Tunnel Junction-based Ultra-violet Light Emitting Diodes

DISSERTATION

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Abstract

This thesis presents the design and demonstration of ultra-wide bandgap AlGaN tunnel junctions and their applications in UV LEDs.

III-Nitrides including AlN, GaN, InN and their alloys have attracted great research interest for high power and high efficiency optoelectronics. Driven by the successful research progress that has been achieved for InGaN based blue light emitting diodes, AlGaN based ultraviolet light emitters are expected to show promising device performance. Efficient and compact solid state ultraviolet light sources could address a wide range of societal needs in the areas of water purification, air disinfection, and sensing. However, widespread adoption of UV LEDs has not occurred, mainly due to the low efficiency associated with poor p-type contact and low p-type conductivity. In this work, we investigate the incorporation of efficient interband tunnel junctions for enhanced hole injection into UV LEDs.

Achieving low tunnel junction resistance for ultra-wide bandgap AlGaN is challenging, because of the high tunnel barrier. The design of low resistance, low voltage consumption wide bandgap AlGaN tunnel junctions was first investigated. Polarization effect is utilized to create high charge density at heterointerfaces to enable strong polarization field, leading to sharp band bending and dramatically reduced tunneling barrier. Simulation results show that efficient AlGaN interband tunnel junctions with Al composition as high as 100% could be achieved based on polarization engineering.
Following the design, tunnel-injected UV LEDs are fabricated using plasma assisted molecular beam epitaxy (MBE). Non-equilibrium hole injection into the active region of the UV LED structures are demonstrated through light emissions ranging from UV-A to UV-C LEDs. Low tunnel junction resistances below 2 mΩ cm² have been achieved for AlGaN tunnel junctions with Al composition as high as 75%. The optimization of the p-type layers led to the demonstration of high on-wafer efficiencies, which are 3.37% (external quantum efficiency) and 1.62% (wall-plug efficiency) for UV-A LEDs, and 2.8% (EQE) and 1.1% (WPE) for UV-B LEDs. The device performance is comparable to state-of-the-art UV LEDs, demonstrating the great potential in the applications for high power and high efficiency UV emitters.

A novel metal/semiconductor tunnel junction structure employing reflective Al-based metal stack is further demonstrated, as an approach that can be better adopted in other material production technologies, especially metal-organic chemical vapour deposition (MOCVD). The effects of Ni and Al contacts on both the electrical and optical performance of the tunnel-injected UV LEDs are compared. High external quantum efficiency and wall-plug efficiency of 2.65% and 1.55% are obtained at the emission wavelength of 325 nm. While further studies in validating their applications toward shorter emission wavelength are necessary, the metal/semiconductor tunnel junction structure provides a novel solution to the p-type contact challenges faced by conventional UV LEDs.
Dedication

Dedicated to my family
Acknowledgments

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Chapter 1

Introduction

III-Nitrides, including InN, GaN and AlN and their alloys, have enabled a broad range of applications, including optoelectronics[1,2], RF and power electronics[3-5]. The wide range of bandgap energy enabled by III-Nitride compounds spans from 0.7 eV (InN)[6] to 6.2 eV (AlN)[7], which covers the light spectrum from far infrared to deep ultra-violet light, making III-Nitrides especially suitable for optoelectronics applications. Since the breakthroughs of p-type doping in GaN in the 1990s[1,8,9], InGaN-based visible light emitting diodes (LEDs) have experienced significant efficiency increase. The wall-plug efficiency, which describes the efficiency of LEDs converting electrical power to optical power, of blue LEDs can be as high as 80%[10], and is significantly higher than that can be achieved for conventional light sources. As a result, semiconductor-based solid state lighting is replacing the incandescent and fluorescent light sources for a significant reduction of the energy cost. At the same time, numerous novel applications have been enabled due to the compact size and high stability of InGaN LEDs. Driven by the great success in InGaN-based blue LEDs, substantial research efforts were devoted to the realization of high efficiency Nitride-based ultra-violet (UV) emitters in the past two decades.
Figure 1 Applications and EQE/WPE of III-Nitride UV LEDs. The wavelength range for the UV spectrum is divided into UV A (400-315 nm), UV B (315-280 nm) and UV C (280-200 nm).

Solid-state UV LEDs and laser diodes are one of the main frontiers in III-nitride research today. Efficient and compact ultraviolet light sources could address a wide range of societal needs in the areas of water purification, air disinfection, and sensing.[11] Current UV sources are predominantly mercury lamps, with many drawbacks due to their bulky nature, environmental concerns and high power consumption. In comparison, UV LEDs are compact, environmental friendly, and require low operation power. They are expected to replace conventional UV lamps in many present applications, and also enable new
applications for which UV lamps can never be used.[12] Great research progress has been achieved in the past decade toward highly efficient UV LEDs covering the full range of UV-A (315 – 400 nm), UV-B (290 – 315 nm), and UV-C (200 – 290 nm).[11,13-15] Thanks to the efforts from many research groups, the external quantum efficiency (EQE) above 20% has been achieved for an emitting wavelength of 280 nm.[16] Here, external quantum efficiency describes the transfer ratio of the number of injected carriers into the UV LED to the number of emitted photons from the device. However, this value still remains much lower than their InGaN-based visible counterparts, whose external quantum efficiency is as high as 80%.[10] Even worse, the power conversion efficiency - wall-plug efficiency - is even lower than EQE, with a highest reported value of ~ 5%. [16-18]

Until now, widespread adoption of UV LEDs has not occurred, mainly due to the low efficiency (10× lower than visible LEDs) and high cost (> 100× higher than visible LEDs), both of which are due to fundamental material limits of AlGaN.

In this thesis, a tunnel-injected UV LED structure will be investigated as a tentative solution to the challenges for achieving high efficiency UV LEDs. The feasibility of achieving efficient interband tunneling for ultra-wide bandgap AlGaN tunnel junctions will be exploited.

1.1. Challenges for UV LEDs

Following nearly two decades of research efforts, significant achievements in UV LEDs have been demonstrated by many research groups, however, the wall-plug efficiency has not fulfilled the commercial expectations, and still remains a major challenge to the
widespread adoption of solid state ultra violet emitters. Figure 1 shows a survey of external quantum efficiency and wall-plug efficiency values for different UV wavelengths. The efficiency values of blue LEDs are also benchmarked on the plot for a direct comparison. Among the wide spectrum of the UV light, UV LEDs targeting for ~ 280 nm light emission attracted more research efforts, driven by the applications in water sterilization and disinfection. Even though this resulted in a remarkable efficiency peak at 280 nm, the power conversion efficiency is still lower than conventional UV lamps, which could be as high as 30%. The challenges for improving the device efficiency can be understood by breaking down the efficiency (or losses) into different components.

The wall-plug efficiency is defined as the conversion ratio from electrical input power ($I \times V$) to optical output power ($P_{out}$) and can be expressed as:

$$WPE = \frac{P_{out}}{I \cdot V} = EQE \times \frac{h \nu}{qV}$$

The external quantum efficiency ($EQE$) can be further described as:

$$EQE = \frac{\text{number of emitted photons}}{\text{number of injected electrons}} = \eta_{inj} \times \eta_{rad} \times \eta_{LEE} = \eta_{IQE} \times \eta_{LEE}$$

Here, $h \nu$ is the emitted photon energy, $\eta_{inj}$, $\eta_{rad}$, $\eta_{IQE}$ and $\eta_{LEE}$ represent for the carrier injection efficiency, radiative efficiency, internal quantum efficiency and light extraction efficiency. The term $h \nu/qV \times \eta_{inj}$ is also referred to as electrical efficiency. The status and challenges of current state-of-the-art UV LEDs will be briefly summarized below based on the analysis of the above parameters.

**Radiative efficiency:**
Radiative efficiency denotes the ratio between spontaneous recombination rates and the total recombination rates including radiative recombination rates and non-radiative recombination rates. Two major non-radiative recombination mechanisms are Shockley–Read–Hall (SRH) recombination and Auger recombination. III-Nitride LEDs are normally grown on non-native sapphire substrates because of the high cost of native AlN or GaN substrates, leading to dislocation density above $10^7$ cm$^{-2}$ in the LED epitaxial stack. High dislocation density and defect density in the active region could potentially cause strong SRH recombination. However, for visible LEDs, InGaN compositional fluctuations could lead to carrier localization and help significantly screen the SRH recombination centers.[19] As a result, the recombination efficiency at low current level is insensitive to the dislocation and defect density in InGaN-based blue LEDs, while Auger recombination becomes a dominant non-radiative recombination mechanism at high current levels and contribute to efficiency droop.[20,21] However, evidence on strong carrier localization effect has not been reported for AlGaN-based UV LEDs. Instead, the internal quantum efficiency of AlGaN quantum wells drops off significantly when the threading dislocation density is above $10^8$ cm$^{-2}$.[18] Therefore, major research efforts have been focusing on the optimization of the material quality using a variety of techniques. Advances in substrate quality and optimization of the active region have enabled high radiative efficiency above 60% for a wide range of UV wavelength spectrum[22,23], making it suitable for high efficiency UV LED applications.

Even though high material quality have been achieved through growth optimizations, the remaining two factors, electrical efficiency (defined as $h\nu/qV \times$ Injection efficiency) and
light extraction efficiency, are the ones that pull down the efficiency below 5%, and both are related to the injection of holes into the LED structure.

**Electrical efficiency and light extraction efficiency:**

Low p-type conductivity and high contact resistance remain a critical problem in wide band gap AlGaN-based ultraviolet light emitters due to the high acceptor ionization energy. The activation energy of acceptors in high composition AlGaN (0.63 eV for AlN)[24] is significantly higher than that in GaN (0.14 eV), making it challenging to achieve efficient hole injection. For example, when the material is doped with [Mg]=1×10^{19} \text{ cm}^{-3}, the thermally activated hole concentration drops from 7×10^{17} \text{ cm}^{-3} in GaN to 6×10^{13} \text{ cm}^{-3} in AlN. As a result, the highly unbalanced populations of electrons and holes injected into the quantum well regions result in severe electron overflow to the p-AlGaN side and contribute to parasitic emission or non-radiative emission. More severe is the drop in injection efficiency since the available hole density decreases exponentially with increasing Al composition and therefore decreasing emission wavelength. The solution to this issue requires excellent blocking of the overflow electrons using an electron blocking layer with high conduction band offset.

Another limitation comes with the poor direct p-type contact due to the low hole density, and low mobility, which is typically below 20 cm²/Vs for high Al composition p-AlGaN.[25] This causes poor current spreading, and severe current crowding problems. The two existing approaches to overcome this are shown in Figure 2. The first approach is to put a p-GaN layer to inject holes, and the second approach is to use p-AlₓGa₁₋ₓN/ AlₓGa₁₋ₚ₁₋ₚN superlattice layer. Unfortunately, while these solutions do enable hole injection, they
come with significant penalties. P-GaN can reduce the resistance and lead to high electrical efficiency but also result in high absorption loss and low light extraction efficiency since the bandgap of GaN is smaller than the energy of the emitted light. The p-AlGaN superlattices have a wide energy bandgap and do not absorb but have high resistance and can therefore reduce the electrical efficiency.

Figure 2 Schematic comparison between conventional UV LED structures and the tunnel junction-based UV LED structure.

Due to the absorption in the p-type contact layer, UV light has to be collected from the substrate side of the devices, for which flip chip bonding is necessary. Moreover, the polarization of emitted light changes from top emission (transverse electric mode) to side emission (transverse magnetic mode) at short wavelengths[26]. The combination of the high internal absorption loss and emission mode switching causes a dramatic reduction of the light extraction efficiency of deep UV LEDs. The highest reported value is only 25% for deep UV LEDs[27], while the value for blue LEDs is as high as 90%[10]. Therefore, improving the electrical efficiency and light extraction efficiency is limited by the intrinsic material properties and device structures, and has remained as a major challenge for UV LED community.
1.2. III-Nitride tunnel junctions

In this work, we explore the use of a tunnel-injected UV LED structure to address the critical challenges faced by the conventional UV LED stacks to achieve comparable efficiencies to blue LEDs. The approach (Figure 2) we propose is to use polarization-engineered tunnel junctions integrated on UV emitters to reduce both absorption and electrical losses. Instead of direct metal contact to p-type layers, we use tunneling contact to p-AlGaN with an n-AlGaN layer as the top most contact layer.

Using low-resistivity tunnel junctions and thin p-regions minimizes the electrical losses for hole injection. Furthermore, the hole availability is not limited by thermal ionization of acceptors since holes can be introduced through *non-equilibrium injection* across the tunnel junction. This can be especially useful for high Al-composition structures where the equilibrium hole concentration is extremely low. The increased availability of holes could have direct impact on the carrier injection efficiency. In addition, the top of the structure is n-type AlGaN, which is transparent and has low spreading resistance. This allows for a significant reduction of the internal light absorption loss compared to conventional UV LEDs and eliminates the need for flip chip bonding. Therefore, the tunnel-injected UV LED structure could enable efficiency carrier injection and, at the same time, improve the light extraction efficiency, making it a superior structure for high efficiency UV LED applications.

The critical component of the tunnel-injected UV LEDs is the tunnel junction structure. Interband tunnel junction was first discovered by Esaki in 1958 when he observed a
negative differential resistance in a heavily doped germanium p+ - n+ junction under forward-bias conditions.[28] A tunneling diode is typically formed by degenerate doping of both the p+ and n+ regions of the junction, forming a small and sharp depletion barrier. The current flow through the junction originates from the quantum-mechanical tunneling of carriers through the thin depletion barrier.

At forward bias, the electrons in the conduction band in the n+ region tunnel through the potential barrier to an empty state in the p+ region. It behaves like electrons and holes recombine at the junction through tunneling. The most important application of forward tunneling is to use as low resistance inter-connecting layer for cascade solar cells.[29]

Figure 3 Schematic demonstration the carrier transport processes of tunnel junctions operated under reverse bias and forward bias

The situation is slightly different when the tunneling diode is reverse biased. Electrons in the valence band in the p+ region tunnel to the conduction band in the n+ region, free holes are thus generated in the p+ region. So the current flow through the reverse biased tunnel junction is accompanied with hole injection into the p+ region. For a reverse biased heavily doped tunnel junction, an ohmic-like current-voltage behavior with very low resistance is
expected. Based on this, we integrate it with UV LEDs to achieve non-equilibrium hole injection.

One problem with the tunneling injection is that the tunneling probability decreases exponentially with increasing depletion barrier, which is determined by the band gap of the semiconductor material used in the tunnel junction. Many reported resistances of tunnel junctions formed by different materials follows an exponential trend with increasing bandgaps. As a result, low tunneling probability is expected for AlGaN tunnel junctions, because of the high tunnel barrier. The design of the AlGaN tunnel junctions based on polarization engineering forms a building block for the work described in this thesis.

1.3. Overview of the thesis

Chapter 2 presents the design of efficient interband tunnel junctions for ultra-wide bandgap AlGaN. The feasibility of achieving low resistance AlGaN tunnel junctions is investigated based on polarization engineering in the entire Al composition range. The method to reduce the tunneling resistances using a graded tunnel junction structure, and its feasibility for UV LED applications is discussed. The effect of polarization grading in improving electron and hole doping efficiency is also presented, and the influence on UV LED performance is discussed.

Chapter 3 describes the growth optimizations and p-type doping of AlGaN layers using MBE. The growth window to obtain smooth surfaces with atomic steps is discussed through a series of growth studies. The influence of the growth conditions on the impurity
incorporation into AlGaN layers is also described. Those optimized growth conditions ensure the successful demonstrations of the tunnel-injected UV LEDs.

Chapter 4 presents experimental demonstrations of ultra-wide bandgap AlGaN tunnel junctions based on the theoretical designs to be discussed in Chapter 2. Experimental demonstrations of AlGaN tunnel junctions with Al composition up to 75% is realized. The tunnel junctions are integrated with UV LEDs to evaluate the ability in achieving efficient interband tunneling in AlGaN. Light emissions in the UV-A to UV-C spectrum driven by tunneling hole injection are demonstrated. The key challenges and the corresponding approaches toward the realization of high efficiency tunnel-injected UV LEDs are discussed. For UV-A LEDs, the effect of the p-AlGaN layers is investigated. By utilizing a compositionally down-graded p-AlGaN layer to take advantage of polarization doping, high device efficiencies are achieved. The realization of p-type dopant-free UV LEDs emitting at 325 nm will also be discussed. The optimization of the p-AlGaN layers are also studied for UV-B and UV-C LEDs. It is found that better electron blocking is necessary because of the extra voltage drop across the tunnel junction layer for the onset of interband tunneling.

