensions: A generalization of the Pauli principle. *Phys. Rev. Lett.*, 67:937–940, Aug 1991.
- [65] JW Harrison and JR Hauser. Theoretical calculations of electron mobility in ternary III-V compounds. *Journal of Applied Physics*, 47(1):292–300, 1976.
- [66] Walter A Harrison. *Solid State Theory*. Dover Publications, 1980.
- [67] R Held, G Nowak, BE Ishaug, SM Seutter, A Parkhomovsky, AM Dabiran, Philip I Cohen, I Grzegory, and S Porowski. Structure and composition of GaN (0001) A and B surfaces. *Journal of Applied Physics*, 85(11):7697–7704, 1999.
- [68] Austin Hickman, Reet Chaudhuri, Samuel James Bader, Kazuki Nomoto, Kevin Lee, Huili Grace Xing, and Debdeep Jena. High breakdown voltage in RF AlN/GaN/AlN quantum well HEMTs. *IEEE Electron Device Letters*, 40(8):1293–1296, 2019.
- [69] Austin Hickman, Reet Chaudhuri, Lei Li, Kazuki Nomoto, Samuel James Bader, James CM Hwang, Huili Grace Xing, and Debdeep Jena. First RF power operation of AlN/GaN/AlN HEMTs with > 3 A/mm and 3 W/mm at 10 GHz. *IEEE Journal of the Electron Devices Society*, 9:121–124, 2020.
- [70] Austin Hickman, Reet Chaudhuri, Neil Moser, Michael Elliott, Kazuki Nomoto, Lei Li, James C. M Hwang, Huili Grace Xing, and Debdeep Jena. Large Signal Response of AlN/GaN/AlN HEMTs at 30 GHz. In *2021 Device Research Conference (DRC)*, pages 1–2, 2021.
- [71] Austin Lee Hickman, Reet Chaudhuri, Samuel James Bader, Kazuki Nomoto, Lei Li, James CM Hwang, Huili Grace Xing, and Debdeep Jena. Next generation electronics on the ultrawide-bandgap aluminum nitride platform. *Semiconductor Science and Technology*, 36(4):044001, 2021.
- [72] W. E. Hoke, A. Torabi, J. J. Mosca, R. B. Hallock, and T. D. Kennedy. Rapid silicon outdiffusion from SiC substrates during molecular-beam epitaxial growth of AlGaIn/GaN/AlN transistor structures. *Journal of Applied Physics*, 98(8):084510, 2005.

- [73] Lindsay Hussey, Ryan M. White, Ronny Kirste, Seiji Mita, Isaac Bryan, Wei Guo, Katherine Osterman, Brian Haidet, Zachary Bryan, Milena Bobea, Ramón Collazo, and Zlatko Sitar. Sapphire decomposition and inversion domains in N-polar aluminum nitride. *Applied Physics Letters*, 104(3):032104, 2014.
- [74] H. Inc. Hexatech launches deep-uv transparent 2-inch diameter aluminum nitride substrates. Accessed: 2021-08-30.
- [75] Tatsuya Isono, Tadatoshi Ito, Ryota Sakamoto, Yongzhao Yao, Yukari Ishikawa, Narihito Okada, and Kazuyuki Tadatomo. Growth of N-Polar Aluminum Nitride on Vicinal Sapphire Substrates and Aluminum Nitride Bulk Substrates. *Physica Status Solidi (b)*, 257(4):1900588, 2020.
- [76] Łukasz Janicki, Jan Misiewicz, Marcin Siekacz, Henryk Turski, Joanna Moneta, Sandeep Gorantla, Czesław Skierbiszewski, and Robert Kudrawiec. Sensitivity of n-polar gan surface barrier to ambient gases. *Sensors and Actuators B: Chemical*, 281:561–567, 2019.
- [77] C. Jarzynski. Nonequilibrium Equality for Free Energy Differences. *Phys. Rev. Lett.*, 78:2690–2693, Apr 1997.
- [78] J. Jasinski, Z. Liliental-Weber, Q. S. Paduano, and D. W. Weyburne. Inversion domains in AlN grown on (0001) sapphire. *Applied Physics Letters*, 83(14):2811–2813, 2003.
- [79] Debdeep Jena. A theory for the high-field current-carrying capacity of one-dimensional semiconductors. *Journal of Applied Physics*, 105(12):123701, 2009.
- [80] Debdeep Jena. *Quantum Physics of Semiconductor Materials and Devices*. Oxford University Press, 2022.
- [81] Debdeep Jena. Ultra-wide bandgap semiconductors for power electronics: which one? Compound Semiconductor Week, 2022.
- [82] Debdeep Jena, Arthur C Gossard, and Umesh K Mishra. Dislocation scattering in a two-dimensional electron gas. *Applied Physics Letters*, 76(13):1707–1709, 2000.
- [83] Debdeep Jena, Sten Heikman, Daniel Green, Dario Buttari, Robert Coffie, Huili Xing, Stacia Keller, Steve DenBaars, James S Speck, Umesh K Mishra, et al. Realization of wide electron slabs by polarization bulk doping in graded iii–v nitride semiconductor alloys. *Applied physics letters*, 81(23):4395–4397, 2002.