Chapter 5 presents a different tunnel-injected UV LED structure employing a metal/InGaN/p-AlGaN tunnel junction for hole injection. The influences of Ni- and Al-based top contact metal stacks on the device performance, including both electrical and optical characterizations, are experimentally studied. The benefit compared to the semiconductor tunnel junctions are discussed.
The thesis concludes with discussions on further improving the tunnel junction performance for potential applications in deep UV LEDs and UV laser diodes based on the work presented. A hybrid growth method employing MOCVD for active region growth and MBE for tunnel junction growth is also proposed.
Chapter 2

Design of III-Nitride tunnel junctions

Tunnel junctions have been studied extensively for both optoelectronics and electronics applications, including cascaded LEDs/ laser diodes[30], tandem solar cells[31] and tunneling field-effect transistors[32]. Following the first report in degenerately-doped Ge PN diodes[28], heavy impurity doping has been utilized for the realization of low resistance tunnel junctions in a wide range of material systems. While degenerate doping can help reduce the depletion width for interband tunneling, the tunnel barrier height increases with the material bandgap. As a result, the tunnel junction resistances follow an exponential increase with increasing bandgap energy. This makes it extremely challenging to achieve efficient interband tunneling in wide bandgap semiconductors, such as GaN or AlGaN.

GaN tunnel junctions have been investigated by multiple research groups aiming for promising applications in visible light emitters. The initial studies on GaN tunnel junctions were reported by Takeuchi et al, Ozden et al, and Jeon et al in 2001 and 2002.[33-35] However, the tunnel junctions showed high turn-on voltage and on-resistance, resulting in poorer LED performance when the standard p-type contact was replaced by the tunnel junction structures. Following that, polarization effect was utilized to reduce the depletion width and enhance the tunneling process through the insertion of a thin AlN layer between
p+ and n+ GaN layers, as developed by Grundmann et al in 2006.[36,37] Later on, polarization engineered n-GaN/InGaN/p-GaN tunnel junction structure grown by plasma assisted molecular beam epitaxy (PA-MBE) was reported by Krishnamoorthy et al in 2010 with low on-resistance.[38-42] Similar tunnel junctions were also demonstrated based on MOCVD growth after successful demonstration of p-GaN sidewall activation.[43-46] By adopting the same tunnel junction structure, cascaded blue LEDs were demonstrated by Akyol et al in 2015 with near ideal turn-on voltages.[47,48] Similar cascaded LED structures were also demonstrated by Chang et al in 2015 with an external quantum efficiency as high as 90%.[49,50] Applications of GaN tunnel junctions in nanowire LEDs have also be realized.[51,52]

Recently, low-resistance homojunction GaN tunnel junctions were also developed.[53-61] By taking advantage of the ultra-high Si and Mg doping or the un-intentional n-type dopants, excellent tunnel junction performance was achieved without the need for polarization engineering. This has led to successful demonstrations of high efficiency blue LEDs with wall-plug efficiency above 70%[57], edge emitting laser diodes[54,59], and vertical-cavity surface-emitting laser diodes[56]. Similar junctions grown by MBE with further increases in both Mg and Si doping concentrations showed high current tunnel diode operations (150 kA/cm²) and repeatable room temperature negative differential resistance.[61] Those successful demonstrations of GaN tunnel junctions have led to increased interest on III-Nitride tunnel junctions.

While significant progress has been achieved for GaN tunnel junctions, AlGaN tunnel junctions have not been studied before this work regardless of their promising applications
for efficient UV emitters. It becomes increasingly challenging to make efficient interband p-n tunnel junctions for ultra-wide bandgap AlGaN materials, due to the wide depletion barriers and doping limitations. In this chapter, the feasibility of achieving low resistance AlGaN tunnel junctions will be discussed. The tunnel junction designs based on polarization engineering will be discussed over the entire Al composition range.

### 2.1. Polarization effect

The polarization effect is a unique property possessed by the III-Nitride material system. It forms the basis for many Nitride-based device structures, and provides a new approach for the design of III-Nitride tunnel junctions. Here, a brief introduction to the polarization effect and a discussion on tunnel junction design based on polarization engineering will be presented.

The deviation of the crystal structure in III-nitride semiconductors from an ideal wurtzite structure and the polar nature of the III-N bonds give rise to strong spontaneous polarization. For most device applications, the epitaxial of III-Nitrides is along +c [0001] direction, and the spontaneous polarization vector points along the -c direction. The spontaneous polarization charge in a unit cell is $1.8 \times 10^{13}$ cm$^{-2}$ in GaN, $2.0 \times 10^{13}$ cm$^{-2}$ in InN and $5.1 \times 10^{13}$ cm$^{-2}$ in AlN. When AlGaN is grown on top of GaN, the AlGaN lattice is subjected to an in-plane tensile strain and a compressive strain along the [0001] direction, because of its smaller in-plane lattice. This leads to a piezoelectric polarization with the same direction as the spontaneous polarization in AlGaN. The total polarization is the sum of those two components. The polarization charge density is given by the gradient of the
polarization as $\sigma = -\nabla P$. This results in a net positive polarization charge at the AlGaN/GaN interface as shown in Figure 4. Therefore, high density of free electrons is attracted to the hetero-interface, leading to the formation of a two dimensional electron gas. This forms the basis for AlGaN/GaN high electron mobility transistors.

Figure 4 Charge distributions and energy band diagrams of pseudomorphically-grown AlGaN or InGaN on GaN substrates.

When InGaN is grown on top of GaN, the piezoelectric polarization in InGaN has an opposite vector direction as compared to the spontaneous polarization, owing to the larger in-plane lattice constants than those of GaN. Since InGaN has similar spontaneous polarization as GaN, the polarization sheet charge at the InGaN/GaN interface is mainly determined by the piezoelectric polarization caused by the strain. As a result, a negative sheet polarization charge exists at the InGaN/GaN interface, leading to an electric field
pointing to the [000-1] direction in the InGaN layer as shown in Figure 4. When the GaN layer is doped with p-type dopants, the negative polarization charge attracts free holes and creates a two dimensional hole gas (2DHG) at the interface.

The electric field \((F)\) in the InGaN layer is determined by the polarization sheet charge following the Gauss’s Law \(F = \sigma/\varepsilon\) (\(\varepsilon\) is the dielectric constant) by neglecting the screening effect from the 2DHG and the surface pinning effect. The energy band bending \((E)\) caused by such polarization field would be \(E/q = F \times t_{InGaN}\), where \(t_{InGaN}\) is the InGaN layer thickness and \(q\) is unit charge. However, the maximum band bending in the InGaN layer is limited by the bandgap energy of InGaN \((E_g_{InGaN})\), giving rise to a critical InGaN layer thickness \(t_{cr}\). When the InGaN layer is thicker than \(t_{cr}\), the band bending is higher than the bandgap energy, pushing the InGaN conduction band below the Fermi level at the surface. As a result, electron accumulation occurs at the InGaN surface, and contributes to screening of the polarization field in InGaN. The critical tunneling thickness can be estimated through \(t_{cr} = \varepsilon E_g_{InGaN} / q\sigma\). As an example, the net polarization charge is \(\sim 2 \times 10^{13}\) cm\(^{-2}\) at the In\(_{0.2}\)Ga\(_{0.8}\)N/GaN interface mainly originated from the high piezoelectric polarization. Therefore, the polarization field in the InGaN layer is nearly 4 MV/cm, which exceeds the material breakdown field, making the structure in the Zener tunneling regime. The critical tunneling thickness is further estimated to be 5 nm. It is worth noting that, when the GaN layer is replaced by AlGaN, which has even higher lattice mismatch with InGaN and therefore higher piezoelectric and spontaneous polarization charge, further increase in the polarization field and reduction in the critical tunneling
thickness are expected. Such a thin barrier, together with the sharp band bending forms the basis for the polarization engineered interband tunnel junctions.

Figure 5 Schematic illustrations of bulk polarization doping.

In addition to the sheet charges enabled by the abrupt changes in both the spontaneous polarization and piezoelectric polarization at the hetero-interfaces, bulk polarization charges can be obtained as well through polarization engineering. Since polarization charge originates from the gradient of polarization, engineering the polarization profile could enable different forms of bulk polarization doping profiles.[62-64] Particularly, when polarization is graded linearly along the epitaxial direction, the resulted polarization charge is nearly uniform. The polarization grading can be achieved through Al compositional grading.
As shown in Figure 5, two situations are illustrated when a linear compositional graded layer is grown pseudomorphically on top of an Al$_{0.3}$Ga$_{0.7}$N layer. When the Al composition is graded from 30% to 0%, the polarization charge in each unit cell reduces as illustrated in Figure 5. As a result, the net polarization charge is negative and remains nearly constant in the graded layer. To balance the bounded polarization charge and achieve charge neutrality, extra free holes are attracted in the compositional grading layer. This contributes to improvements in p-type doping and pushes the Fermi level closer to the valence band edge. On the other hand, if such a grading scheme presents in the n-type doped layers, the polarization charge behaves as compensating dopants, therefore, extra n-type doping is necessary to overcome the compensation and achieve n-type conductivity.

Similarly, when the Al composition is graded upward from 30% to 60%, the total polarization in the unit cells increases linearly, leading to the formation of a three-dimensional positive polarization charge. Free electrons are thereby attracted to the compositional graded layer, and contributes to enhanced n-type doping.

It is worth noting that, the sources for the attracted free holes or electrons by the fixed polarization charges are not limited by intentional dopants, instead, they could be surface states or dopants in the bulk. Compare to thermal activated carriers, the density of the electrons/holes attracted by polarization charges only depends on the bulk polarization charge density, and is insensitive to the dopant activation energy. This makes the polarization doping especially critical for the devices with ultra-wide bandgap AlGaN involved. As discussed in Chapter 1, the thermal activated hole concentration is extremely low (below 10$^{15}$ cm$^{-3}$) in high Al composition AlGaN, regardless of the high p-type dopant
concentration. In comparison, the polarization doping could enable hole density of $3\sim5\times10^{18}$ cm$^{-3}$ when the Al composition is graded over 10% within 10 nm. This technique could be especially beneficial for deep UV LED applications. In this thesis, we utilize the polarization effect in the design of tunnel junctions for ultra-wide bandgap AlGaN.

2.2. Polarization engineered tunnel junctions

In the previous section, we have discussed the strong band bending in the InGaN layer when pseudomorphically grown on p-GaN. One step forward by adding an n-type GaN layer on top of InGaN will lead to an effective tunnel junction structure. Optimizations of the n-GaN/InGaN/p-GaN tunnel junction structures have enabled low resistance tunnel junctions with resistance below $10^{-4}$ $\Omega$ cm$^2$.[39] Similar tunnel junction resistances have also been achieved using pn tunnel junctions by doping the acceptors and donors to their doping limits of $3\sim5\times10^{20}$ cm$^{-3}$.[60,61] The formation of band tail states in the forbidden energy gap and the bandgap narrowing effect because of extremely high doping are recognized as the key enablers for the efficient interband tunneling.[61] However, whether those two methods will work for ultra-wide bandgap AlGaN remained unexplored.

2.2.1. P-N tunnel junction vs polarization-assisted tunnel junction

The standard AlGaN p-n tunnel junctions and the polarization engineered n-AlGaN/InGaN/ p-AlGaN tunnel junctions are first compared based on the calculations of tunneling currents. Simulation of tunnel junctions was carried out using a two dimensional device simulator. We assumed linear change of acceptor activation energy from 140 meV in GaN
to 630 meV in AlN, constant donor activation energy of 15 meV for AlGaN with Al composition lower than 80%, and donor activation energy of 200 meV for Al compositions of 80% and greater.\[65] The band diagrams were calculated by self-consistently solving Schrödinger-Poisson equations. Wentzel–Kramers–Brillouin (WKB) approximation was used for tunneling probability calculation, and tunneling current was calculated by considering all possible contributions by carriers with different energies, through the expression:

\[
J_T = \frac{4\pi q m^*}{(2\pi)^3 \hbar^3} \int_0^\infty dE_z T(E_z) \int_0^\infty dE_t (f_n^p(E_z, E_t) - f_n^n(E_z, E_t))
\]

Here, \(E_z\) and \(E_t\) are the electron energies along and perpendicular to the tunnel direction, \(v_z = \sqrt{2E_z/m_z}\) is the electron velocity along the tunneling direction. \(f_n^p\) and \(f_n^n\) are the Fermi-Dirac distributions of electrons, \(\rho^p\) and \(\rho^n\) are the density of states, while the superscripts denote p and n regions on either side of the TJ. \(T(E_z)\) is the tunnel probability calculated for the electrons with energy \(E_z\). Here, band tail states and bandgap narrowing effect due to heavy impurity doping are not included in the simulations. While those effects could lead to increase in the tunneling probability, achieving heavy doping to reach the onset of those effects could result in high density of defects in AlGaN and thereby severe self-compensation effect.

An \(\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}\) p-n tunnel junction with acceptor doping density of \(N_A=5 \times 10^{19}\) cm\(^{-3}\), and donor doping density of \(N_D=1 \times 10^{20}\) cm\(^{-3}\) was first simulated. The depletion width for a p-n tunnel junction under equilibrium condition could be described by \(w_d = \sqrt{2eV_{bi}(N_A + N_D)/qN_A N_D}\), where \(N_A\) and \(N_D\) are p- n- type doping concentrations in the
junction, $\varepsilon$ is material dielectric constant, and $V_{bi}$ is the build-in voltage. Even with the high doping densities in the Al$_{0.7}$Ga$_{0.3}$N p-n junction, a depletion width of 12 nm is expected due to the high build-in voltage, as shown in Figure 6(a). This results in a wide depletion barrier with a barrier height of the bandgap of Al$_{0.7}$Ga$_{0.3}$N $\sim$ 5.2 eV. For a simplified estimation, the tunneling probability has an exponential dependence on the bandgap energy and the depletion width, as described by:

$$T \propto \exp \left( - \frac{4}{3} \sqrt{\frac{2m^*E_s}{\hbar^2}} * t_{dep} \right)$$

Compare to GaN pn tunnel junctions, whose barrier height is 3.4 eV and depletion width could be $\sim$ 4 nm with degenerate doping, the theoretical tunneling probability in Al$_{0.7}$Ga$_{0.3}$N is 25 orders of magnitude lower than that in GaN tunnel junctions at zero bias, and this prevents effective interband tunneling in AlGaN tunnel junctions.
Figure 6 Comparison of tunnel junction structures formed by (a) heavily doped p-n homojunction, (b) heterojunction with thin InGaN layer inserted between AlGaN layers, (c) heterojunction further with graded Al composition layers. The Al/In mole fraction profiles, charge profiles and band diagrams of Al$_{0.7}$Ga$_{0.3}$N (/ In$_{0.3}$Ga$_{0.7}$N) tunnel junctions are compared.

To surmount the high tunneling barrier, we investigated the use of heterostructure and polarization engineering. A thin In$_y$Ga$_{1-y}$N layer is inserted between p- and n-type Al$_x$Ga$_{1-x}$N layers to reduce the tunneling barrier energy and width (Figure 6(b)). Due to the polarization discontinuity, sheet charges with density over $10^{13}$ cm$^{-2}$ are induced at the AlGaN/InGaN heterointerfaces and this reduces the tunneling barrier to less than 3 nm.
At the same time, the tunnel barrier height is reduced from the bandgap energy of AlGaN (5.2 eV) to that of InGaN (~ 2.1 eV). The drastic reduction of the tunnel barrier leads to much higher tunneling probability compared to the homojunction tunnel junction. However, wide depletion barriers are present in both n- and p-AlGaN sides due to the large band offsets between AlGaN and InGaN. Moreover, the high acceptor activation energy in AlGaN pushes the Fermi level into the forbidden gap even with heavy Mg doping, making it hard to align the valence band edge in the p-side to the conduction band edge in the n-side of the tunnel junction structure. This makes it challenging to achieve effective interband tunneling at low reverse bias. It is also found that the depletion width in the p-AlGaN layer increases under reverse bias (shown for 20 A/cm²) leading to extra voltage drop to achieve effective interband tunneling.

2.2.2. Graded tunnel junction structure

To reduce the depletion-related tunneling barrier, we introduce compositionally graded AlGaN layers. In the scheme investigated here, for each AlₓGa₁₋ₓN layers (Figure 6(c)), the region adjacent to the tunnel junction is graded from AlₓGa₁₋ₓN to Alₓ₋₀.₁Ga₁₋ₓ+₀.₁N on the p-side, and from Alₓ₋₀.₁Ga₁₋ₓ+₀.₁N to AlₓGa₁₋ₓN on the n-side (Figure 6(c)). This is to ensure the graded AlGaN layers have higher energy than the emitted UV light from the quantum wells, to minimize light absorption. The compositional grading leads to a gradient in the polarization (P), which creates a three dimensional (3D) polarization charge \( \rho(x) = -\nabla \cdot P = -\nabla \cdot \left| P_{AlₓGaN}(x) - P_{Alₓ₋₀.₁Ga₁₋ₓN}(x) \right| / t \), where \( t \) is the grading distance). For linear grading
within 3 nm, this results in $3 \sim 5 \times 10^{19}$ cm$^{-3}$ polarization charge density, which ensures
degenerate doping.

To demonstrate the effect of the compositional grading layers, the band diagrams of
$\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}/\text{In}_{0.3}\text{Ga}_{0.7}\text{N}$ tunnel junction structures without and with grading layers are
compared in Figure 6 (b) and (c). The depletion barriers in both n- and p- sides are reduced
since the grading induced 3D polarization bound charges attract electrons in the n-AlGaN
side and holes in the p-AlGaN side, results in degenerate carrier distributions on either side.
This also enables the alignment of band edges, leading to substantial increase in the
tunneling probability even at small reverse bias. It is also found that a significant depletion
layer is formed in the p-AlGaN layer at reverse bias for the TJ structure without grading,
leading to much higher voltage drop to achieve effective interband tunneling as compared
by the band diagrams extracted at 20 A/cm$^2$ in Figure 6 (b) and (c). One drawback is the
lower sheet polarization charge density at the $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}/\text{In}_{0.3}\text{Ga}_{0.7}\text{N}$ interfaces for the
graded TJ structure as shown schematically in the polarization charge profiles in Figure
6(c), as compared to the $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}/\text{In}_{0.3}\text{Ga}_{0.7}\text{N}$ interfaces without grading. This results in
slight reduction in the polarization field in InGaN layer, which could lead to an increase in
the InGaN tunneling barrier. However, it could show very minimal influence in the
tunneling probability since the polarization charge density remains to be high at
$\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}/\text{In}_{0.3}\text{Ga}_{0.7}\text{N}$ interfaces.
Figure 7 Calculated current-voltage curves for the Al$_{0.7}$Ga$_{0.3}$N ($/\text{In}_{0.3}\text{Ga}_{0.7}$N) tunnel junctions (Figure 6). The homojunction tunnel junction is highly resistive, while polarization engineered tunnel junction structures enable much lower tunneling resistances.

As shown from the calculated current-voltage curves for Al$_{0.7}$Ga$_{0.3}$N tunnel junctions in Figure 7, the resistance for homojunction tunnel junction was found to be high, with 4 A/cm$^2$ under 50 V reverse bias, suggesting that unlike GaN, homojunctions may not be a viable solution for high composition ultra-wide bandgap AlGaN. In comparison, high tunneling current can be achieved for ultra-wide bandgap AlGaN using polarization engineered tunnel junction structure. More significantly, the graded tunnel junction structure leads to a further reduction in the reverse bias from 1.8 V to 0.12 V, and in the tunneling resistance from $2.8 \times 10^{-4} \text{ } \Omega \text{ cm}^2$ to $3.7 \times 10^{-5} \text{ } \Omega \text{ cm}^2$ at 1 kA/cm$^2$, both of which have important consequences for device efficiency.
Figure 8 Simulated tunneling resistance and reverse voltage drop at a current density of 1 kA/cm² for AlGaN/InGaN tunnel junction structures without and with the compositional grading layers. Experimental results of graded Al₀.₅₅Ga₀.₄₅N/In₀.₂Ga₀.₈N, graded Al₀.₃Ga₀.₇N/In₀.₂₅Ga₀.₇₅N[66], GaN/In₀.₂₅Ga₀.₇₅N[39], and GaN p+-n+[61] tunnel junctions are marked in the figures.

To further explore the design space for ultra-wide bandgap tunnel junctions, various combinations of AlGaN/InGaN compositions (constant thicknesses and doping levels same as that in Figure 6(b) and 6(c)) were modeled. Figure 8 shows the calculated tunneling resistance and reverse bias at 1 kA/cm² for tunnel junctions with and without compositional grading layers. InGaN interband tunneling barrier is dominant at low In compositions (<10%), leading to high resistance for both graded and non-graded tunnel junctions. Lower
tunneling resistance is observed when 10% to 80% In mole fraction is used, but the graded tunnel junction structure is critical to ensure lower tunneling resistance and voltage drop, especially for high Al composition (> 50%). In the structures that are feasible from lattice mismatch considerations (up to 30% In mole fraction), for the entire Al composition range, tunneling resistance in the $10^{-4} \, \Omega \, \text{cm}^2$ range are achievable, with a voltage drop less than 1 V at 1 kA/cm$^2$.

The experimental (red stars) tunneling resistance and voltage drop of various AlGaN/InGaN, GaN/InGaN, and GaN p+-n+ tunnel junctions are shown together with the simulation predictions in Figure 8. The experimental values are of the same order of magnitude as the simulated results for the tunnel junction structures. The discrepancy could be attributed to the approximations made in the simulations, as well as non-idealities in growth and material quality.

The simulation results show the possibility to achieving efficient interband tunneling hole injection through a graded TJ structure, which could enable low tunneling resistances for ultra-wide bandgap AlGaN tunnel junctions that are suitable for UV LED applications. It shows great potential to integrate the graded TJs to UV LEDs for tunneling hole injection.

### 2.3. Conclusions

In this chapter, the feasibility of achieving low resistance AlGaN tunnel junctions were investigated. Polarization effect was exploited to explore the design space. In addition to the high density polarization sheet charge arose from sharp hetero-interfaces, the bulk polarization charges were also utilized to reduce the depletion barriers for interband
tunneling. It was found that low tunnel junction resistances of $\sim 10^{-4} \, \Omega \, \text{cm}^2$ could be achieved for AlGaN tunnel junctions in a wide Al composition range. This makes it suitable for UV LED applications. The investigated tunnel junction structures form the building block for the tunnel-injected UV LEDs studied in this thesis.

The polarization doping approach discussed in this chapter also provides a design method for efficient p-type doping, which is found to be critical in the realization of high efficiency UV LEDs.
Chapter 3

Molecular beam epitaxy growth of AlGaN

GaN growth using plasma-assisted molecular beam epitaxy (PA-MBE) have been well-studied. The optimized GaN growth temperature was found to be ~700 °C, and the best surface morphology and material quality can be obtained at a slight Ga-rich growth condition when 1-2 ML of excess Ga exists at the epitaxial surface.[67] However, in growth practices, maintaining a constant thickness of Ga coverage is challenging without growth interruptions. Therefore, techniques such as interruptions of Ga flux and thermal desorption of excess Ga during the growth were developed to avoid the formation of Ga droplets while maintaining slight Ga-rich growth condition. However, for the growth of AlGaN, such growth interruptions could result in unexpected variations in the atomic mole fractions. Because of the stronger bonding energy between Al and N than that of Ga-N bonding, Al has a higher priority to incorporate to the lattice and the remaining metal sites will be occupied by Ga.[68] As a result, any interruption in either Ga or Al flux will result in an immediate change in the Al content in the lattice. Therefore, it is critical to control the growth to avoid either surface roughening due to Ga deficit or the formation of metal droplets because of excess Ga. Besides, due to the strong Al-N bonding, the Al ad-atom mobility is significantly lower than that of Ga or In. Therefore, high growth temperatures are preferred for the epitaxial growth of AlGaN with high material quality. The growth
kinetics for AlGaN at the elevated temperatures, and their influences on the surface morphology and impurity incorporations remain to be explored. In this chapter, the MBE growth of AlGaN is investigated systematically. The optimized growth conditions are adopted for the UV LED growths using MBE.

3.1. AlGaN growth optimization

A series of samples with the same epitaxial stack as shown in Figure 9 were grown using PA-MBE. The growths were initiated with 10 nm AlN grown using migration enhanced epitaxy method on AlN/sapphire substrate from Nitride Solutions Inc. This was followed by 200 nm AlGaN growth aiming for 80% of Al content. The surface morphology and Al composition were characterized using AFM and XRD, respectively.

![Figure 9 Epitaxial stack adopted for the AlGaN growth study.](image)

3.1.1. Influence of substrate temperature

As we discussed earlier, higher substrate temperature could be beneficial for increasing Al ad-atom mobility and enhancing the uniformity of the material. Therefore, the influence of the substrate temperatures on AlGaN growth were first investigated. Here, the substrate
temperatures referred in this thesis are the actual surface temperatures read from a pyrometer which was calibrated to the melting point of Al. Five samples grown at different substrate temperatures ranging from 700 °C to 810 °C with the same stack as shown in Figure 9 are compared. The growth rate was fixed to be 5.6 nm/min, corresponding to a Ga stoichiometric flux of ~ 2×10^{-7} Torr. The Al flux was fixed to be 9.8×10^{-8} Torr for samples aiming for ~80% Al composition. In order to maintain a similar Ga-rich growth mode, the Ga fluxes were increased from 3.5×10^{-7} Torr to 9×10^{-7} Torr with increasing growth temperatures to compensate the exponential increase in the desorption rate of Ga atoms. At the growth temperatures of 790 °C and 810 °C, even with a high Ga flux of 9×10^{-7} Torr, which is nearly the highest flux feasible in our MBE system, excess Ga coverage was absent as evidenced from bright RHEED patterns during the growths.

The surface morphologies of the samples are presented in Figure 10. The samples grown below 760 °C showed similar morphologies with a random distribution of spiral patterns, which have been correlated to screw dislocations with a dislocation core located at the center of the spiral. The density of the screw dislocations can be estimated to be approximated 1×10^9 cm^{-2}. Additionally, clear atomic steps can be observed in the samples. When the growth temperature was increased from 700 °C to 730 °C, there is a noticeable increase in the width of the atomic terraces. This is attributed to an increase in the Al ad-atom mobility and therefore longer diffusion length at higher temperatures. However, distinct changes in surface morphology is observed for the samples grown above 790 °C. The sample grown at 790 °C showed dendritic features, which is a typical morphology
grown under nitrogen rich conditions. This indicates that Ga is not incorporated sufficiently at such high temperatures.

Figure 10 AFM images of AlGaN layers grown at different substrate temperatures.

The XRD results of those samples are shown in Figure 11. Even though the same Al fluxes were used in the growths, a significant shift of the Al composition with increasing growth temperature was observed. The dependence of the extracted Al composition on the growth temperature follows an exponential trend. This is attributed to the increased thermal decomposition of the Ga-N bonding and desorption of the Ga atoms at high temperatures.

This series of samples points to a conclusion that AlGaN can be grown with clear atomic steps in the temperature range of 700 - 760 °C in the MBE system.
Figure 11 XRD results and the extracted Al compositions of the AlGaN samples grown at different temperatures.

![XRD results](image1)

![Al composition vs. growth temperature](image2)

Figure 12 SIMS profile of oxygen and carbon in high composition AlGaN grown at different substrate temperatures.

![SIMS profile](image3)
AlGaN has been known to have higher impurity incorporation. The dependence of the background impurities (O and C) was characterized using secondary ion mass spectrometry (SIMS) is shown in Figure 12. When the substrate temperature was increased from 700 °C to 750 °C, a significant increase of both O and C concentration was observed at various Al compositions. This could originate from a reduction of the Ga wetting layer on the growth front, which could help screen the incorporation of the impurities. Therefore, the determination of the optimized AlGaN growth temperature requires the balance of two situations: a) high growth temperature could enable more uniform material because of higher Al ad-atom mobility, b) sufficient excess Ga coverage need to be maintained. This sets an upper limit for the growth temperature ~ 740 °C, which could vary slightly with the supplied Ga flux.

3.1.2. Influence of Ga flux

![Comparison between the samples with different Ga fluxes.](image)

The influence of Ga flux on the AlGaN growth was further investigated. Two samples grown at 760 °C with the same Al flux but different Ga fluxes are compared. When the Ga
flux was reduced from $6 \times 10^{-7}$ Torr to $4 \times 10^{-7}$ Torr, the spiral features and the atomic steps disappeared. In addition to that, the Al composition increased from 85% to 95%, which is attributed to the deficit of Ga incorporation into the lattice.

The indication from those two samples is that: a) maintaining Ga-rich condition is critical for achieving atomically smooth surfaces; b) growing AlGaN under intermediate conditions could result in an increase in the Al composition because of the decomposition of the Ga-N bonding.

3.1.3. Influence of growth rate

Figure 14 Dependence of AlGaN surface morphology on the growth rate

The influence of the growth rate on AlGaN surface morphology was studied at a growth temperature of 760 °C. The AFM images of three samples grown at 3 nm/min, 4.5 nm/min and 5.6 nm/min are compared in Figure 14. An increase in the terrace size with reducing growth rate can be observed. This is attributed to a longer diffusion length of Al atoms because of the lower amount of incoming effective nitrogen atoms.
To conclude, reducing the growth rate can help increase the lateral diffusion of Al atoms, and thereby enhance the uniformity of the AlGaN layers.

### 3.1.4. Sub-monolayer digital alloy

During the UV LED growth, abrupt changes of the Al compositions is inevitable. This includes the transitions from quantum barriers to quantum wells, and to the electron blocking layers. From the growth point of view, those abrupt transitions of Al composition normally require growth interruptions especially when multiple Al cells are not available in the MBE systems. However, growth interruptions could introduce sheet charges of unexpected impurities, which are especially detrimental to the quantum well active region because of the formation of non-radiative recombination centers. Therefore, techniques to achieve abrupt compositional transitions, and at the same time to avoid any growth interruptions are critical for the MBE growth of UV LED structures. Here, a sub-monolayer (sub-ML) digital alloy method was adopted for the realization of AlGaN compositional variations.[69-72] In this method, a periodical stack of sub-monolayer GaN and AlN is grown to target for an averaged AlGaN composition. For example, a stack of 0.4 ML GaN/1 ML AlN is expected to result in an Al composition of ~71% in AlGaN.
Two AlGaN samples grown using the sub-monolayer digital alloy method are compared in Figure 15. The samples were grown at 760 °C, with the only difference being the pulsing time of a period, which are 0.4 ML GaN/ 1 ML AlN in the first sample and 0.8 ML GaN/2 ML AlN in the second sample. The Al flux was kept close to its stoichiometric flux during the growths to avoid accumulation of excess Al metal. Both samples showed smooth surface morphology, with rms values lower than the continuous growths as shown earlier. The extracted Al compositions from the measured XRD curves are 85% for both samples. This is higher than the expected Al composition of 71%, however, it can be understood by considering decomposition of Ga-N bonds and desorption of the Ga metal at the high growth temperature. Regardless of that, the samples indicate that the submonolayer digital alloy method could provide abrupt changes of Al composition and at the same time maintain smooth surface morphology.
Figure 16 The growth methods for the quantum wells and the electron blocking layer and the corresponding transmission electron microscope (TEM) images.

One example of the shutter pulsing sequences during the actual growth of the quantum wells and the electron blocking layer (EBL) is shown in Figure 16. The Al composition of the quantum barrier and the cladding layer is 65%. Each quantum well contains 6 periods of $0.24 \text{ ML GaN}/0.8 \text{ ML Al}_{0.65}\text{Ga}_{0.35}\text{N}$ to aim for an average Al composition of 50%. The high resolution TEM image indicates the growth of sharp quantum wells. Using this method, light emissions in UV A to UV C spectrum range have been achieved. However, compare to the quantum barriers, the quantum wells show higher Al compositional fluctuations, and indicate the existence of sub-monolayers of GaN. The light emission in a wide UV spectrum range from sub-monolayers of GaN has been studied by several groups.\[71,73-75\] It was demonstrated to be beneficial for maintaining a transverse electric polarized light emission pattern even for deep UV LEDs.\[75,76\] Therefore, the adopted sub-monolayer digital alloy method could potentially take advantage of this effect.

The growth method for the electron blocking layer is presented in Figure 16 as well. To increase the Al composition, the Al shutter was open for an extra time in each period while
the other shutters were kept closed. The TEM image showed atomically sharp interfaces for the electron blocking layer.

3.2. P-type doping of AlGaN

Effective p-type doping is critical in reducing the p-AlGaN depletion barrier for interband tunneling. While higher temperatures are preferred for AlGaN growth to enhance the material uniformity, the incorporation of Mg at high temperatures becomes increasingly challenging. There are several possible ways to increase Mg doping concentrations, including increasing Mg flux, changing growth temperature and growth rate. Those methods were investigated by means of SIMS measurements.

The dependence of Mg doping concentration on the substrate temperature and the Mg flux is shown in Figure 17. The doping concentration drops exponentially with increasing substrate temperature. By increasing the Mg flux, the doping concentration above $10^{19}$ cm$^{-3}$ can be achieved at substrate temperature of 700 - 750 ºC. At 670 ºC, the doping density can be as high as $7 \times 10^{19}$ cm$^{-3}$. 
Figure 17 Dependence of Mg doping concentration on the growth temperature.