- [84] Debdeep Jena, Sten Heikman, James S. Speck, Arthur Gossard, Umesh K. Mishra, Angela Link, and Oliver Ambacher. Magnetotransport properties of a polarization-doped three-dimensional electron slab in graded AlGa_N. *Phys. Rev. B*, 67:153306, Apr 2003.
- [85] Debdeep Jena, Sten Heikman, James S Speck, Arthur Gossard, Umesh K Mishra, Angela Link, and Oliver Ambacher. Magnetotransport properties of a polarization-doped three-dimensional electron slab in graded algan. *Physical Review B*, 67(15):153306, 2003.
- [86] Edward A Jones, Fei Fred Wang, and Daniel Costinett. Review of commercial gan power devices and gan-based converter design challenges. *IEEE Journal of Emerging and Selected Topics in Power Electronics*, 4(3):707–719, 2016.
- [87] Edward A. Jones, Fei Fred Wang, and Daniel Costinett. Review of Commercial GaN Power Devices and GaN-Based Converter Design Challenges. *IEEE Journal of Emerging and Selected Topics in Power Electronics*, 4(3):707–719, 2016.
- [88] Agata Kaminska, Kamil Koronski, Pawel Strak, Aleksandra Wierzbicka, Marta Sobanska, Kamil Klosek, Dmitrii V Nechaev, Vladimir Pankratov, Kirill Chernenko, Stanislaw Krukowski, et al. Defect-related photoluminescence and photoluminescence excitation as a method to study the excitonic bandgap of aln epitaxial layers: Experimental and ab initio analysis. *Applied Physics Letters*, 117(23):232101, 2020.
- [89] R. J. Kaplar, A. A. Allerman, A. M. Armstrong, M. H. Crawford, J. R. Dickerson, A. J. Fischer, A. G. Baca, and E. A. Douglas. Review—Ultra-Wide-Bandgap AlGa_N power electronic devices. *ECS Journal of Solid State Science and Technology*, 6(2):Q3061–Q3066, dec 2016.
- [90] A Keerthi, AK Geim, A Janardanan, AP Rooney, A Esfandiar, S Hu, SA Dar, IV Grigorieva, SJ Haigh, FC Wang, et al. Ballistic molecular transport through two-dimensional channels. *Nature*, 558(7710):420–424, 2018.
- [91] S Keller, NA Fichtenbaum, F Wu, D Brown, A Rosales, SP DenBaars, JS Speck, and UK Mishra. Influence of the substrate misorientation on the properties of n-polar gan films grown by metal organic chemical vapor deposition. *Journal of Applied Physics*, 102(8):083546, 2007.
- [92] Stacia Keller, Nicholas Fichtenbaum, Feng Wu, Grace Lee, Steven P DenBaars, James S Speck, and Umesh K Mishra. Effect of the nucleation conditions on the polarity of AlN and GaN films grown on C-face 6H–SiC. *Japanese Journal of Applied Physics*, 45(3L):L322, 2006.

- [93] Stacia Keller, Haoran Li, Matthew Laurent, Yanling Hu, Nathan Pfaff, Jing Lu, David F Brown, Nicholas A Fichtenbaum, James S Speck, Steven P DenBaars, et al. Recent progress in metal-organic chemical vapor deposition of N-polar group-III nitrides. *Semiconductor Science and Technology*, 29(11):113001, 2014.
- [94] Dolar Khachariya, Seiji Mita, Pramod Reddy, Saroj Dangi, J. Houston Dycus, Pegah Bagheri, M. Hayden Breckenridge, Rohan Sengupta, Shashwat Rathkanthiwar, Ronny Kirste, Erhard Kohn, Zlatko Sitar, Ramón Collazo, and Spyridon Pavlidis. Record >10MV/cm mesa breakdown fields in Al_{0.85}Ga_{0.15}N/Al_{0.6}Ga_{0.4}N high electron mobility transistors on native AlN substrates. *Applied Physics Letters*, 120(17):172106, 2022.
- [95] M Asif Khan, Q Chen, MS Shur, BT Dermott, JA Higgins, J Burm, W Schaff, and LF Eastman. Short-channel gan/algan doped channel heterostructure field effect transistors with 36.1 cutoff frequency. *Electronics Letters*, 32(4):357–358, 1996.
- [96] Eungkyun Kim, Zexuan Zhang, Jimmy Encomendero, Jashan Singhal, Kazuki Nomoto, Austin Hickman, Cheng Wang, Patrick Fay, Masato Toita, Debdeep Jena, et al. N-polar gan/algan/aln high electron mobility transistors on single-crystal bulk aln substrates. *Applied Physics Letters*, 122(9):092104, 2023.
- [97] Eungkyun Kim, Zexuan Zhang, Jashan Singhal, Kazuki Nomoto, Austin Hickman, Masato Toita, Debdeep Jena, and Huili Grace Xing. First demonstration of n-polar gan/algan/aln hemt on single crystal aln substrates. In *2022 Device Research Conference (DRC)*, pages 1–2. IEEE, 2022.
- [98] Brianna A Klein, Albert G Baca, Stephan M Lepkowski, Christopher D Nordquist, Joel R Wendt, Andrew A Allerman, Andrew M Armstrong, Erica A Douglas, Vincent M Abate, and Robert J Kaplar. Saturation velocity measurement of al 0.7 ga 0.3 n-channel high electron mobility transistors. *Journal of Electronic Materials*, 48:5581–5585, 2019.
- [99] G. Koblmüller, R. Averbeck, L. Geelhaar, H. Riechert, W. Hösler, and P. Pongratz. Growth diagram and morphologies of AlN thin films grown by molecular beam epitaxy. *Journal of Applied Physics*, 93(12):9591–9596, 2003.
- [100] G. Koblmüller, C. S. Gallinat, and J. S. Speck. Surface kinetics and thermal instability of N-face InN grown by plasma-assisted molecular beam epitaxy. *Journal of Applied Physics*, 101(8):083516, 2007.
- [101] Gregor Koblmüller, Jay Brown, Robert Averbeck, Henning Riechert, Peter Pongratz, and James S. Speck. Ga Adlayer Governed Surface Defect Evolution