The dependence of Mg doping density on the growth rate is less trivial. Figure 18 shows a SIMS profile of the Mg-doped AlGaN layers grown at different growth rates while the Mg flux was fixed. As the growth rate reduces from 9 nm/min to 2.5 nm/min, the Mg doping concentration remained to be similar. This indicates that the Mg incorporation rate does not show clear dependence on the Mg:N ratio, instead it might be related to the solubility in the liquid Ga present on the growth surface.
Figure 18 SIMS profile of Mg-doped AlGaN layers grown under different conditions as marked in the figure.

3.3. Conclusions

This chapter described the growth optimizations and p-type doping of AlGaN using MBE. Smooth surfaces with atomic steps were obtained in a substrate temperature range of 700 °C to 760 °C. It was found that supplying sufficient Ga flux to obtain liquid Ga coverage is critical in maintaining smooth surface morphology and reducing impurity incorporation. Reducing the growth rate can lead to smoother surfaces, but it was found to have very minimal impact on the Mg doping concentration. The optimized growth temperature for the realization of p-AlGaN was chosen to be 660 to 720 °C. Those optimized growth methods ensure the successful demonstrations of the tunnel-injected UV LEDs.
Chapter 4

Tunnel-injected III-Nitride UV LEDs

Figure 19 Comparison between conventional UV LED structure and the tunnel-injected UV LED structure. Lower part of the figure shows the schematic energy band diagram of the tunnel-injected UV LED under operation.

The incorporation of interband tunnel junctions on UV LEDs is schematically presented in Figure 19. As shown in the schematic band diagram, when negative voltage is applied on the top contact, the active region is reverse biased, and there is no current flow. By applying
positive bias on the top contact, holes can be injected through the reverse biased tunnel junction layer into the forward biased active region, resulting in radiative recombination. The potential advantages of tunnel-injected UV LEDs were analyzed in Chapter 1. It was discussed that the tunnel-injected UV LED structure could solve both the absorption and electrical loss issues faced by the conventional UV LED structures. In this structure, a transparent n-AlGaN top contact layer is connected to the p-AlGaN layer through an abrupt tunnel junction layer. This avoids the absorbing p-type contact layers and enables efficient non-equilibrium hole injection. Since the structure is terminated with an n-AlGaN layer, which has low spreading resistance, the top metal electrode coverage can be minimized to allow light extraction from the top surface. Besides, aluminum, as the only UV reflective metal with a high reflectivity above 90% in the deep UV range, can be used to form n-type reflective top contact. This provides flexibility in the development of optimized light extraction schemes based on the tunnel-injected UV LED structure. Another benefit of the tunnel-injected UV LED structure is that holes are injected through interband tunneling, which resists the influence of extremely low thermal activation rate of Mg acceptors in AlGaN. This is critical for deep UV LEDs, as the thermally activated hole concentration decreases significantly with increasing Al content in the p-AlGaN layer. While conventional UV LEDs have encountered a substantial efficiency reduction when lowering the emission wavelength in the deep UV wavelength range[14-16,18,27,77-82], the tunnel-injected UV LED structure could potently solve the problem and lead to efficient deep UV emitters.
The design of the tunnel junction structure for ultra-wide bandgap AlGaN using polarization engineering was further discussed in Chapter 2. Prior to this work, the incorporation of III-Nitride tunnel junctions on visible LEDs has been demonstrated, however, AlGaN-based tunnel junctions and their applications in UV LEDs have not been studied. In this chapter, experimental demonstrations of the AlGaN tunnel junctions and their integrations with UV LEDs will be presented.

4.1. UV-A LEDs

The incorporation of tunnel junctions for UV-A LEDs was studied first[66,83,84]. Two generations of devices will be discussed in this section. All the investigated samples were grown by N$_2$ plasma assisted molecular beam epitaxy on Si-doped metal-polar Al$_{0.3}$Ga$_{0.7}$N templates, which were grown by metalorganic chemical vapor deposition (MOCVD) with a threading dislocation density of 1.5 ~ 3×10$^9$ cm$^{-2}$. The first generation of devices has a constant Al composition in the p-AlGaN, while the second generation of devices has a polarization graded p-AlGaN layer.

4.1.1. 1st generation: constant Al composition in p-AlGaN

Epitaxy and device fabrication:

The first generation of devices has a constant Al composition in the p-AlGaN layer.[66] The epitaxial structure and energy band diagram investigated in this work are shown in Figure 20. It contains a UV LED active region, a TJ layer, and a top n-AlGaN transparent contact layer. The UV LED active region has three 4.5 nm Al$_{0.2}$Ga$_{0.8}$N QWs, and a 12 nm
p type Al$_{0.46}$Ga$_{0.54}$N electron blocking layer (EBL). A p+ Al$_{0.3}$Ga$_{0.7}$N/ 4 nm In$_{0.25}$Ga$_{0.75}$N/ graded n+ Al$_{0.3}$Ga$_{0.7}$N TJ layer was grown for tunneling contact and hole injection. The InGaN layer growth condition was calibrated XRD fitting of bulk InGaN growth under the same growth conditions. The Al composition in the n+ AlGaN layer was graded from 22% to 30% in 15 nm, to lower the depletion barrier and avoid light absorption/ re-emission, while there is no compositional grading in the p-AlGaN side. The high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) image of a typical TJ-based UV LED structure (Figure 20) show that flat and sharp heterointerfaces were achieved for the quantum wells and the In$_{0.25}$Ga$_{0.75}$N interband tunneling layer.

Figure 20 (a) TEM image, (b) epitaxial stack, and (c) equilibrium energy band diagram of TJ-based UV LED structure.
Figure 20(c) shows the band diagram of the TJ-UV LED structure calculated using a one dimensional Schrodinger-Poisson solver. A TJ layer on top of p-AlGaN layer enables tunneling contact. The high polarization charge density at the AlGaN/InGaN interface builds up high electric fields, causing band bending across the thin InGaN layer to align the band edges of n+ and p+ AlGaN over just a few nanometers. When the LED is forward biased, the top TJ layer is reverse biased, electrons tunnel from the valence band in p-AlGaN to the conduction band in n-AlGaN, and the remnant holes are then injected into p-AlGaN. As shown in Fig. 20(c), the tunnel barrier consists of the (interband) tunnel barrier across the InGaN bandgap and (intraband) depletion barriers in the p+ and n+ AlGaN layers. Since the depletion barrier in the n side is higher, a graded n+ AlGaN layer was used to reduce the barrier height and increase effective tunneling probability as discussed in Chapter 2.

Inductively coupled plasma reactive ion etching (ICP-RIE) with BCl3/Cl2 chemistry was used for device mesa isolation. Bottom contact evaporation was done with a metal stack of Ti(20 nm)/Al(120 nm)/Ni(30 nm)/Au(50 nm). Rapid thermal annealing under N2 atmosphere at 850 °C for 30 seconds was then carried out to form ohmic contact to the bottom contact layer. Al(20 nm)/Ni(20 nm)/Au(80 nm) was then deposited for top contact. Full metal coverage was used for measuring the electrical behavior, while partial metal coverage was used for optical power measurements. For 50 × 50 µm² devices, ~ 28% of the device region is covered with L shape metal to minimize the blocked light intensity. The electroluminescence and emission power were obtained from on-wafer measurement.
at room temperature using a calibrated Ocean Optics USB 2000 spectrometer with a coupled fiber optic cable.

**Electrical characteristics:**

The electrical characteristics of devices (50 × 50 µm²) with full and partial top metal coverage are shown in Figure 21(a). At a current density of 2 kA/cm², the voltage drop was 7.47 V, while the voltage drop at 20 A/cm² was 4.8 V. In the case of the device with partial metal coverage, we observed a slightly higher voltage drop, which we attribute to the spreading resistance in the n-type AlGaN top contact layer. Increasing the thickness of the Al₀.₃Ga₀.₇N top contact layer would reduce the spreading resistance.

![Figure 21](image)

Figure 21 (a) Electrical characteristics of TJ-UV LED devices (50 × 50 µm²) with full and partial top metal coverage. (b) Differential resistance as a function of current density (full top metal coverage).

The differential resistance is extracted to be 7.5×10⁻⁴ Ohm cm² at 1 kA/cm². To estimate the contribution of the tunnel junction to this total resistance, we de-embedded the other various components in the resistance. The contact resistance for the top and bottom regions

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were estimated (from transfer length method measurements) to be $\sim 1.4 \times 10^{-6}$ Ohm cm$^2$ and $\sim 4.6 \times 10^{-6}$ Ohm cm$^2$, respectively, and the series resistance of the p-AlGaN layer was estimated to be $\sim 1.9 \times 10^{-4}$ Ohm cm$^2$ (acceptor activation energy = 220 meV, and hole mobility = 1 cm$^2$/Vs)[85]. The resistance of n-AlGaN layers is ignored. Therefore, the resistance of the p+ AlGaN/InGaN/n+ AlGaN TJ layer can be estimated as $5.6 \times 10^{-4}$ Ohm cm$^2$.

**Optical characteristics:**

Figure 22 (a) Electroluminescence of the TJ-UV LED structure with dc current injection from 0.1 mA to 20 mA at room temperature, single peak emission at 327 nm is shown. The inset shows an optical micrograph of a TJ-UV LED device ($50 \times 50 \mu$m$^2$) with partial top metal coverage operated at 10 mA. (b) Output power, (c) EQE and WPE of the 50 × 50 µm$^2$ TJ-UV LED device. The powers were measured on wafer without integrating sphere from the top surface.

As shown in Figure 22, single peak emission at 327 nm was obtained with a full width at half maximum of around 14.7 nm, and no significant long wavelength peaks were observed. A small blue shift with increasing current due to the quantum confined Stark
effect is evident. The inset to Figure 22(a) shows an optical micrograph of a TJ-UV LED device showing a $50 \times 50 \mu m^2$ mesa with top contact metal along the borders (dark L-shape), and no metal in the remaining region. When operated at 10 mA, emission is evident over the entire mesa showing that the LED operates in regions without any metal coverage since the n-AlGaN is efficient at spreading the current.

The emission power as a function of injected current (continuous wave) is shown in Figure 22(b). The measured output power of 0.58 mW at 20 mA, corresponds to a normalized optical power of 23 W/cm$^2$ at 800 A/cm$^2$. The maximum external quantum efficiency and wall plug efficiency of the sample are 1.5% and 1.08% as shown in Fig. 22(c).

![Figure 22](image22.png)

Figure 23 Electrical and optical characteristics of the 300×300 µm$^2$ devices.

While most large devices suffer from high shunt leakage because of high density of dislocations, the devices with 300×300 µm$^2$ showed an emission power near 2.5 mW at an
injection current of 100 mA as shown in Figure 23. The microscope image showed uniform light emission from the whole mesa region, indicating the capability of current spreading in the n-AlGaN top contact layer.

Those results were the first reported demonstration of tunnel-injected UV LEDs employing an AlGaN tunnel junction structure.[66]

4.1.2. 2nd generation: optimization of p-AlGaN

Following the successful demonstration of tunnel-injected UV LEDs, we further explored the engineering of the p-AlGaN cladding layers toward more efficient UV LEDs. Here, graded p-AlGaN layers were adopted to take advantage of the polarization charge. We show that capacitance-voltage measurements can provide information about background compensation and doping in p-AlGaN layers.[84] By increasing the p-type doping concentration to overcome the background compensation, on-wafer external quantum efficiency and wall-plug efficiency of 3.37% and 1.62% were further achieved for tunnel-injected UV LEDs emitting at 325 nm. Moreover, we show that interband tunneling hole injection can be used to realize UV LEDs without any acceptor doping.

Epitaxial stack

The epitaxial stack of the tunnel injected UV LED structure investigated here is shown in Fig. 24(a). The structure is similar to the 1st generation of devices, with the major difference being the p-AlGaN layer, which was changed from a constant Al composition to a graded composition. A compositional grading from 75% to 30% in the p-AlGaN layer was adopted to take advantage of the 3D polarization charge. The equilibrium fixed and depletion
charge profile and band diagrams of the tunneling injected UV LED structures with varying effective dopant density \( N_A^* = N_A - N_{\text{imp}} \) in the p-AlGaN layer are shown in Fig. 24(b). Due to the strong polarization effect, band alignment of the tunnel junction can be achieved by inserting a thin InGaN layer. However, the tunneling probability can be greatly reduced by the depletion barrier in the p-AlGaN layer due to the difficulty in achieving degenerate p-type doping, and the large valence band offset between InGaN and AlGaN as shown in the energy band diagram in Fig. 24(b). Increasing the Mg concentration is therefore important to achieve high ionized acceptor (or negative) charge density, and low depletion barrier in the p-AlGaN layer.

Figure 24 (a) Epitaxial stack of the tunneling injected UV LED structure. (b) Equilibrium fixed and depletion charge profile (mobile charges are not shown) and band diagrams of
the tunneling injected UV LED structures with varying effective dopant density \( N_A^* = N_A - N_{imp} \) in the p-AlGaN layer.

As discussed in Chapter 2, linear grading of Al mole fraction from 75% to 30% in 20 nm p-AlGaN results in \( \sim 1.5 \times 10^{19} \) cm\(^{-3}\) 3D polarization charge, as determined by the gradient of the polarization \( \rho = -\nabla \cdot P \). The 3D polarization charge in p-AlGaN allows the formation of a p-n diode even without Mg doping. On the other hand, field ionization due to polarization grading in p-AlGaN further assists the activation of Mg dopants, leading to near degenerate p-type doping, which is beneficial for enhanced tunneling probability across the tunnel junction.

One challenge to achieving conductive p-type AlGaN lies in the severe compensation of the acceptors due to crystal imperfections including native defects such as N vacancies, and the incorporation of donor-type impurities (O/ C).[86] This degrades both the tunnel junction and UV LED active region performance. The band diagrams with different net dopant concentrations \( N_A^* = N_A - N_{imp} \) are compared in Fig. 24(b). Near degenerate p-type AlGaN can be achieved with \( N_A^* \) above \( 5 \times 10^{18} \) cm\(^{-3}\) due to the effect of 3D polarization charge. Even at zero net impurity doping \( N_A^* = 0 \), the negative polarization charges at the InGaN/p-AlGaN interface and in the graded p-AlGaN layer lead to the valence band being close to the Fermi level with relatively low depletion barrier for tunneling in the p-AlGaN layer.

If the p-AlGaN layer has an effective n-type doping \( N_A^* < 0 \), the AlGaN can still function as a hole injection layer for low effective donor concentrations, as shown in the case when \( N_A - N_{imp} = -5 \times 10^{18} \) cm\(^{-3}\). However, for higher effective donor concentrations (such as
\(N_A - N_{imp} = -1 \times 10^{19} \text{ cm}^{-3}\), the entire p-AlGaN layer is depleted. In both these cases, higher voltage would be needed for tunneling.

**Epitaxy and device fabrication**

To study the influence of the donor-type compensating impurities, four tunnel-injected UV LED structures, as shown in Fig. 22(a), with different p-AlGaN layers were grown under similar growth conditions as described earlier. Three samples with 20 nm p-AlGaN were doped with different Mg doping levels, which are 0 (A), \(7 \times 10^{18}\) (B) and \(3 \times 10^{19}\) (C) \text{ cm}^{-3}, respectively. Another sample (D) with 50 nm p-AlGaN and \(3 \times 10^{19}\) \text{ cm}^{-3} Mg doping density was grown to study the influence of the graded p-AlGaN layer thickness on the device performance. The Mg doping densities were achieved by increasing the incoming Mg flux during growth as discussed in Chapter 3.

The samples were fabricated into UV LED devices with partial top contact coverages. The Al-based top contact covers 25%, 37% and 52% of the mesa areas for 50 \(\times\) 50, 30 \(\times\) 30, and 20 \(\times\) 20 \(\mu\text{m}^2\) devices, respectively. Both bottom and top contact resistances are below \(5 \times 10^{-6}\) \(\Omega\) cm\(^2\) for the samples based on TLM measurements. On-wafer electroluminescence and power measurements were carried out at room temperature under continuous wave operation. The light was collected from the top surface of the devices using a calibrated Ocean Optics USB 2000+ spectrometer.

**Electrical characterization: Capacitance-voltage measurement**

Capacitance-voltage (CV) measurements were carried out by reverse biasing the top contact, with excitation frequency of 1 MHz and amplitude of 30 mV. The measured CV curves of full metal covered devices are plotted in Fig. 25(a). Sample A ([Mg] = 0) and B
([Mg] = 7×10^{18} \text{ cm}^{-3}) show nearly constant capacitances with increasing reverse bias especially at low voltage range (< 2.5 V). In comparison, when the p-AlGaN layer is heavily doped to 3×10^{19} \text{ cm}^{-3} (C and D), the capacitance drops greatly with increasing reverse bias.

Figure 25 (a) Measured CV curves and (b) extracted effective depletion charges (\(N_{\text{eff}}\)) of the tunneling injected UV LED devices. Sample A and B show near constant capacitance and depletion width indicating modulation of high density charges. Sample C and D show larger increase in the depletion width with reverse bias.

The measured capacitance (\(C_{\text{total}}\)) can be modeled as two series capacitances due to the tunnel junction (\(C_{\text{TJ}}\)) and the p-QWs-n junction (\(C_{\text{PN}}\)) as shown in Fig. 24(b). Because of the strong polarization field in the InGaN layer, the tunnel junction capacitance is much larger than the p-n junction capacitance and is expected to remain nearly constant with
applied bias. Therefore, the overall capacitance $C_{\text{total}} = C_{TJ} C_{PN} / (C_{TJ} + C_{PN})$ can be approximated as $C_{\text{total}} \sim C_{PN}$. The p-n junction capacitance ($C_{PN}$) is determined by the effective doping densities ($N_A^*$ in p-AlGaN and $N_D$ in n-AlGaN) and the reverse bias ($V_{rev}$) across the junction, as expressed by \( \frac{1}{C_{PN}^2} = \frac{2}{q\varepsilon} \frac{N_A^* N_D}{N_A^* + N_D} (V_{bi} - V_{rev}) \), where $V_{bi}$ is the built-in voltage, $\varepsilon$ is the dielectric constant and $q$ is unit charge. Based on the above equation, effective doping density $N_{\text{eff}} = \frac{N_A^* N_D}{N_A^* + N_D}$ can be extracted.

As shown in Fig. 25(b), sample A and B show nearly constant capacitance and depletion width, indicating modulation of high density charges. This corresponds to full depletion of the graded p-AlGaN layers, with 2D electron gases originated at the AlN/ Al$_{0.3}$Ga$_{0.7}$N or Al$_{0.3}$Ga$_{0.7}$N/ Al$_{0.2}$Ga$_{0.8}$N heterointerfaces in the active region. As determined from the calculated equilibrium band diagrams (Fig. 24(b)), a net donor-type compensating charge density ($N_{\text{imp}} - N_A$) of $5 \times 10^{18}$ cm$^{-3}$ is required to deplete the graded p-AlGaN layer by compensating the negative polarization charge. In Sample B, where the p-AlGaN layer was doped to $[\text{Mg}] = 7 \times 10^{18}$ cm$^{-3}$, the donor-type compensating impurity density can be estimated to be at least $N_{\text{imp}} = 1.2 \times 10^{19}$ cm$^{-3}$. This is similar to previously reported compensating impurity density in p-type GaN layer grown by ammonia MBE.[87] SIMS measurement of the MBE-grown AlGaN films with either p-type or n-type doping under similar conditions showed that both the oxygen and carbon concentrations were $\sim 3 \times 10^{17}$ cm$^{-3}$ as shown in Chapter 3, indicating their minimal contribution to the compensation effect. Therefore, the high compensation impurity density could come from dislocation related traps, or native defects such as vacancies.[88,89] Optimizing the AlGaN material
quality is expected to greatly lower the defect density in both the active region and the p-AlGaN layers.

Since Sample A does not have any Mg doping, it is also depleted, and shows similar (constant) C-V profiles. The small difference in the absolute value of capacitance and depletion width may be due to variations in the growth. The compensating charge was overcome by heavy doping in sample C and D with $[\text{Mg}] = 3 \times 10^{19} \text{ cm}^{-3}$, leading to a net acceptor doping density ($N_A^*$) of $1.8 \times 10^{19} \text{ cm}^{-3}$. Therefore, the extracted effective doping density can be approximated as $N_{\text{eff}} = N_D$ due to much higher net acceptor density in the p-AlGaN layer than the donor density in n-AlGaN ($N_A^* \gg N_D$). Figure 25(b) shows that the effective doping concentrations in both heavily doped samples (C and D) drop with increasing depletion width and stabilize at $\sim 3 \times 10^{18} \text{ cm}^{-3}$, which matches the doping density in the quantum barriers and the n-Al$_{0.3}$Ga$_{0.7}$N cladding layer. This indicates depletion in the n-AlGaN layer due to achieved effective doping in p-AlGaN.

**Electrical characterization: Current-Voltage characteristics**

Current-voltage characteristics of the samples are shown in Figure 26. The tunnel-injected UV LED devices showed similar reverse leakage current, but the turn-on voltage varied with different p-AlGaN layers. For the samples (A, B and C) with 20 nm graded p-AlGaN, the voltages at 20 A/cm$^2$ were 5.98 V (A), 6.22 V (B) and 5.75 V (C), respectively. The lowest voltage was obtained for sample C due to reduced depletion barrier for tunneling resulting from heavy p-type doping. By contrast, because of the absence of acceptors in sample A, the wide depletion barrier in p-AlGaN prevents effective interband tunneling at low bias, leading to severe electron overflow and soft turn-on of the devices. The samples
showed a reduction in the overall resistance with increasing Mg doping level as shown in Figure 26(b). This is attributed to contributions from both reduced p-AlGaN series resistance and tunneling resistance due to increased doping levels.

Figure 26 (a) I-V characteristics and (b) differential resistances of the tunnel-injected UV LED samples.

When p-AlGaN thickness was increased to 50 nm (sample D), the voltage at 20 A/cm² increased to 6.56 V. The differential resistance was higher than that for sample C as well. The underlying reason is attributed to the lower 3D polarization charge density ($\rho_{3D} = 0.6 \times 10^{19}$ cm$^{-3}$) due to thicker grading, and correspondingly lower polarization field for field-assisted acceptor ionization. This results in wider tunneling barrier as confirmed from CV measurement, and further leads to higher tunneling resistances and higher voltage to turn on the tunnel junction.
Optical characteristics

On-wafer electroluminescence (EL) and optical power measurements were carried out at room temperature. As shown in Fig. 27, all samples showed single peak emission at approximately 325 nm. This demonstrates effective interband tunneling hole injection through AlGaN/InGaN tunnel junction. Sample A and B showed highly non-uniform emission from the devices, which is attributed to conduction through low tunneling barrier paths associated with AlGaN and InGaN compositional fluctuations. In comparison, the heavily doped samples C and D showed uniform emission over the entire device region.

Figure 27 EL spectrums and corresponding microscope images of the tunnel-injected UV LED devices.
Figure 28 (a) Output power, (b) EQE and (c) WPE of the tunnel-injected UV LED devices.

The schematic band diagrams under device operation for the samples with different p-AlGaN grading thicknesses are shown in the inset of (a). Thicker grading of the p-AlGaN layer could lead to lower tunneling leakage through the thin electron blocking layer.

The output power showed abrupt increase with increasing Mg doping level from less than 1 µW in the acceptor-free LED (A) to above 1 mW in the heavily doped samples (C and D). Both the external quantum efficiency (EQE) and wall-plug efficiency values were two orders of magnitude higher in the higher doped samples (C and D) than in the low and undoped samples (A and B). The maximum measured power was 1.38 mW at 12 mA, corresponding to 55 W/cm² at 480 A/cm². The highest external quantum efficiency of 3.37% was obtained from sample D, while sample C has the highest peak wall-plug efficiency of 1.62%. The efficiency curves did not show saturation and droop for the samples with thin p-AlGaN layers (A, B, C), while the sample (D) with thicker p-AlGaN layer showed saturation near 200 A/cm². We attribute this to better electron confinement and lower tunneling leakage through the thin electron blocking layer by using thicker p-AlGaN grading as depicted in the inset of Figure 28(a).
To summarize, the design of the p-AlGaN cladding layer towards efficient tunneling injected UV LEDs is discussed in this section. The achieved EQE and WPE of 3.37% and 1.62% are among the highest reported values for this wavelength range. It is shown that the tunnel-injected UV LED structure enables the analysis of background impurities using CV measurements. It was found that increasing the Mg doping concentration together with the use of polarization doping is beneficial for improving UV LED efficiencies.

4.1.3. Light extraction efficiency enhancement

One important factor limiting UV LED performance is the low light extraction efficiency caused by light absorption in the p-type contact region and internal light reflection at the interfaces.[90] Conventional UV LEDs use either p-GaN or p-Al\textsubscript{1-x}Ga\textsubscript{x}N/ Al\textsubscript{y}Ga\textsubscript{1-y}N superlattice layer for top contact, which induces light absorption loss or increases operating voltage.[80] As a solution, light is most efficiently extracted from the substrate side of the devices using flip chip bonding. To reduce internal reflection, micro-structure patterning has to be done on the back side of the devices, and device encapsulation and packaging is necessary. Despite these techniques, the achieved light extraction efficiency is only 25%[27], which is much lower than the visible LEDs (> 80%). The difference is largely attributed to the fact that the thick p- GaN contact layer absorbs UV light, but is transparent to visible light. In comparison, the tunnel-injected UV LED structure avoids the absorbing p-type contact layers, making it possible to improve the light extraction efficiency close to that can be achieved for visible LEDs. In this section, attempts on improving the light extraction efficiency through top surface roughening will be discussed.[83]
The tunnel-injected UV LEDs adopted in this study are from the 1st generation of the devices, while the only difference is a thicker (~ 300 nm) top contact layer. The epitaxial stack is shown in Figure 29(a).

![Figure 29 Schematic device processing flow.](image)

(a) Growth stack of the tunnel junction UV LED structure. (b) Deposition of 300 nm SiO\(_2\) and 10 nm Ni. (c) Annealing to form Ni nano-clusters. (d) ICP-RIE etch of SiO\(_2\) and n-AlGaN top layer to form nano-columns, and Ni removal using Nitric acid. (e) Define mesa region and wet etch of SiO\(_2\). (PR represents photoresist) (f) Device finalization.
Top surface roughening was carried out using self-assembled Ni nano-clusters as etching mask.[91-94] The device process flow is schematically shown in Figure 29. First, 300 nm SiO$_2$ was deposited on the as-grown sample using plasma-enhanced chemical vapor deposition (PECVD), followed by 10 nm Ni on SiO$_2$ using e-beam evaporator. The sample was annealed at 860 °C for 90 s under N$_2$ ambient to form nano-sized Ni clusters.[91-94] The self-assembled Ni nano-clusters were used as nanoscale etch masks for ICP-RIE etching of both SiO$_2$ and Al$_{0.3}$Ga$_{0.7}$N. CF$_4$ and BCl$_3$/ Cl$_2$ based etch chemistries were used to dry etch SiO$_2$ and Al$_{0.3}$Ga$_{0.7}$N, respectively. The etch depth was controlled to remove 300 nm SiO$_2$ and 150 nm Al$_{0.3}$Ga$_{0.7}$N, retaining 150 nm of the n-Al$_{0.3}$Ga$_{0.7}$N top contact layer. The Ni nano-clusters were then etched using dilute nitric acid. The remaining SiO$_2$ nano-columns out of the device mesa were etched using buffered oxide etch (BOE) as shown in Figure 29(e). The device mesas were then isolated using ICP-RIE etch, followed by bottom contact deposition of Ti(20 nm)/ Al(120 nm)/ Ni(30 nm)/ Au(50 nm) and subsequent annealing at 850 °C for 30 sec, and Al(20 nm)/ Ni (20 nm)/ Au(80 nm) top contact deposition. Partial metal coverage (23% electrode coverage for 50 × 50 µm$^2$ devices) for top contacts was used to minimize light absorption in the metal contact. Devices with and without surface roughening were compared on the same sample by avoiding Ni deposition in half of the sample area.

Figure 30 shows the scanning electron microscopy (SEM) images of the sample surface after roughening. The roughening process creates randomly distributed nano-columns composed of 300 nm SiO$_2$ and 150 nm n-Al$_{0.3}$Ga$_{0.7}$N, with the interface seen clearly in the SEM images. The average diameter of the nano-columns is 300 nm, and the distance
between them varies in the range of 50 nm to 100 nm. The controlled anisotropic etch profile resulted in SiO₂ whiskers with tapered sidewalls that increases light extraction. In addition, the higher refractive index of SiO₂ \((n_s \approx 1.5)\) compare to air increases the critical angle of the UV light at the Al₀.₃Ga₀.₇N/ SiO₂ interface.

![Figure 30](image)

Figure 30 Scanning electron microscopy (SEM) image of the roughened top surface after 300 nm SiO₂/ 150 nm Al₀.₃Ga₀.₇N selective etch and Ni removal using Nitric acid.

The electrical characteristics were measured for 50 × 50 µm² devices with partial metal coverage. Pulsed measurements with pulse width and period of 1 ms and 100 ms were performed to reduce self-heating effects. The smooth and roughened devices show similar electrical behavior, with a voltage drop of 5.15 V at 20 A/cm² (Figure 31). Top surface roughening on the p-GaN layer for standard visible LEDs has been reported, however, increases in both the turn-on voltage and on-resistance have been observed, which have been attributed to the surface depletion of the p-GaN layer due to plasma induced surface
This effect is minimized in the case of tunnel-injected UV LEDs since the surface roughening was applied on the n-AlGaN layer, which is less sensitive to the plasma damage.

Figure 31 Electrical characteristics for smooth and roughened tunnel junction UV LED devices (50 × 50 µm²) under both CW and pulse (pulse width and period of 1 ms and 100 ms) measurements.

Figure 32 Optical characteristics for smooth and roughened tunnel junction UV LED devices (50 × 50 µm²) under CW and pulse modes.
On-wafer optical power measurements of the devices with/without surface roughening were carried out at room temperature to compare the change in light extraction efficiency. As shown in Figure 32, single peak emission from the active region with peak wavelength at 326 nm was achieved. Both devices showed uniform light emission (inset of Figure 32). At the same injection current of 5 mA, the rough region gives a higher emission peak due to increased light scattering at the surface. The inset to Fig. 32(a) shows the EL peak in log scale in a broad wavelength range. There is a weak peak at 510 nm for both devices, which could come from the thin InGaN layer or from a defect level in the p-AlGaN layer. The device with surface roughening reaches 1.39 mW at 20 mA under pulse mode, corresponds to a power density of 55.6 W/cm² at 800 A/cm².

As shown in Figure 32(b) and (c), the external quantum efficiency (EQE) and wall-plug efficiency (WPE) curves indicate a light extraction enhancement of ~43%. The peak EQE and WPE of the roughened device are 2.21% and 1.36% under CW operation, while the values are 1.55% and 1.00% for the smooth device.

While many approaches have been used to increase the light extraction efficiency of UV LEDs, all those methods are based on back-side processing and flip-chip bonding.[80,96,97] The absorbing p-type contact layer is an important reason that the light extraction efficiency of UV LEDs remains much lower than visible LEDs. The tunneling injected UV LED structure mitigates the absorption loss issues in UV LEDs, since the InGaN interband tunneling layer used (<4 nm) is significantly thinner than typical p-GaN capping layers (>20 nm). Previous work on light extraction in conventional UV LEDs showed that for a p-GaN contact layer thickness of 4 nm, light extraction efficiency as high
as 60% can be achieved for transverse-electric (TE) polarized light.[90] We may expect similar light extraction efficiency in tunnel-injected UV LEDs when a thin InGaN layer (≤ 4 nm) is used by assuming similar absorption coefficients of low In content InGaN and GaN for the emitted UV light. Therefore, the tunnel-injected UV LEDs are expected to enable much higher efficiency through further optimization. This makes it possible to achieve UV light extraction efficiency comparable to the visible counterparts, and reduces the complexity and cost of device fabrication. Engineering the active region design could lead to preferential surface emission instead of side-emission for deep UV LEDs emitting longer wavelengths than 240 nm.[98] In this sense, the enhanced top surface emission enabled by tunnel junction UV LED structure could be efficiently applied to UV LEDs emitting at a wide UV range.

4.2. UV-B LEDs

Following the successful demonstration of tunneling hole injection for UV-A LEDs, the feasibility of achieving low resistance AlGaN tunnel junctions for UV-B LEDs was further investigated.[99-101] Because of larger AlGaN bandgap energy, achieving efficient interband tunneling became more difficult. Specifically, the doping difficulties, especially the challenges in p-type doping, could result in extended depletion barriers for interband tunneling. Therefore, the optimization of the p-AlGaN layer and the tunnel junction layer was treated as major points of focus for the realization of tunnel-injected UV-B LEDs. In this section, three generations of device designs will be discussed.
4.2.1. 1\textsuperscript{st} generation: graded p-AlGaN

In the first attempt for UV-B LEDs, the optimized UV-A LED structure with graded p-AlGaN layer was adopted. The active region consists of 3 periods of Al\textsubscript{0.55}Ga\textsubscript{0.45}N/Al\textsubscript{0.7}Ga\textsubscript{0.3}N quantum wells/barriers. The electron blocking layer is 8 nm AlN, and the p-AlGaN layer has an Al compositional grading from 92\% to 70\% to create a 3D polarization charge. However, the devices showed soft turn-on and high leakage current as shown in Figure 33. Correspondingly, the devices showed very dim light emission at ~285 nm.