- of (0001) {GaN} Films Grown by Plasma-Assisted Molecular Beam Epitaxy. *Japanese Journal of Applied Physics*, 44(No. 28):L906–L908, jul 2005.
- [102] Junji Kotani, Junya Yaita, Kenji Homma, Shirou Ozaki, Atsushi Yamada, Masaru Sato, Toshihiro Ohki, and Norikazu Nakamura. 24.4 w/mm x band gan hemts on aln substrates with the lpcvd grown high breakdown field sinx layer. *IEEE Journal of the Electron Devices Society*, 2023.
 - [103] Herbert Kroemer. Heterostructure bipolar transistors and integrated circuits. *Proceedings of the IEEE*, 70(1):13–25, 1982.
 - [104] S Kurtin, TC McGill, and CA Mead. Fundamental transition in the electronic nature of solids. *Physical Review Letters*, 22(26):1433, 1969.
 - [105] K. Köhler, S. Müller, R. Aidam, P. Waltereit, W. Pletschen, L. Kirste, H. P. Mennner, W. Bronner, A. Leuther, R. Quay, M. Mikulla, O. Ambacher, R. Granzner, F. Schwier, C. Buchheim, and R. Goldhahn. Influence of the surface potential on electrical properties of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures with different Al-content: Effect of growth method. *Journal of Applied Physics*, 107(5):053711, 2010.
 - [106] Lev Davidovich Landau and Evgenii Mikhailovich Lifshitz. *Statistical Physics Part 1*. Pergamon Press, 2013.
 - [107] R Landauer. Conductance determined by transmission: probes and quantised constriction resistance. *J. Phys. Condens. Matter*, 1(43):8099–8110, oct 1989.
 - [108] Oleg Ledyayev, Mahesh Pandikunta, and Sergey Nikishin. N-polar AlN thin layers grown on Si (111) by plasma-assisted MBE. *Japanese Journal of Applied Physics*, 53(5):050306, 2014.
 - [109] Kevin Lee, YongJin Cho, Leo J. Schowalter, Masato Toita, Huili Grace Xing, and Debdeep Jena. Surface control and MBE growth diagram for homoepitaxy on single-crystal AlN substrates. *Applied Physics Letters*, 116(26):262102, 2020.
 - [110] Jori Lemettinen, Nadim Chowdhury, Hironori Okumura, Iurii Kim, Sami Suihkonen, and Tomás Palacios. Nitrogen-polar Polarization-Doped Field-Effect Transistor Based on $\text{Al}_{0.8}\text{Ga}_{0.2}\text{N}/\text{AlN}$ on SiC with drain current over 100 mA/mm. *IEEE Electron Device Letters*, 40(8):1245–1248, 2019.
 - [111] Jori Lemettinen, Hironori Okumura, I Kim, C Kauppinen, T Palacios, and

- S Suihkonen. MOVPE growth of N-polar AlN on 4H-SiC: Effect of substrate miscut on layer quality. *Journal of Crystal Growth*, 487:12–16, 2018.
- [112] Jori Lemettinen, Hironori Okumura, Tomás Palacios, and Sami Suihkonen. N-polar AlN buffer growth by metal–organic vapor phase epitaxy for transistor applications. *Applied Physics Express*, 11(10):101002, 2018.
- [113] Dongsheng Li, M Sumiya, S Fuke, Deren Yang, Duanlin Que, Y Suzuki, and Y Fukuda. Selective etching of GaN polar surface in potassium hydroxide solution studied by x-ray photoelectron spectroscopy. *Journal of Applied Physics*, 90(8):4219–4223, 2001.
- [114] DS Li, H Chen, HB Yu, HQ Jia, Q Huang, and JM Zhou. Dependence of leakage current on dislocations in gan-based light-emitting diodes. *Journal of Applied Physics*, 96(2):1111–1114, 2004.
- [115] Guowang Li, Yu Cao, Huili Grace Xing, and Debdeep Jena. High mobility two-dimensional electron gases in nitride heterostructures with high Al composition AlGaN alloy barriers. *Applied Physics Letters*, 97(22):222110, 2010.
- [116] Guowang Li, Bo Song, Satyaki Ganguly, Mingda Zhu, Ronghua Wang, Xiaodong Yan, Jai Verma, Vladimir Protasenko, Huili Grace Xing, and Debdeep Jena. Two-dimensional electron gases in strained quantum wells for AlN/GaN/AlN double heterostructure field-effect transistors on AlN. *Applied physics letters*, 104(19):193506, 2014.
- [117] Weili Liu and Alexander A Balandin. Thermal conduction in $\text{al}_x\text{ga}_{1-x}\text{n}$ alloys and thin films. *Journal of Applied Physics*, 97(7):073710, 2005.
- [118] ZK Liu, Bo Zhou, Yong Zhang, ZJ Wang, HM Weng, Dharmalingam Prabhakaran, S-K Mo, ZX Shen, Zhong Fang, Xi Dai, et al. Discovery of a three-dimensional topological Dirac semimetal, Na_3Bi . *Science*, 343(6173):864–867, 2014.
- [119] Bin Lu, Elison Matioli, and Tomas Palacios. Tri-gate normally-off gan power misfet. *IEEE Electron Device Letters*, 33(3):360–362, 2012.
- [120] L Lu, ZY Gao, B Shen, FJ Xu, S Huang, ZL Miao, Y Hao, ZJ Yang, GY Zhang, XP Zhang, et al. Microstructure and origin of dislocation etch pits in GaN epilayers grown by metal organic chemical vapor deposition. *Journal of Applied Physics*, 104(12):123525, 2008.