Figure 33 Epitaxial stack, I-V characteristics and the energy band diagram under operation for the 1\textsuperscript{st} generation of UV-B LEDs.

The poor device performance was investigated based on the analysis of carrier transport. The energy band diagram of the tunnel-injected UV-B LED structure under forward bias is shown in Figure 33. In the ideal case of device operation, the tunneling hole injection process happens with very minimal voltage drop across the tunnel junction layer, and the electron blocking layer ensures negligible amount of electron overflow. As a result, balanced amount of electrons and holes are injected into the quantum well active region.
However, high reverse bias could be necessary to reach the onset of interband tunneling for ultra-wide bandgap AlGaN tunnel junctions. This leads to excess electron accumulation in the active region and higher possibility of electron overflow. For UV-A LEDs, the AlN electron blocking layer on top of the Al$_{0.3}$Ga$_{0.7}$N quantum barrier provides high barrier for the overflowing electrons, and therefore lead to high device efficiency. However, for UV-B LEDs, the barrier height is significantly reduced by the lower conduction band offset between AlN and the Al$_{0.7}$Ga$_{0.3}$N quantum barrier. This, in combination with the poorer tunnel junction performance, leads to severe electron overflow. The overflowed electrons either recombine in the p-AlGaN layer, or get accelerated by the electric field in the p-AlGaN layer and further injected into the n-AlGaN top contact layer and contribute to leakage current. Therefore, two design considerations are critical for the tunnel-injected UV LEDs:

a) Efficient interband tunnel junctions are necessary. This includes low on-resistance and low voltage drop to start the tunneling process.

b) Effective electron blocking layer is critical to avoid electron overflow before the onset of interband tunneling hole injection.

Following those design considerations, the first attempt was carried out using a graded p-AlGaN superlattice (SL) structure as depicted in the band diagram as shown in Figure 34. Here, the polarization grading and short period superlattice approaches are combined to achieve both enhanced acceptor activation rate and reduced electron overflow. The superlattice structure enhances the Mg doping efficiency through a periodic oscillation of the valence band edge.\textsuperscript{[102,103]} Therefore, the depletion barrier in the p-AlGaN layer can
be reduced, making it easier for interband tunneling. At the same time, the graded SL structure provides polarization barriers for the overflowing electrons and could potentially contribute to a reduction of electron overshoot.[15,104]

Figure 34 Energy band diagram of the tunnel-injected UV LED structure employing a graded p-AlGaN superlattice structure.

The effect of the graded p-AlGaN superlattice in the tunnel-injected UV LEDs was studied experimentally. The tunneling injected UV LEDs were grown by plasma assisted molecular beam epitaxy on metal polar Al₀.₇Ga₀.₃N templates with threading dislocation density of 2.5×10⁹ cm⁻². The UV LEDs contain three periods of 3 nm Al₀.₅₈Ga₀.₄₂N quantum wells/ 8 nm Al₀.₇Ga₀.₃N quantum barriers, 50 nm graded p-AlGaN layer, thin tunnel junction layer with 4 nm In₀.₂Ga₀.₈N, and 150 nm n-Al₀.₇Ga₀.₃N top contact layer. Four samples were grown under similar growth conditions, but with different p-AlGaN structure. Sample A has continuous grading from 92% to 64% Al mole fraction in p-
AlGaN, while Sample B, C and D have graded Al$_x$Ga$_{1-x}$N/Al$_y$Ga$_{1-y}$N superlattice structures, with $x$ grading from 92% to 64% and $y$ grading from 100% to 75%. The widths of the SL barrier/well are 0.5/0.5 nm, 1.8/1.8 nm and 3.0 nm/3.0 nm for Sample B, C and D, respectively. 30 × 30 um$^2$ devices with ~25% top metal coverage were used for electrical and optical measurements.

Figure 35 Epitaxial stack of the UV LEDs with graded p-AlGaN SL structures.

The electrical characteristics are shown in Figure 36. Sample A showed soft turn-on with a voltage drop of 3.96 V at 20 A/cm$^2$, while the current increases sharply at high current density, indicating severe electron overflow. In comparison, when short period superlattices are adopted, the electron overflow at high current is greatly reduced. Sample B and C showed similar electrical characteristics at high current levels, however, an increase of the voltage drop at 20 A/cm$^2$ from 4.58 V (B) to 6.87 V (C) was observed when the SL barrier/well thicknesses are increased, which is attributed to better electron blocking and higher acceptor activation rate by using thicker barrier/well SL. Further
increasing the SL thicknesses to 3.0 nm in sample D resulted in a soft turn-on but higher on-resistance. This is attributed to poor vertical transport in the p-AlGaN layer as blocked by the valence band fluctuations.

Figure 36 Electrical characteristics of the UV LED samples with different SL thicknesses in the p-AlGaN layer.

On-wafer electroluminescence measurements confirmed non-equilibrium hole injection into the active regions for all the samples. The samples showed similar emission peak wavelength at 282 nm. However, Sample A showed minimal emission power, further confirming severe electron overflow. The efficiency curves for Sample C peaked at approximately 250 A/cm², while Sample B showed much lower efficiencies at low current injection, and did not show droop till high current levels (1 kA/cm²). The higher efficiency in sample C (1.8/1.8 nm SL) is attributed to lower electron overflow to top n-type contact compared to sample B (0.5/0.5 nm SL). When the SL thickness is further increased to 3.0 nm in sample D, the device showed low efficiency at low current levels, but highest efficiency near 1.2 kA/cm². This confirms that even though thick SL periods can introduce...
higher hole density, the strong valence band fluctuation can detriment hole transport and lead to high on-resistance.

Figure 37 EL spectrum, output power and EQE of the samples with different p-AlGaN layers.

This demonstration shows that effective interband tunnel junction could be achieved for UV-B LEDs, and graded p-AlGaN superlattice structure could be favorable for reducing electron overflow in tunnel-injected UV LEDs. However, further optimizations in the structural design and material quality are necessary to further improve the device efficiency.

4.2.2. 2nd generation: graded tunnel junctions

As discussed in the last section, achieving efficient interband tunnel junctions is critical for the realization of high efficiency UV LEDs. In this generation of UV LEDs, a graded tunnel
junction structure is utilized to reduce the tunneling barrier and improve the device performance.[99]

Figure 38 Epitaxial stack, TEM image and equilibrium energy band diagram of the 2nd generation of tunnel-injected UV-B LEDs.

A graded tunnel junction was integrated on a UV LED structure as shown in Figure 38. The device structure consisted of a 600 nm Al$_{0.55}$Ga$_{0.45}$N bottom contact layer with Si doping density of $1.2 \times 10^{19}$ cm$^{-3}$, three periods of 2 nm Al$_{0.4}$Ga$_{0.6}$N/ 6nm Al$_{0.55}$Ga$_{0.45}$N quantum wells (QWs)/ barriers, 8 nm Al$_{0.72}$Ga$_{0.28}$N p-type electron blocking layer, 25 nm p-Al$_{0.55}$Ga$_{0.45}$N, graded tunnel junction layer, and 300 nm n-type top contact layer. The graded tunnel junction structure consisted of 4 nm In$_{0.2}$Ga$_{0.8}$N, and AlGaN grading from 45% (55%) to 55% (45%) Al mole fraction on the n- (p-) side. Since the compositional grading was achieved by varying Al cell temperature, the grading thickness was estimated to be approximately 10 nm, which could provide $\sim 5 \times 10^{18}$ cm$^{-3}$ polarization charge. Apart from the polarization grading, high doping concentrations of [Mg]= $5 \times 10^{19}$ cm$^{-3}$ and [Si]= $1 \times 10^{20}$ cm$^{-3}$ were adopted in the p- and n-AlGaN sides, respectively. Self-consistent energy
band calculations show that the p-AlGaN side of the tunnel junction structure is degenerate benefiting from the polarization field ionization of the acceptors.

Light emitting diodes for on-wafer measurements were fabricated on the epitaxial structure described above. Partial metal coverage (~ 25% electrode coverage for 30 × 30 µm² devices) for top contacts was used to minimize light absorption since light was collected from the top surface. On-wafer electroluminescence (EL) and power measurements were carried out at room temperature under continuous wave mode.

![Current-voltage characteristic for the 30 × 30 µm² device](image)

**Figure 39** Electrical characteristics of the tunnel-injected UV LED devices (30 × 30 µm²).

The measured current-voltage characteristic for the 30 × 30 µm² device is shown in Figure 39. The device showed a current density of 10 A/cm² at 6.8 V. The additional voltage drop (2.4 V) over the quantum well band gap (Al0.4Ga0.6N – 4.4 eV) is attributed to voltage drop across the electron blocking layer and the graded tunnel junction layer. The device reached 1 kA/cm² at 11.2 V, with a differential resistance of 1.5×10⁻³ Ω cm². The top contact resistance was extracted to be 5.6 ×10⁻⁴ Ω cm² based on transfer length method.
measurements. The bottom contact resistance and spreading resistances are neglected. By subtracting the contact resistance from the total series resistance, it gives an upper bound of the tunnel junction resistance of $9.4 \times 10^{-4} \Omega \text{ cm}^2$ at 1 kA/cm$^2$.

Figure 40 (a) Electroluminescence of the tunneling injected UV LED structure with dc current injection from 0.3 mA to 6 mA at room temperature, showing single peak emission at 292 nm. (b) EQE and WPE of the $30 \times 30 \mu \text{m}^2$ device. The inset to (a) shows the output power, and the inset to (b) is an optical micrograph image of a device ($30 \times 30 \mu \text{m}^2$) operated at 5 mA.

Tunneling hole injection was confirmed by light emission from the devices. As shown in Figure 40(a), single peak emission at 292 nm was achieved across the entire device area, with emission power of 0.1 mW at 6 mA injection current for the $30 \times 30 \mu \text{m}^2$ device (Fig. 40(a) inset). The maximum external quantum efficiency and wall-plug efficiency values were 0.41% and 0.16%, respectively. The output power and device efficiency are both higher than the achieved values in the 1st generation of devices. This is attributed to higher interband tunneling probabilities achieved using the graded tunnel junction structure.
However, the external quantum efficiency and wall-plug efficiency did not show droop until high current density, suggesting high non-radiative recombination in the active region. This is consistent with the measured TEM image, which shows high density of dislocations formed during MBE growth initialization. Further optimizations of growth initialization and the material quality are important to increase the internal quantum efficiency of the devices.

4.2.3. 3rd generation: AlN electron blocking layer

Following the successful demonstration of AlGaN tunnel junctions for UV-B LEDs, further attempts on achieving better electron blocking were developed.[101] As discussed at the beginning of this section, a balance of the tunneling hole injection and electron blocking is critical in improving the device efficiency. However, based on the results from the 2nd generation of devices, extra-voltage drop was inevitable for the current tunnel junction design, which could originate from background compensation from the unintentional impurities or Ga/N vacancies and the high depletion barriers. This necessitates a corresponding improvement in the electron blocking layer to reduce electron overshoot. In the 3rd generation of devices, better electron blocking was attempted through the use of a thick AlN layer and will be discussed in this section.
Figure 41 (a) Epitaxial stack, (b) HAADF-STEM image, and (c) equilibrium energy band diagram of the tunnel-injected UV LED grown using MBE.

The tunnel-injected UV LED structure investigated here is shown in Figure 41. The structure was grown by N$_2$ plasma assisted MBE on metal-polar Al$_{0.7}$Ga$_{0.3}$N template. The threading dislocation density in the substrate was estimated as $3 \times 10^9$ cm$^{-2}$. As shown in Figure 41, the Al composition in the cladding layer is 65%, and the QW active region has an asymmetric quantum barrier design to account for the drift mobility difference between electrons and holes, with three periods of 2 nm Al$_{0.5}$Ga$_{0.5}$N QWs separated by 6 nm Al$_{0.65}$Ga$_{0.35}$N barriers while a 3 nm Al$_{0.65}$Ga$_{0.35}$N barrier was adopted right below the EBL. Here, 18 nm of p-AlN was grown as an electron blocking layer to reduce electron overshoot. This was followed by a thin p-Al$_{0.65}$Ga$_{0.35}$N layer of 35 nm, the tunnel junction layer, 200 nm n$^{++}$-Al$_{0.65}$Ga$_{0.35}$N and 40 nm reverse graded n$^{++}$-AlGaN top contact layer.
with Al mole fraction grading from 65% to 15%. The tunnel junction layer consists of $p^+$-AlGaN with $[\text{Mg}]=5\times 10^{19} \text{ cm}^{-3}$, 4 nm In$_{0.2}$Ga$_{0.8}$N and 5 nm $n^+$-AlGaN ($[\text{Si}]=1\times 10^{20} \text{ cm}^{-3}$) with Al composition grading from 58% to 65%. The simulated energy band diagram confirms a sharp band alignment obtained through such a tunnel junction design. Meanwhile, the reverse-graded top contact layer provides a flat conduction band for electron transport and enables the formation of low resistance Ohmic contact without the necessity of metal annealing. The benefit of such a graded-contact structure will be discussed later. The TEM image of the tunnel-injected UV LED structure showed abrupt heterointerfaces for the QWs, EBL and the tunnel junction layer. No sign of lattice relaxation was observed for the AlGaN/InGaN tunnel junction layer from the STEM images.

Device mesa was defined by etching to the bottom contact layer using inductively coupled plasma reactive ion etching (ICP-RIE). V(20 nm)/Al(80 nm)/Ti(40 nm)/Au(100 nm) metal stack was evaporated and annealed at 860 °C for 4 min to form bottom contact. The top contact was formed using Al(30nm)/Ni(30 nm)/Au(200 nm)/Ni(20 nm) non-alloyed metal stack. The top contact metal covered 37% of the $30 \times 30 \mu\text{m}^2$ device mesa area. To minimize internal light absorption, a low power ICP-RIE etch was then used to remove the reverse graded top contact layer in the area without top metal contact as shown in the inset to Figure 41(c). Then, electrical and optical characterizations were carried out for the on-wafer devices.

The bottom contacts and top contacts were characterized using circular transfer length measurement (CTLM) and TLM measurements, respectively. The contact resistances are
extracted to be $1.2 \times 10^{-5} \ \Omega \text{ cm}^2$ for the bottom contacts, and $2.2 \times 10^{-6} \ \Omega \text{ cm}^2$ for the top contacts. The sheet resistances are extracted to be 411 and 216 $\Omega/\square$ for the bottom and top $\text{Al}_{0.65}\text{Ga}_{0.35}\text{N}$ contact layers, respectively. This ensures sufficient current spreading in the contact layers.

Figure 42 Electrical characteristics of the tunnel-injected UV LEDs.

The low contact resistances enable the analysis of the tunnel-junction resistances. The current-voltage (IV) characteristics of the $30 \times 30 \ \mu\text{m}^2$ tunnel-injected UV LED device are shown in Figure 42. For ideal tunnel junctions, efficient interband tunneling should happen at low reverse bias. However, the tunnel-injected UV LED device showed a high voltage drop of 10.5 V at 20 A/cm$^2$. This is 5.9 V higher than the ideal turn-on voltage determined from the quantum well bandgap ($E_g = 4.6$ V). The excess voltage drop could have major contribution from the tunnel junction layer because of low tunnel probability at low bias. As discussed in the earlier sections, background compensation in the p-$\text{AlGaN}$ layer could lead to extended depletion barrier, and therefore contribute to the increased voltage drop across the tunnel junction layer for efficient tunneling. However, the difference in this UV
LED structure compare to the 2nd generation of devices is the use of a thick AlN layer as the electron blocking layer. This provides high barrier to prevent electron overflow under excess forward voltages. Therefore, improving the tunnel junction design to reduce the voltage required for the onset of effective interband tunneling is critical.

The device reached a high current level of 1 kA/cm² at 15.6 V with a low differential resistance of $1.9 \times 10^{-3} \, \Omega \, \text{cm}^2$. This can be estimated as the tunnel junction resistance by neglecting the contributions from the spreading resistances, contact resistances and the p-n junction series resistances. This indicates that even though high reverse bias was still necessary to turn-on the interband tunneling, low differential resistances can be obtained under further reverse bias across the tunnel junctions.

Capacitance-voltage measurements were further carried out to monitor the doping information. As discussed earlier, when the device is reverse biased, the voltage drop across the tunnel junction region is minimal because of the small depletion width and thereby the high capacitance. Therefore, the capacitance profile describes the p-QW-n junction. The depletion width at zero bias was extracted to be 53 nm, which matches well with the simulated energy band diagram as shown in Figure 43. The extracted charge profile showed a constant concentration of $1.2 \times 10^{18} \, \text{cm}^3$. This is close to the doping concentration in the n-AlGaN cladding layer. The increase of the charge density at higher reverse bias is attributed to the higher doping concentration below the n-AlGaN cladding layer. This serves as a useful tool for the probe of the charge profile near the active region.
Figure 43 Capacitance-voltage measurements and the extracted charge profile of the tunnel-injected UV-B LEDs.