- [121] Mark S Lundstrom and Changwook Jeong. *Near-Equilibrium Transport: Fundamentals and Applications*, volume 2. World Scientific Publishing Company, 2012.
- [122] Jun Ma and Elison Matioli. High performance tri-gate gan power moshemts on silicon substrate. *IEEE Electron Device Letters*, 38(3):367–370, 2017.
- [123] Ryota Maeda, Kohei Ueno, Atsushi Kobayashi, and Hiroshi Fujioka. AlN/Al_{0.5}Ga_{0.5}N HEMTs with heavily Si-doped degenerate GaN contacts prepared via pulsed sputtering. *Applied Physics Express*, 15(3):031002, feb 2022.
- [124] D. Maier, M. Alomari, N. Grandjean, J.-F. Carlin, M.-A. Diforte-Poisson, C. Dua, S. Delage, and E. Kohn. InAlN/GaN HEMTs for Operation in the 1000 °C Regime: A First Experiment. *IEEE Electron Device Letters*, 33(7):985–987, 2012.
- [125] F. Medjdoub, J.-F. Carlin, M. Gonschorek, E. Feltin, M.A. Py, D. Ducatteau, C. Gaquiere, N. Grandjean, and E. Kohn. Can InAlN/GaN be an alternative to high power / high temperature AlGaIn/GaN devices? In *2006 International Electron Devices Meeting*, pages 1–4, 2006.
- [126] MS Miao, PG Moses, JR Weber, A Janotti, and CG Van de Walle. Effects of surface reconstructions on oxygen adsorption at AlN polar surfaces. *EPL (Europhysics Letters)*, 89(5):56004, 2010.
- [127] J. Millan, P. Godignon, X. Perpina, A. Perez-Tomas, and J. Rebollo. A survey of wide bandgap power semiconductor devices. *IEEE Transactions on Power Electronics*, 29(5):2155–2163, 2014.
- [128] Takashi Mimura. The early history of the high electron mobility transistor (hemt). *IEEE Transactions on microwave theory and techniques*, 50(3):780–782, 2002.
- [129] Umesh K Mishra, Likun Shen, Thomas E Kazior, and Yi-Feng Wu. Gan-based rf power devices and amplifiers. *Proceedings of the IEEE*, 96(2):287–305, 2008.
- [130] Umesh K. Mishra, Likun Shen, Thomas E. Kazior, and Yi-Feng Wu. GaN-based RF Power Devices and Amplifiers. *Proceedings of the IEEE*, 96(2):287–305, 2008.
- [131] Makoto Miyoshi, Shu Fujita, and Takashi Egawa. Numerical and experimental analyses of two-dimensional electron mobility in al (in, ga) n/algan heterostructures. *Applied Physics Express*, 8(5):051003, 2015.

- [132] Makoto Miyoshi, Shu Fujita, and Takashi Egawa. Numerical and experimental analyses of two-dimensional electron mobility in Al(In,Ga)N/AlGaN heterostructures. *Applied Physics Express*, 8(5):051003, apr 2015.
- [133] E. Monroy, T. Andreev, P. Holliger, E. Bellet-Amalric, T. Shibata, M. Tanaka, and B. Daudin. Modification of GaN(0001) growth kinetics by Mg doping. *Applied Physics Letters*, 84(14):2554–2556, 2004.
- [134] E Monroy, E Sarigiannidou, F Fossard, N Gogneau, E Bellet-Amalric, J-L Rouvière, S Monnoye, H Mank, and B Daudin. Growth kinetics of N-face polarity GaN by plasma-assisted molecular-beam epitaxy. *Applied Physics Letters*, 84(18):3684–3686, 2004.
- [135] Hadis Morkoc and Paul M Solomon. The hemt: A superfast transistor: An experimental gaas-algoas device switches in picoseconds and generates little heat. this is just what supercomputers need. *IEEE spectrum*, 21(2):28–35, 1984.
- [136] Shuji Nakamura and Michael R Krames. History of gallium–nitride-based light-emitting diodes for illumination. *Proceedings of the IEEE*, 101(10):2211–2220, 2013.
- [137] Takuma Nanjo, Misaichi Takeuchi, Muneyoshi Suita, Yuji Abe, Toshiyuki Oishi, Yasunori Tokuda, and Yoshinobu Aoyagi. First Operation of AlGaIn Channel High Electron Mobility Transistors. *Applied Physics Express*, 1(1):011101, dec 2007.
- [138] Kenji Natori. Ballistic metal-oxide-semiconductor field effect transistor. *J. Appl. Phys.*, 76(8):4879–4890, 1994.
- [139] Jörg Neugebauer, Tosja K. Zywietz, Matthias Scheffler, John E. Northrup, Huajie Chen, and R. M. Feenstra. Adatom Kinetics On and Below the Surface: The Existence of a New Diffusion Channel. *Phys. Rev. Lett.*, 90:056101, Feb 2003.
- [140] Madhab Neupane, Su-Yang Xu, Raman Sankar, Nasser Alidoust, Guang Bian, Chang Liu, Ilya Belopolski, Tay-Rong Chang, Horng-Tay Jeng, Hsin Lin, et al. Observation of a three-dimensional topological Dirac semimetal phase in high-mobility Cd₃As₂. *Nature communications*, 5(1):1–8, 2014.
- [141] Atsushi Nishikawa, Kazuhide Kumakura, and Toshiki Makimoto. High critical electric field exceeding 8 mv/cm measured using an algan p–i–n vertical conducting diode on n-sic substrate. *Japanese journal of applied physics*, 46(4S):2316, 2007.

- [142] Kazuki Nomoto, Bo Song, Zongyang Hu, Mingda Zhu, Meng Qi, Naoki Kaneda, Tomoyoshi Mishima, Tohru Nakamura, Debdeep Jena, and Huili Grace Xing. 1.7 kv and $0.55 \text{ m}\omega.\text{cm}^2$ gan pn diodes on bulk gan substrates with avalanche capability. *IEEE Electron Device Letters*, 37(2):161–164, 2015.
- [143] Hironori Okumura, Tsunenobu Kimoto, and Jun Suda. Growth of Nitrogen-Polar 2H-AlN on Step-Height-Controlled 6H-SiC (000 $\bar{1}$) substrate by Molecular-Beam Epitaxy. *Japanese Journal of Applied Physics*, 51(2S):02BH02, 2012.
- [144] S. Ozaki, J. Yaita, A. Yamada, Y. Kumazaki, Y. Minoura, T. Ohki, N. Okamoto, N. Nakamura, and J. Kotani. First demonstration of x-band algan/gan high electron mobility transistors using free-standing aln substrate over 15 w mm-1 output power density. *Applied Physics Express*, 14, 4 2021.
- [145] JW Palmour, HS Kong, and RF Davis. High-temperature depletion-mode metal-oxide-semiconductor field-effect transistors in beta-sic thin films. *Applied physics letters*, 51(24):2028–2030, 1987.
- [146] Nick Pant, Zihao Deng, and Emmanouil Kioupakis. High electron mobility of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ evaluated by unfolding the DFT band structure. *Applied Physics Letters*, 117(24):242105, 2020.
- [147] Nick Pant, Woncheol Lee, Nocona Sanders, and Emmanouil Kioupakis. Increasing the mobility and power-electronics figure of merit of AlGaN with atomically thin AlN/GaN digital-alloy superlattices. *Applied Physics Letters*, 121(3):032105, 2022.
- [148] P. S. Park, D. N. Nath, and S. Rajan. Quantum capacitance in N-polar GaN/AlGaN/GaN heterostructures. *IEEE Electron Device Letters*, 33(7):991–993, 2012.
- [149] Shashank Patwal, Manvi Agrawal, K. Radhakrishnan, Tian Long Alex Seah, and Nethaji Dharmarasu. Enhancement of 2D Electron Gas Mobility in an AlN/GaN/AlN Double-Heterojunction High-Electron-Mobility Transistor by Epilayer Stress Engineering. *Physica Status Solidi (a)*, 217(7):1900818, 2020.
- [150] Max Planck. *The Theory of Heat Radiation*. Dover Publications, 2013.
- [151] C. Poblenz, P. Waltereit, S. Rajan, U. K. Mishra, J. S. Speck, P. Chin, I. Smorchkova, and B. Heying. Effect of AlN nucleation layer growth conditions on buffer leakage in AlGaN/GaN high electron mobility transistors grown by molecular beam epitaxy (MBE). *Journal of Vacuum Science & Technology B*:

Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena, 23(4):1562–1567, 2005.

- [152] Meng Qi, Guowang Li, Satyaki Ganguly, Pei Zhao, Xiaodong Yan, Jai Verma, Bo Song, Mingda Zhu, Kazuki Nomoto, Huili Xing, and Debdeep Jena. Strained GaN quantum-well FETs on single crystal bulk AlN substrates. *Applied Physics Letters*, 110(6):063501, 2017.
- [153] Meng Qi, Kazuki Nomoto, Mingda Zhu, Zongyang Hu, Yuning Zhao, Vladimir Protasenko, Bo Song, Xiaodong Yan, Guowang Li, Jai Verma, et al. High break-down single-crystal gan pn diodes by molecular beam epitaxy. *Applied Physics Letters*, 107(23):232101, 2015.
- [154] S. Rajan, A. Chini, M. H. Wong, J. S. Speck, and U. K. Mishra. N-polar GaNAl-GaN high electron mobility transistors. *Journal of Applied Physics*, 102(4), 2007.
- [155] Siddharth Rajan, Huili Xing, Steve DenBaars, Umesh K Mishra, and Debdeep Jena. Algan/gan polarization-doped field-effect transistor for microwave power applications. *Applied physics letters*, 84(9):1591–1593, 2004.
- [156] Pramod Reddy, Isaac Bryan, Zachary Bryan, James Tweedie, Shun Washiyama, Ronny Kirste, Seiji Mita, Ramon Collazo, and Zlatko Sitar. Charge neutrality levels, barrier heights, and band offsets at polar algan. *Applied Physics Letters*, 107(9):091603, 2015.
- [157] Luis G. C. Rego and George Kirczenow. Quantized Thermal Conductance of Dielectric Quantum Wires. *Phys. Rev. Lett.*, 81:232–235, Jul 1998.
- [158] Luis G. C. Rego and George Kirczenow. Rego and Kirczenow Reply:. *Phys. Rev. Lett.*, 81:5038–5038, Nov 1998.
- [159] Luis G. C. Rego and George Kirczenow. Fractional Exclusion Statistics and the Universal Quantum of Thermal Conductance: A Unifying Approach. *Phys. Rev. B*, 59(20):13080, 1999.
- [160] B. Romanczyk, M. Guidry, X. Zheng, H. Li, E. Ahmadi, S. Keller, and U. K. Mishra. Bias-dependent electron velocity extracted from n-polar gan deep recess hemts. *IEEE Transactions on Electron Devices*, 67(4):1542–1546, April 2020.
- [161] Brian Romanczyk, Xun Zheng, Matthew Guidry, Haoran Li, Nirupam Hatui, Christian Wurm, Athith Krishna, Elaheh Ahmadi, Stacia Keller, and Umesh K

- Mishra. W-band power performance of SiN-passivated N-polar GaN deep recess HEMTs. *IEEE Electron Device Letters*, 41(3):349–352, 2020.
- [162] Keith Schwab, EA Henriksen, JM Worlock, and Michael L Roukes. Measurement of the quantum of thermal conductance. *Nature*, 404(6781):974–977, 2000.
- [163] Xu She, Alex Q Huang, Oscar Lucia, and Burak Ozpineci. Review of silicon carbide power devices and their applications. *IEEE Transactions on Industrial Electronics*, 64(10):8193–8205, 2017.
- [164] Xu She, Alex Q. Huang, Óscar Lucía, and Burak Ozpineci. Review of Silicon Carbide Power Devices and Their Applications. *IEEE Transactions on Industrial Electronics*, 64(10):8193–8205, 2017.
- [165] K Shibahara, T Takeuchi, T Saitoh, S Nishino, and H Matsunami. Inversion-type mos field effect transistors using cvd grown cubic sic on si. *MRS Online Proceedings Library (OPL)*, 97, 1987.
- [166] Keisuke Shinohara, Dean C Regan, Yan Tang, Andrea L Corrion, David F Brown, Joel C Wong, John F Robinson, Helen H Fung, Adele Schmitz, Thomas C Oh, et al. Scaling of gan hemts and schottky diodes for submillimeter-wave mmic applications. *IEEE Transactions on Electron Devices*, 60(10):2982–2996, 2013.
- [167] W. Shockley. Hot electrons in germanium and ohm’s law. *Bell System Technical Journal*, 30(4):990–1034, 1951.
- [168] William Shockley. The theory of p-n junctions in semiconductors and p-n junction transistors. *Bell System Technical Journal*, 28(3):435–489, 1949.
- [169] Kanako Shojiki, Kenjiro Uesugi, Shigeyuki Kuboya, and Hideto Miyake. Reduction of threading dislocation densities of N-polar face-to-face annealed sputtered AlN on sapphire. *Journal of Crystal Growth*, 574:126309, 2021.
- [170] Jia Si, Jin Wei, Wanjun Chen, and Bo Zhang. Electric field distribution around drain-side gate edge in algan/gan hemts: Analytical approach. *IEEE Transactions on Electron Devices*, 60(10):3223–3229, 2013.
- [171] John Simon, Vladimir Protasenko, Chuanxin Lian, Huili Xing, and Debdeep Jena. Polarization-induced hole doping in wide-band-gap uniaxial semiconductor heterostructures. *Science*, 327(5961):60–64, 2010.