The electroluminescence of the on-wafer devices were further characterized. The light was collected from the top surface of the tunnel-injected UV LED device (30 × 30 μm²). Efficient light emission at 287 nm with a full width at half maximum of ~ 12 nm was obtained. The inset shows the logarithmic plot of an EL spectrum. No parasitic emission was observed except for a weak emission peak at 510 nm, which was also detected in the tunnel-injected UV-A LEDs emitting at 325 nm. This could come from defect emission, or light emission from the thin InGaN layer due to photoexcitation. The microscope image shows uniform light emission from the whole mesa region even though only 37% of the
mesa region was covered by the top metal contact. While the reverse graded AlGaN contact layer was etched in most of the mesa area and did not contribute to light absorption, inevitable absorption persisted below the top metal contacts. Further optimizations in reducing the metal contact area while maintaining sufficient current spreading is necessary to maximize the light extraction efficiency.

Figure 44 (a) Electroluminescence spectra, (b) output power, (c) EQE and WPE of the tunnel-injected UV LEDs. The microscope image of a 30×30 μm² device under operation is shown in the inset of (a). The results were measured on-wafer under CW operation.

The output power was measured on-wafer under continuous wave (CW) operation. The measured power values are normalized to device mesa area, and are plotted in Fig. 44(b). A high power density of 54.4 W/cm² was obtained at 1 kA/cm². The peak external quantum efficiency of 2.8% and wall-plug efficiency of 1.1% were measured at 30 A/cm². Even though the measured power and efficiency values are underestimated by the on-wafer measurement, the efficiency values are comparable to state-of-the-art device results obtained for conventional UV LEDs.
The improvement of the device performance compare to the first two generations of devices is attributed to better electron blocking using the thick AlN EBL. A noticeable difference in this set of samples is the significantly lower current level for the peak device efficiencies. The current density to achieve peak efficiencies was 1.2 kA/cm² for the first generation of devices, and it was reduced to 440 A/cm² for the second generation of devices, but it was only 30 A/cm² for the third generation of devices. This serves as a clear indication of reduced electron leakage through the optimization of both the electron blocking layer and the tunnel junction layer.

While even better device performance is expected by introducing surface patterning and device packaging for improved light extraction efficiency, the wall-plug efficiency of the devices is still limited by the high turn-on voltage. Therefore, optimization of the tunnel junction layer to reduce the extra voltage drop is critical in achieving high wall-plug efficiency.

4.3. UV-C LEDs

UV-C LEDs have attracted remarkable research efforts because of the wide range of applications, especially in air disinfection and water sterilization. Compare to UV-A and UV-B LEDs, UV-C LEDs necessitate higher Al composition in the AlGaN layers, as a result, there is low lattice mismatch between the LED epitaxial layer and the AlN substrate. This makes it possible to achieve pseudomorphic growth without introducing dislocations or defects due to strain relaxation. The critical layer thickness for pseudomorphic growth on AlN could be above 1.5 µm for AlₐGaₐN, while it reduces to ~ 0.5 µm for AlₐGaₐN.
This enables the growth of high quality active regions, and has resulted in high radiative efficiencies above 60% for a wide range of UV-C spectrum.[105] However, UV-C LEDs suffer from severe challenges in hole injection because of the extremely low acceptor ionization rate. As a result, the device efficiencies are still below 10% at emission wavelength below 270 nm, and exhibit an exponential drop-off with shorter wavelengths. The tunnel-injected UV LED structure featuring non-equilibrium hole injection and low internal absorption is thus of critical importance in improving the device efficiency.

Figure 45 Challenges for the realization of tunnel-injected UV-C LEDs

The tunnel-injected UV-C LEDs face several challenges as depicted in Figure 45. Firstly, the use of high Al composition AlGaN in the material results in difficulties in achieving ohmic contact to both the bottom and top contact layers. Secondly, the high bandgap energy results in poor tunnel junction performance with low tunneling probability. Thirdly, the Fermi level in the p-AlGaN layer sits above the valence band edge because of the high acceptor activation energy, making it difficult to initiate band-to-band tunneling at low reverse bias. While there are more challenges related to the improvement of the material
quality and the radiative efficiency, those three issues are treated as the major aspects to be investigated in this study.

4.3.1. Low resistance top contact

The tunnel-injected UV LED structure enables n-type contacts for both bottom and top contact layers. However, the fabrication of low resistance ohmic contact to high Al composition AlGaN layers has been challenging.[106-108] Even though vanadium or Titanium based metal contacts have been developed for optimized contact resistance, low contact resistance below $1 \times 10^{-4} \, \Omega \, \text{cm}^2$ for high Al content (>75%) AlGaN has not been achieved.[106] The reason behind this is the low electron affinity (< 2.6 eV for Al$_{0.7}$Ga$_{0.3}$N) of ultra-wide bandgap AlGaN material, while the metal work function for n-type contacts is typically ~ 4 eV. As depicted in Figure 46, when making direct metal contact to the n-AlGaN layer, the mismatch in the work function energies between the AlGaN layer and the metal contact results in a high depletion barrier at the interface.[109] The barrier height increases with increasing Al composition in the AlGaN layer. This significantly limits the formation of ohmic contact to the AlGaN layer, as a result, the contact resistance stays above 0.01 $\Omega \, \text{cm}^2$ for direct metal contact to AlGaN with Al composition above 75%.[106] Meanwhile, all of them require high temperature annealing and correspondingly metal spike into the material. This is not feasible for the top contact of UV LEDs since the metal spike could ruin the active region.
Figure 46 Comparison between metal contacts to UWBG AlGaN with and without the reverse graded n^{++}-AlGaN contact layer.

The approach to circumvent the high contact resistance to high composition AlGaN is to adopt a compositionally graded heavily n-type doped AlGaN layer with Al composition grading from the channel composition to \( \sim 0 \) as shown in Figure 46.[109-111] In this way, the electron affinity of the n-AlGaN is increased through the compositional grading, and it minimizes the Schottky barrier between the metal and the top n-AlGaN contact layer. While the reverse compositional grading could result in a negative polarization sheet charge as discussed in Chapter 2, the polarization charge can be compensated through heavy n-type doing. This results in a flat conduction band profile, enabling smooth electron injection through the metal contact and transport in the n-AlGaN layer. Meanwhile, this approach does not require metal annealing for the formation of ohmic contact, making it compatible to UV LEDs. Low contact resistance of \( \sim 1 \times 10^{-6} \ \Omega \text{cm}^2 \) to ultra-wide bandgap Al\(_{0.75}\)Ga\(_{0.25}\)N has been demonstrated using this method.[109] This is four orders of
magnitude lower than that can be achieved using annealed metal contact. In this section, the alloyed contacts directly formed on high composition AlGaN and the non-alloyed contacts formed through the graded AlGaN contact layer are compared.

For the device fabrication of tunnel-injected UV-C LEDs, the bottom contacts are formed using a V(20 nm)/Al(80 nm)/Ti(40 nm)/Au(100 nm) metal stack deposited by e-beam evaporation, and annealed at 860 °C for 3 min under N₂ ambient. The top contact are formed using non-alloyed Al(30 nm)/Ni(30 nm)/Au(150 nm)/Ni(20 nm) metal stack on top of the graded AlGaN contact layer. The non-alloyed top contact and alloyed bottom contact are analyzed by transfer length measurement (TLM) and circular TLM (CTLM) methods, respectively.

The metal contacts to n⁺-Al₀.₆₅Ga₀.₃₅N and n⁺-Al₀.₇₅Ga₀.₂₅N were studied. The TLM measurement results for the contacts on n⁺-Al₀.₆₅Ga₀.₃₅N are shown in Figure 47. The alloyed contacts to n⁺-Al₀.₆₅Ga₀.₃₅N showed near ohmic performance, with slight non-linear behavior at low bias. The resistances are extracted from the linear portion of the CTLM curves, and are plotted with gap spacing after correction. The extracted bottom contact specific resistance is 1.2×10⁻⁵ Ω cm². In comparison, the Al-based non-alloyed top contact showed ohmic behavior, and a lower contact resistance of 2.2×10⁻⁶ Ω cm² to the n⁺⁺-Al₀.₆₅Ga₀.₃₅N top contact layer was extracted. It should be noted that the reversed graded AlGaN contact layer was removed using plasma etching in between the metal contacts as depicted in the inset to Figure 47(c). This is expected to originate from the lowering of the Schottky barrier formed at the metal-AlGaN interface, and the resulted flat conduction band profile in the heavily n-type doped reversed graded top contact layer. In the meantime,
the sheet resistances are extracted to be 411 and 216 Ω/□ for the bottom and top Al$_{0.65}$Ga$_{0.35}$N contact layers, respectively. This enables sufficient current spreading in the contact layers.

Figure 47 Characterizations of the contacts to n$^+$-Al$_{0.65}$Ga$_{0.35}$N. The alloyed bottom contacts are characterized using CTLM ((a) and (b)), and non-alloyed top contacts are characterized using TLM measurement ((c) and (d)). The insets to (a) and (c) shows the schematic structures for the measurements. The resistances in (b) are extracted from the linear portion of the CTLM curves, and are plotted with gap spacing after correction.

Figure 48 Characterizations of the contacts to n$^+$-Al$_{0.75}$Ga$_{0.25}$N. (a) Circular TLM measurement result for annealed bottom contact, and (b) the extracted sheet resistance at different current levels. (c) Top contact TLM measurement result, and (d) the change of extracted resistances with TLM pattern spacing.
The metal contacts to n$^+$-Al$^{0.75}$Ga$^{0.25}$N were further studied. The annealed bottom contact exhibits Schottky performance, which is consistent with recent investigations on metal/AlGaN contacts with high Al content. This is attributed a dramatic increase in the activation energy of the donors at Al compositions above 75%. Nevertheless, the sheet resistance of the bottom contact layer is estimated to be 2.3 to 2.5 kΩ/□ based on the CTLM measurement. The estimated sheet resistance drops with increased current flow as shown in Fig. 48(b). The deviation is attributed to the influence of the Schottky contact resistance on the adopted CTLM model. In comparison, the top contact, formed through non-alloyed contacts on the graded AlGaN contact layer, showed Ohmic behavior with an extracted contact resistance of 4.8×10$^{-5}$ Ω cm$^2$, which represents a combination of the resistance at metal/AlGaN interface and the resistance of the graded contact layer. The sheet resistance extracted for the n$^{++}$ Al$^{0.75}$Ga$^{0.25}$N top current spreading layer is 1.1 kΩ/□. The abrupt contrast between the non-alloyed Ohmic top contact and the alloyed Schottky bottom contact demonstrates the benefit of using a down-graded AlGaN contact layer on high Al content n-AlGaN layers.

4.3.2. Effect of p-type doping on UV-C LEDs

In the earlier section, the approach for obtaining ohmic electrode contacts on high Al composition AlGaN was discussed. Built upon those results, the tunnel-injected UV-C LEDs were fabricated and characterized. Significant influence of p-type doping concentration on the device performance was noticed.[112] In this section, the effect of p-type doping on the tunnel-injected UV-C LEDs will be discussed.
Figure 49 (a) Epitaxial stack of the tunnel-injected UV-C LED. (b) Schematic structure of the top contact layer after device fabrication. The down-graded n++ AlGaN top contact layer remains only under the top contact metal. (c) Forward biased energy band diagram under the top metal contact region.

The investigated tunnel-injected UV LED structure is shown in Figure 49(a). The structure was grown by N\textsubscript{2} plasma assisted molecular beam epitaxy (MBE) on Si-doped metal-polar Al\textsubscript{0.72}Ga\textsubscript{0.28}N template with a threading dislocation density of 3×10\textsuperscript{9} cm\textsuperscript{-2}. The MBE growth started with a 600 nm n+-Al\textsubscript{0.75}Ga\textsubscript{0.25}N bottom contact layer with [Si]=1.8×10\textsuperscript{19} cm\textsuperscript{-3}, followed by 50 nm n-Al\textsubscript{0.75}Ga\textsubscript{0.25}N cladding layer ([Si]=4×10\textsuperscript{18} cm\textsuperscript{-3}), three periods of 2 nm Al\textsubscript{0.6}Ga\textsubscript{0.4}N/ 6 nm Al\textsubscript{0.73}Ga\textsubscript{0.27}N quantum wells/barriers, 6 nm AlN electron blocking layer, 50 nm compositionally graded p-AlGaN layer, 4 nm In\textsubscript{0.25}Ga\textsubscript{0.75}N, 5 nm graded n++ AlGaN with Al content increasing from 62% to 75%, 200 nm n++ Al\textsubscript{0.75}Ga\textsubscript{0.25}N, and a 40 nm graded n++ AlGaN top contact layer. The p-AlGaN layer has a linear Al compositional grading from 95% to 65% to create a negative bulk polarization.
charge. The 40 nm graded n++ AlGaN top contact layer has a similar Al compositional grading from 75% to 15%. The negative polarization charges behave like p-type doping in this layer, therefore, heavy Si doping to \([\text{Si}]=1 \times 10^{20} \text{cm}^{-3}\) is used to compensate them. This leads to a flat conduction band profile and effectively n-type doped layer.

ICP-RIE was used for device mesa isolation. The bottom and top contacts were formed as discussed in the last section. The top contact was designed to have partial metal coverage on the mesa area. For the investigated 30 × 30 µm² devices, the metal contact covers 37% of the mesa region. This was followed by a low power ICP-RIE etch to remove the down-graded n++ AlGaN top contact layer in the device mesa region that has no metal contact to minimize internal light absorption. The schematic structure of the finalized top contact is shown in Fig. 49(b).

Two tunnel-injected UV LEDs were grown and fabricated under similar conditions as discussed above, whereas, Mg doping concentration in the p-AlGaN layers was designed to be the only difference. Mg doping was varied by controlling Mg flux during growth, and was calibrated using SIMS measurement as shown in Fig. 50(b). An exponential increase in the Mg doping concentration was observed with increasing Mg cell temperature at the p-AlGaN growth temperature of 715 °C. Because of the high growth temperature, Mg cell was operated at an upper temperature limit to provide sufficient doping concentrations in the two samples, resulting in \([\text{Mg}]=6.2 \times 10^{18} \text{cm}^{-3}\) and \(1.5 \times 10^{19} \text{cm}^{-3}\) in sample A and B, respectively.
Figure 50 (a) Current-voltage characteristics of the tunnel-injected UV-C LEDs with different Mg doping concentrations ([Mg]=6.2×10^{18} \text{ cm}^{-3} \text{ and } 1.5×10^{19} \text{ cm}^{-3} \text{ in sample A and B, respectively}). The inset shows the current in log scale. (b) Mg concentration in Al_{0.75}Ga_{0.25}N as a function of Mg cell temperature at the growth temperature of 715 °C as determined from SIMS measurement.

The current-voltage characteristics for the 30 \times 30 \mu\text{m}^2 devices are shown in Fig. 50(a). The samples showed similar voltage drop at 20 A/cm², which are 10.4 V (A) and 10.2 V (B). This is ~ 4.5 V higher than the quantum well bandgap energy (E_{g,QW}=4.9 \text{ eV}), and is attributed to contributions from the tunnel junction layer. In contrast, the electrical characteristics exhibited an abrupt difference at high current levels. The voltage at 1 kA/cm² is reduced from 30.9 V to 19.2 V as the Mg doping concentration is increased. This is attributed to an extended depletion in the p-AlGaN layer due to the low Mg concentration in sample A when the tunnel junction layer is reverse-biased. Since the tunneling probability drops exponentially with increasing barrier width, a high voltage drop across the tunnel junction layer is required to obtain efficient interband tunneling.
Figure 51 (a) EL spectrums, (b) output power and EQE of the 30 × 30 μm² tunnel-injected UV-C LED measured under continuous-wave operation.

On-wafer EL measurement was carried out to confirm interband tunneling hole injection. The emission spectrum was obtained using a calibrated Ocean optics spectrometer by collecting light from the top surface of the 30 × 30 μm² devices. The EL result of sample B with \([\text{Mg}]=1.5\times10^{19} \text{ cm}^{-3}\) is shown in Figure 51. Single peak light emission at 257 nm was obtained. The microscope image shows uniform light emission from the whole device area, indicating sufficient current spreading in the top contact layer. The devices exhibited low efficiency, with a measured peak external quantum efficiency of 0.035%. Nevertheless, this is the first demonstration of interband tunnel injected UV-C LED emitting at 257 nm using an AlGaN/ InGaN tunnel junction for hole injection.

The difficulty to achieving efficient hole injection through the AlGaN/ InGaN tunnel junction could have exerted limitations on the UV LED performance. High density of background compensating impurities has been demonstrated to be a critical challenge in realizing efficient interband tunnel junctions. Further increasing the Mg doping
concentration and utilizing the polarization doping is expected to greatly enhance the tunneling probability.