- [172] John Simon, Albert (Kejia) Wang, Huili Xing, Siddharth Rajan, and Debdeep Jena. Carrier transport and confinement in polarization-induced three-dimensional electron slabs: Importance of alloy scattering in AlGa_N. *Applied Physics Letters*, 88(4):042109, 2006.
- [173] Jashan Singhal, Reet Chaudhuri, Austin Hickman, Vladimir Protasenko, Huili Grace Xing, and Debdeep Jena. Toward algan channel hemts on aln: Polarization-induced 2degs in aln/algan/aln heterostructures. *APL Materials*, 10(11):111120, 2022.
- [174] Jashan Singhal, Jimy Encomendero, Yongjin Cho, Len van Deurzen, Zexuan Zhang, Kazuki Nomoto, Masato Toita, Huili Grace Xing, and Debdeep Jena. Molecular Beam Homoepitaxy of N-polar AlN on bulk AlN substrates. *arXiv preprint arXiv:2206.11370*, 2022.
- [175] U. Singiseti, M. H. Wong, and U. K. Mishra. High-performance N-polar GaN enhancement-mode device technology. *Semiconductor Science and Technology*, 28(7):074006, 2013.
- [176] U. Sivan and Y. Imry. Multichannel Landauer formula for thermoelectric transport with application to thermopower near the mobility edge. *Phys. Rev. B*, 33(1):551–558, 1986.
- [177] A. R. Smith, R. M. Feenstra, D. W. Greve, J. Neugebauer, and J. E. Northrup. Reconstructions of the GaN(000 $\bar{1}$) surface. *Phys. Rev. Lett.*, 79:3934–3937, Nov 1997.
- [178] A. R. Smith, R. M. Feenstra, D. W. Greve, M.-S. Shin, M. Skowronski, J. Neugebauer, and J. E. Northrup. Determination of wurtzite gan lattice polarity based on surface reconstruction. *Applied Physics Letters*, 72(17):2114–2116, 1998.
- [179] Arthur C Smith, James F Janak, and Richard B Adler. *Electronic Conduction in Solids*. McGraw-Hill, 1967.
- [180] IP Smorchkova, L Chen, T Mates, L Shen, S Heikman, B Moran, S Keller, SP DenBaars, JS Speck, and UK Mishra. AlN/GaN and (Al, Ga) N/AlN/GaN two-dimensional electron gas structures grown by plasma-assisted molecular-beam epitaxy. *Journal of Applied Physics*, 90(10):5196–5201, 2001.
- [181] N Stolyarchuk, T Markurt, A Courville, K March, O Tottereau, P Vennéguès, and M Albrecht. Impact of sapphire nitridation on formation of Al-polar inversion domains in N-polar AlN epitaxial layers. *Journal of Applied Physics*, 122(15):155303, 2017.

- [182] N Stolyarchuk, T Markurt, A Courville, K March, J Zúñiga-Pérez, P Vennéguès, and M Albrecht. Intentional polarity conversion of AlN epitaxial layers by oxygen. *Scientific Reports*, 8(1):1–8, 2018.
- [183] HL Störmer, R Dingle, AC Gossard, W Wiegmann, and MD Sturge. Two-dimensional electron gas at a semiconductor-semiconductor interface. *Solid state communications*, 29(10):705–709, 1979.
- [184] M. Sumiya, K. Yoshimura, K. Ohtsuka, and S. Fuke. Dependence of impurity incorporation on the polar direction of GaN film growth. *Applied Physics Letters*, 76(15):2098–2100, 2000.
- [185] Pil Sung Park, Digbijoy N Nath, Sriram Krishnamoorthy, and Siddharth Rajan. Electron gas dimensionality engineering in algan/gan high electron mobility transistors using polarization. *Applied Physics Letters*, 100(6):063507, 2012.
- [186] Simon M Sze and Kwok K Ng. *Physics of Semiconductor Devices*. John Wiley & Sons, 2006.
- [187] Marko J. Tadjer. Toward gallium oxide power electronics. *Science*, 378(6621):724–725, 2022.
- [188] Maher B. Tahhan, John A. Logan, Matthew T. Hardy, Mario G. Ancona, Brian Schultz, Brian Appleton, Thomas Kazior, David J. Meyer, and Eduardo M. Chumbes. Passivation schemes for scaln-barrier mm-wave high electron mobility transistors. *IEEE Transactions on Electron Devices*, 69(3):962–967, 2022.
- [189] M Takeuchi, H Shimizu, R Kajitani, K Kawasaki, T Kinoshita, K Takada, H Murakami, Y Kumagai, A Koukitu, T Koyama, et al. Al-and N-polar AlN layers grown on c-plane sapphire substrates by modified flow-modulation MOCVD. *Journal of Crystal Growth*, 305(2):360–365, 2007.
- [190] M Takeuchi, H Shimizu, R Kajitani, K Kawasaki, Y Kumagai, A Koukitu, and Y Aoyagi. Improvement of crystalline quality of N-polar AlN layers on c-plane sapphire by low-pressure flow-modulated MOCVD. *Journal of Crystal Growth*, 298:336–340, 2007.
- [191] Shunya Tanaka, Yuta Kawase, Shohei Teramura, Sho Iwayama, Kosuke Sato, Shinji Yasue, Tomoya Omori, Motoaki Iwaya, Tetsuya Takeuchi, Satoshi Kamiyama, Isamu Akasaki, and Hideto Miyake. Effect of dislocation density on optical gain and internal loss of AlGaIn-based ultraviolet-B band lasers. *Applied Physics Express*, 13(4):045504, mar 2020.

- [192] Morris Tanenbaum and DE Thomas. Diffused emitter and base silicon transistors. *Bell System Technical Journal*, 35(1):1–22, 1956.
- [193] Richard Chace Tolman. *The Principles of Statistical Mechanics*. Dover Publications, 1979.
- [194] J. Y. Tsao, S. Chowdhury, M. A. Hollis, D. Jena, N. M. Johnson, K. A. Jones, R. J. Kaplar, S. Rajan, C. G. Van de Walle, E. Bellotti, C. L. Chua, R. Collazo, M. E. Coltrin, J. A. Cooper, K. R. Evans, S. Graham, T. A. Grotjohn, E. R. Heller, M. Higashiwaki, M. S. Islam, P. W. Juodawlkis, M. A. Khan, A. D. Koehler, J. H. Leach, U. K. Mishra, R. J. Nemanich, R. C. N. Pilawa-Podgurski, J. B. Shealy, Z. Sitar, M. J. Tadjer, A. F. Witulski, M. Wraback, and J. A. Simmons. Ultrawide-Bandgap Semiconductors: Research Opportunities and Challenges. *Advanced Electronic Materials*, 4(1):1600501, 2018.
- [195] Jeffrey Y Tsao, Jung Han, Roland H Haitz, and P Morgan Pattison. The blue led nobel prize: Historical context, current scientific understanding, human benefit. *Annalen der Physik (Leipzig)*, 527(SAND-2015-4440J), 2015.
- [196] Lawrence E. Turner. Generalized classical equipartition theorem. *Am. J. Phys.*, 44(1):104–105, 1976.
- [197] Henryk Turski, Shyam Bharadwaj, Huili (Grace) Xing, and Debdeep Jena. Polarization control in nitride quantum well light emitters enabled by bottom tunnel-junctions. *Journal of Applied Physics*, 125(20):203104, 2019.
- [198] Yasuhiro Uemoto, Masahiro Hikita, Hiroaki Ueno, Hisayoshi Matsuo, Hidetoshi Ishida, Manabu Yanagihara, Tetsuzo Ueda, Tsuyoshi Tanaka, and Daisuke Ueda. Gate injection transistor (git)—a normally-off algan/gan power transistor using conductivity modulation. *IEEE Transactions on Electron Devices*, 54(12):3393–3399, 2007.
- [199] Len van Deurzen, Ryan Page, Vladimir Protasenko, Kazuki Nomoto, Huili (Grace) Xing, and Debdeep Jena. Optically pumped deep-UV multimode lasing in AlGa_N double heterostructure grown by molecular beam homoepitaxy. *AIP Advances*, 12(3):035023, 2022.
- [200] Tien-Yu Wang, Wei-Chih Lai, Syuan-Yu Sie, Sheng-Po Chang, Cheng-Huang Kuo, Jinn-Kong Sheu, and Jong-Shing Bow. Algan-based deep ultraviolet light-emitting diodes with thermally oxidized al_xga_{2–x}o₃ sidewalls. *ACS Omega*, 7(17):15027–15036, 2022.

- [201] Man Hoi Wong, Stacia Keller, Sansaptak Dasgupta Nidhi, Daniel J Denninghoff, Seshadri Kolluri, David F Brown, Jing Lu, Nicholas A Fichtenbaum, Elaheh Ahmadi, Uttam Singiseti, et al. N-polar GaN epitaxy and high electron mobility transistors. *Semiconductor Science and Technology*, 28(7):074009, 2013.
- [202] Man Hoi Wong, Yi Pei, Rongming Chu, Siddharth Rajan, Brian L Swenson, David F Brown, Stacia Keller, Steven P DenBaars, James S Speck, and Umesh K Mishra. N-face metal–insulator–semiconductor high-electron-mobility transistors with AlN back-barrier. *IEEE Electron Device Letters*, 29(10):1101–1104, 2008.
- [203] Man Hoi Wong, Uttam Singiseti, Jing Lu, James S. Speck, and Umesh K. Mishra. Anomalous output conductance in n-polar gan high electron mobility transistors. *IEEE Transactions on Electron Devices*, 59(11):2988–2995, 2012.
- [204] Colin Wood and Debdeep Jena. *Polarization effects in semiconductors: from ab initio theory to device applications*. Springer Science & Business Media, 2007.
- [205] Chris J.H. Wort and Richard S. Balmer. Diamond as an electronic material. *Materials Today*, 11(1):22–28, 2008.
- [206] Yong-Shi Wu. Statistical Distribution for Generalized Ideal Gas of Fractional-Statistics Particles. *Phys. Rev. Lett.*, 73:922–925, Aug 1994.
- [207] Christian Wurm, Elaheh Ahmadi, Feng Wu, Nirupam Hatui, Stacia Keller, James Speck, and Umesh Mishra. Growth of high-quality N-polar GaN on bulk GaN by plasma-assisted molecular beam epitaxy. *Solid State Communications*, 305:113763, 2020.
- [208] Runjie Lily Xu, Miguel Muñoz Rojo, SM Islam, Aditya Sood, Bozo Vareskic, Ankita Katre, Natalio Mingo, Kenneth E Goodson, Huili Grace Xing, Debdeep Jena, et al. Thermal conductivity of crystalline aln and the influence of atomic-scale defects. *Journal of Applied Physics*, 126(18):185105, 2019.
- [209] Hao Xue, Kamal Hussain, Towhidur Razzak, Mikhail Gaevski, Shahadat Hasan Sohel, Shahab Mollah, Vishank Talesara, Asif Khan, Siddharth Rajan, and Wu Lu. Al_{0.65}Ga_{0.35}N/Al_{0.4}Ga_{0.6}N Micro-Channel Heterojunction Field Effect Transistors With Current Density Over 900 mA/mm. *IEEE Electron Device Letters*, 41(5):677–680, 2020.
- [210] Hao Xue, Choong Hee Lee, Kamal Hussian, Towhidur Razzak, Mamun Abdullah, Zhanbo Xia, Shahadat Hasan Sohel, Asif Khan, Siddharth Rajan, and

- Wu Lu. $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ heterojunction field effect transistor with f_T of 40 GHz. *Applied Physics Express*, 12(6):066502, may 2019.
- [211] N. Yafune, S. Hashimoto, K. Akita, Y. Yamamoto, H. Tokuda, and M. Kuzuhara. AlN/AlGa N HEMTs on AlN substrate for stable high-temperature operation. *Electronics Letters*, 50(3):211–212, 2014.
- [212] Norimasa Yafune, Shin Hashimoto, Katsushi Akita, Yoshiyuki Yamamoto, and Masaaki Kuzuhara. Low-Resistive Ohmic Contacts for AlGa N Channel High-Electron-Mobility Transistors Using Zr/Al/Mo/Au Metal Stack. *Japanese Journal of Applied Physics*, 50(10R):100202, oct 2011.
- [213] Honggang Ye, Guangde Chen, Youzhang Zhu, and Su-Huai Wei. Asymmetry of adsorption of oxygen at wurtzite AlN (0001) and (000 $\bar{1}$) surfaces: First-principles calculations. *Physical Review B*, 77(3):033302, 2008.
- [214] Lu You, Wataru Matsumura, Kazuya Ataka, Shunsuke Matsuda, Daisuke Inahara, Koki Hanasaku, Ryo Okuno, Taketo Kowaki, Yongzhao Yao, Yukari Ishikawa, et al. Growth and characterization of nitrogen-polar algan/aln and demonstration of field effect transistor. *Japanese Journal of Applied Physics*, 62(SA):SA1018, 2022.
- [215] Feng Yun, Michael A. Reshchikov, Lei He, Thomas King, Hadis Morkoç, Steve W. Novak, and Luncun Wei. Energy band bowing parameter in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. *Journal of Applied Physics*, 92(8):4837–4839, 2002.
- [216] ARA Zauner, E Aret, WJP Van Enckevort, JL Weyher, S Porowski, and JJ Schermer. Homo-epitaxial growth on the n-face of gan single crystals: the influence of the misorientation on the surface morphology. *Journal of crystal growth*, 240(1-2):14–21, 2002.
- [217] L Zhang, K Ding, JC Yan, JX Wang, YP Zeng, TB Wei, YY Li, BJ Sun, RF Duan, and JM Li. Three-dimensional hole gas induced by polarization in (0001)-oriented metal-face iii-nitride structure. *Applied Physics Letters*, 97(6):062103, 2010.
- [218] Zexuan Zhang, Jimy Encomendero, Reet Chaudhuri, Yongjin Cho, Vladimir Protasenko, Kazuki Nomoto, Kevin Lee, Masato Toita, Huili Grace Xing, and Debdeep Jena. Polarization-induced 2d hole gases in pseudomorphic undoped gan/aln heterostructures on single-crystal aln substrates. *Applied Physics Letters*, 119(16):162104, 2021.

- [219] Zexuan Zhang, Jimmy Encomendero, Eungkyun Kim, Jashan Singhal, YongJin Cho, Kazuki Nomoto, Masato Toita, Huili Grace Xing, and Debdeep Jena. High-density polarization-induced 2d electron gases in n-polar pseudomorphic undoped gan/al_{0.85}ga_{0.15}n heterostructures on single-crystal aln substrates. *Applied Physics Letters*, 121(8):082107, 2022.
- [220] Zexuan Zhang, Yusuke Hayashi, Tetsuya Tohei, Akira Sakai, Vladimir Protasenko, Jashan Singhal, Hideto Miyake, Huili Grace Xing, Debdeep Jena, and YongJin Cho. Molecular beam homoepitaxy of n-polar aln: Enabling role of aluminum-assisted surface cleaning. *Science Advances*, 8(36):eabo6408, 2022.
- [221] Ziyi Zhang, Maki Kushimoto, Tadayoshi Sakai, Naoharu Sugiyama, Leo J. Schowalter, Chiaki Sasaoka, and Hiroshi Amano. A 271.8 nm deep-ultraviolet laser diode for room temperature operation. *Applied Physics Express*, 12(12):124003, nov 2019.
- [222] John M Ziman. *Principles of the Theory of Solids*. Cambridge University Press, 1972.
- [223] Tom Zimmermann, Yu Cao, Jia Guo, Xiangning Luo, Debdeep Jena, and Huili Xing. Top-down aln/gan enhancement-& depletion-mode nanoribbon hemts. In *2009 Device Research Conference*, pages 129–130. IEEE, 2009.
- [224] Tosja Zywietz, Jörg Neugebauer, and Matthias Scheffler. Adatom diffusion at GaN (0001) and (000 $\bar{1}$) surfaces. *Applied Physics Letters*, 73(4):487–489, 1998.
- [225] Tosja K Zywietz, Jörg Neugebauer, and Matthias Scheffler. The adsorption of oxygen at GaN surfaces. *Applied Physics Letters*, 74(12):1695–1697, 1999.