4.4. Conclusions

This chapter presented the development of tunnel-injected UV LEDs employing the polarization engineered tunnel junction structures. Light emissions in the UV-A to UV-C spectrum driven by tunneling hole injection were demonstrate. The key challenges and the corresponding approaches toward the realization of high efficiency tunnel-injected UV LEDs were discussed. Low tunnel junction resistances below $2 \times 10^{-3} \, \Omega \, \text{cm}^2$ were achieved for AlGaN tunnel junctions with Al composition up to 75%, however, it was realized that the current AlGaN tunnel junctions require extra reverse bias, therefore, the balance between effective hole injection and minimal electron overflow is critical during device operation. This was treated as a design rule for the tunnel-injected UV LEDs.

For UV-A LEDs, the effect of the p-AlGaN layers were investigated. The highest device efficiencies were realized by utilizing a compositionally down-graded p-AlGaN layer. This also led to the demonstration of a p-type dopant-free UV LED emitting at 325 nm. High Mg doping concentration to overcome the background compensation was found to be beneficial in improving the device efficiency. Attempts on improving the light extraction efficiency through top surface roughening led to 43% improvement in the device efficiency. High EQE and WPE of 3.37% and 1.62% have been achieved for the optimized devices.
The optimization of the p-AlGaN layers were also studied for UV-B LEDs. It was found that better electron blocking is necessary because of the extra voltage drop across the tunnel junction layer for the onset of interband tunneling. Through the use of thick AlN electron blocking layer, peak EQE of 2.8% and WPE of 1.1% were achieved.

The challenges faced by UV-C LEDs were discussed in the last part of this Chapter. A graded top contact layer was adopted to obtain non-alloyed ohmic contact. The p-type doping concentration in the p-AlGaN layer was also found to be critical in improving the device efficiency. It was demonstrated that tunnel junctions for ultra-wide bandgap AlGaN can be achieved. While further optimizations in the tunnel junction performance are still necessary, the observation of interband tunneling demonstrates the feasibility for high efficiency UV LED applications using tunnel junctions.
Chapter 5

Metal/ semiconductor tunnel junctions

In the previous chapters, the design and demonstration of the tunnel-injected UV LEDs were presented. The potential advantages of those devices include efficient non-equilibrium hole injection and minimized internal light absorption. However, those device topologies were demonstrated based on MBE growth, which is not employed as a major mass production technology. In the following section, the challenges in realizing the tunnel-junction UV LED stack using the mass production technique, such as MOCVD, will be discussed, and a modified tunnel junction structure that could be more compatible with the MOCVD growth will be demonstrated.[113]

While MOCVD has been used as a major growth technique for UV LEDs, it faces great challenges in the growth and fabrication of the tunnel-injected UV LED structures. The existence of hydrogen atoms in the MOCVD reaction chamber leads to inevitable passivation of the Mg acceptors.[8] Several approaches have been proposed to achieve p-type conduction, including low-energy electron beam irradiation and thermal annealing.[114,115] Those methods have led to the breakthrough in visible LEDs. However, in the tunnel-injected UV LED structure, the n-type top contact layer impedes Hydrogen diffusion, making it difficult to achieve Mg activation.[45] To circumvent this problem, lateral Mg activation from etched sidewalls was developed for MOCVD-grown tunnel-injected blue LEDs.[45] However, increases in both the turn-on voltage and the differential resistance as compared to standard LEDs without tunnel junctions were observed. Another challenge comes with the fact that the high growth temperature
difference makes it difficult to grow AlGaN layers (typically at ~ 1200 °C)[116,117] on top of the thin InGaN layer (typically grown at ~ 750 °C)[118] using MOCVD. The InGaN layer has to suffer from severe decomposition when the growth temperature is increased to prepare for the AlGaN growth. This could lead to poor tunnel junction performance. In comparison, molecular beam epitaxy (MBE) growth does not require p-AlGaN activation after growth, and provides much lower growth temperature difference between AlGaN and InGaN layers. Utilizing those benefits, low resistance, low turn-on voltage tunnel-injected visible and UV LEDs have been demonstrated based on MBE growth.

In this work, we show a more MOCVD-compatible tunnel-injected UV LED structure employing a polarization engineered metal/InGaN/p-AlGaN tunnel junction.

5.1. Design considerations

Ohmic contacts using p-GaN capping on top of p-AlGaN or p-InGaN capping on top of p-GaN have been well-studied.[15,119,120] However, those p-type contacts were demonstrated inevitably with high work function metal layers, such as Ni- or Pd-based metal stacks, which have low reflectivity for UV light. In comparison, aluminum provides high reflectivity above 90% for UV light in a wide spectrum range.[121,122] Nevertheless, the use of Al as a reflective p-type contact is severely limited by the low work function. In this chapter, the feasibility of forming p-type tunneling contact between Al and p-AlGaN will be investigated.

The structure proposed here is presented in Figure 52. The difference as compared to the previously used n-AlGaN/InGaN/p-AlGaN tunnel junction structure is to replace the n-
AlGaN top contact layer with a metal layer that has a proper work function to enable band alignments and reduce the tunneling barrier as depicted in Figure 52. Similar to the semiconductor tunnel junction structure, the high density polarization charge at the InGaN/p-AlGaN interface creates a strong band bending in the InGaN layer, and leads to a similar tunneling barrier as shown in Figure 52. Under reverse bias across the junction, the electrons in the valence band of the p-AlGaN layer can tunnel into the empty states above the Fermi level in the metal layer and give rise to hole injection. As a result, even though Al has a low work function, the tunnel barrier formed at the metal/semiconductor interface is significantly reduced, making it feasible to achieve UV reflective p-type contact for UV LEDs.

Figure 52 Comparison between semiconductor tunnel junction and metal/semiconductor tunnel junction
5.2. Epitaxy and device fabrication

The metal/semiconductor tunnel junction design were studied experimentally for UV-A LEDs. The optimized epitaxial stack for UV-A LEDs discussed in Chapter 4 (4.1.2) was adopted in this study. It consists of n+ Al$_{0.3}$Ga$_{0.7}$N bottom contact layer, three periods of 2.5 nm Al$_{0.2}$Ga$_{0.8}$N/7.5 nm Al$_{0.3}$Ga$_{0.7}$N quantum wells (QWs)/ barriers, 1.5 nm AlN electron blocking layer (EBL), 50 nm graded p-AlGaN with Al content grading down from 75% to 30%, and 4 nm unintentionally doped In$_{0.25}$Ga$_{0.75}$N capping layer. Immediately after the InGaN layer growth, the substrate temperature was ramped down to room temperature to avoid InGaN decomposition.

Figure 53: Epitaxial stack, cross-sectional TEM image and energy band diagram of the tunnel-injected UV LED with a metal/semiconductor tunnel junction

The LED devices were fabricated by mesa etching using inductively coupled plasma reactive ion etching (ICP-RIE), Ti/Al/Ni/Au bottom metal deposition and subsequent annealing at 750 °C, and deposition of top metal stack. The influence of two different top
metal stacks were studied by depositing Al(30 nm)/ Ni(30 nm)/ Au(150 nm)/ Ni(20 nm) contact to one region of the sample, and Ni(30 nm)/ Au(150 nm)/ Ni(20 nm) contact to another region of the same sample to avoid sample to sample variation. To further investigate the effect of InGaN layer thickness on device electrical performance, low power plasma etch was used to recess the InGaN layer before top metal contact deposition. The etch rates were calibrated to be 10.4 nm/min and 4.5 nm/min for the Al$_{0.3}$Ga$_{0.7}$N and In$_{0.25}$Ga$_{0.75}$N layers, respectively. This has been ascribed to the difference in the volatility of the etch product during ICP-RIE etch.[123] Based on the etch time, the remaining InGaN layer thicknesses were estimated to be 3.2, 2.0, 0.9, 0.2 nm in different devices. A same Al/Ni/Au/Ni top metal stack was then evaporated on those devices to form top contact.

Figure 53(b) shows the HAADF-STEM image of the device with Al-based top contact. Smooth interfaces are observed for QWs, EBL and the InGaN tunneling layer. This indicates that the device fabrication process did not cause noticeable material degradation of the InGaN layer. The contrast gradient in the p-AlGaN layer reflects effective Al-compositional grading, which is critical to the formation of the three-dimensional negative polarization charge. The graded p-AlGaN layer leads to a flat valence band for hole transport, but contributes to a high barrier to block electron overflow as shown in the equilibrium energy band diagram with Al top contact in Figure 53(c). This is beneficial for enhanced carrier injection efficiency. Even though Al has a work function close to InGaN electron affinity, the sharp band bending in the InGaN layer aligns Al work function to the p-AlGaN valence band edge within a short distance (< 4 nm). As a result, holes can be tunnel-injected into the p-AlGaN layer by forward biasing the Al top contact layer.
5.3. Electrical characterization

Figure 54 (a) Current-voltage characteristics and (b) differential resistances of the 10×10 μm² tunnel-injected UV LED devices with different top metal contacts. The electrical characteristics of an identical UV LED with an n-AlGaN/InGaN/p-AlGaN semiconductor tunnel junction layer are shown as dashed lines for comparison.

The current-voltage characteristics of 10×10 μm² micro-LEDs with different top contact metal stacks are shown in Figure 54(a). They showed similar reverse leakage, however, the devices with Al-based top contact turn on at higher voltage. The voltages at 20 A/cm² are 4.63 V and 5.85 V for the devices with Ni- and Al-based contact, respectively. The voltage difference increases from 1.22 V at 20 A/cm² to 2.05 V at 1 kA/cm². This is due to higher differential resistance for the devices with Al-based contacts as shown in Fig. 54(b). The differential resistances are \(6.9 \times 10^{-4} \) Ω cm² and \(7.7 \times 10^{-4} \) Ω cm² at 1 kA/cm² for the devices with Ni- and Al-based contacts, respectively. Both values are similar to our previous tunnel-injected UV LEDs with n-AlGaN/InGaN/p-AlGaN tunnel junctions, and are much lower as compared to conventional UV LEDs with direct p-type contacts.
The effect of Ni- and Al-based contacts can be understood based on the equilibrium energy band diagrams near the metal/semiconductor interface as shown in Figure 54(c). Here, we assume there is no surface pinning effect. The band alignment is calculated by taking Ni and Al work functions ($W_m$) as 5.01 eV and 4.08 eV, respectively. Regardless of the large work function difference between the metal layers and the p-AlGaN layer ($W_{p-AlGaN} > 7.5eV$), both Ni and Al contacts cause very minimal depletion in the p-AlGaN layer. This is enabled by the sharp band banding in the InGaN layer, which acts as an ultra-thin tunneling barrier for hole injection. The barrier height ($\Phi_B$) is determined by the energy difference between metal and InGaN valence band edge as $\Phi_B = \chi_{InGaN} + E_g - W_m$, where $\chi_{InGaN}$ and $E_g$ represent electron affinity and bandgap of the InGaN layer, respectively. Since Al has lower work function, a higher tunneling barrier is expected for the Al/InGaN/AlGaN tunnel junction as shown in Figure 54(c). The tunneling probability drops exponentially with increasing barrier height, therefore, higher reverse bias across the tunnel junction layer is required to achieve sufficient hole injection when Al top contact is used. This leads to higher operation voltage for the UV LEDs with Al top contact as observed in Fig. 54(a). Nonetheless, this demonstrates that Al, as a conventional n-type contact metal, could enable p-type contact through the metal/semiconductor tunnel junction.
Figure 55 (a) I-V characteristics of the UV LEDs with Al/InGaN/p-AlGaN tunnel contact, where the InGaN layer thickness is varied by low power plasma etch. (b) The change of voltage drop at 20 A/cm² with the InGaN layer thickness. A dramatic increase in the turn-on voltage is observed with reducing InGaN layer thickness below 2 nm.

As shown in Figure 55, the electrical characteristics of the devices with different InGaN layer thicknesses are compared. As the InGaN layer thickness is reduced by plasma etching, both the turn-on voltage and on-resistance increase. While plasma etching could create donor states at the etch surface and possibly affect the electrical performance of the devices, the observed shift in the turn-on voltage for the devices is largely due to the change in the polarization-induced band-bending since similar plasma damages were expected. An abrupt increase from 6.35 V to 9.08 V occurs when the InGaN layer is reduced from 2.0 nm to 0.9 nm. This indicates a sharp increase in the tunnel barrier for hole injection, which might correspond to evident depletion in the p-AlGaN layer. The dramatic increase in the forward voltage from 5.85 V (4 nm InGaN) to 9.91 V (0.2 nm InGaN) at 20 A/cm² clearly
demonstrates that the InGaN layer enhances tunneling significantly by reducing the tunnel barrier so that Al-based contact can be used for hole injection.

5.4. Optical characterization

Figure 56 (a) Electroluminescence spectra, and (b) output power of 10×10 µm² tunnel-injected UV LED devices with different top metal contacts obtained on-wafer under continuous-wave operation. It shows single peak emission at ~ 326 nm. The inset to (a) is a microscope image of the device with Al-based top contact operated at 500 A/cm².

The electroluminescence (EL) spectrum of the device with Al-based top contact is shown in Figure 56. It shows single peak emission with a blue shift of the peak wavelength from 328.3 nm to 325.1 nm with increasing injection current due to the quantum confined Stark effect. The microscope image indicates efficient light emission from the tunnel-injected UV LED device. The emission power of the devices was measured on-wafer under continuous-wave operation. The devices with Al-based top contact exhibited higher power...
and efficiency as shown in Figure 57. At the injection current of 1200 A/cm\(^2\), high emission power density of 83.7 W/cm\(^2\) and 49.2 W/cm\(^2\) were measured for the devices with Al- and Ni-based top contact, respectively. The peak external quantum efficiency and wall-plug efficiency are 2.65% and 1.55% for the device with Al top contact, and 1.42% and 1.00% for the device with Ni top contact. The device with Al top contact exhibited 87% and 55% increases in the peak external quantum efficiency and wall-plug efficiency respectively as compared to the device with Ni top contact. This is attributed to higher light extraction efficiency associated with the high UV reflectivity of the Al top contact layer. However, a sharper efficiency droop was observed for the devices with Al top contact as shown in Figure 57(b) and (c). This might be a result of increased heating effect because of the higher voltage drop across the device as shown in Figure 54.

Figure 57 (a) EQE, and (b) WPE of the 10×10 \(\mu\)m\(^2\) tunnel-injected UV LED devices with different top metal contacts. The results were measured on-wafer under continuous-wave operation. The higher emission efficiency from the devices with Al-based top contact is attributed to enhanced light extraction due to high reflectivity of Al to the UV light.

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The above results demonstrate that efficient tunneling hole injection can be achieved using the metal/InGaN/p-AlGaN tunnel junction structure. This structure provides growth flexibilities for various growth methods, including MBE and MOCVD techniques. At the same time, it replaces the widely used absorbing p-type contact layers using Al-based tunneling contact. Since Al is highly reflective (reflectivity ~ 90%) to UV light over the whole wavelength range from 400 nm down to 200 nm, this structure could potentially lead to significant increase in the light extraction efficiency for the UV emitters. The low tunnel junction resistance makes it especially useful in laser diode applications.

5.5. Conclusions

In this chapter, a tunnel-injected UV LED structure employing a metal/InGaN/p-AlGaN tunnel junction for hole injection was demonstrated. The influence of Ni- and Al-based top contact metal stacks on the device performance was experimentally studied. Higher turn-on voltage and differential resistance was observed using Al-based contacts, and it is attributed to higher tunnel barrier originating from the lower work function of Al. Nonetheless, the device with Al top contact exhibited 87% and 55% increases in the peak external quantum efficiency and wall-plug efficiency, respectively, as compared to the device with Ni top contact. Through tunneling hole injection, we achieved light emission at 326 nm with on-wafer peak EQE and WPE of 2.65% and 1.55%, respectively. A high power density of 83.7 W/cm² was measured at 1200 A/cm². This work demonstrates the potential application of metal/semiconductor tunneling contact for hole injection towards high efficiency UV emitters. Compare to the semiconductor tunnel junctions, the metal/
semiconductor tunnel junction provides more flexibility in material epitaxy, and it is expected to be a more compatible structure for the current mass-production technology using MOCVD.
Chapter 6

Conclusions and future work

6.1. Conclusions

The work presented in this dissertation focused on the design and development of AlGaN tunnel junctions and their applications in UV LEDs to achieve non-equilibrium hole injection through interband tunneling.

The design of III-Nitride tunnel junctions through polarization engineering was first investigated, and it formed the basis for the study presented in this dissertation. Achieving low tunnel junction resistance is challenging for ultra-wide bandgap AlGaN material because of the high/wide tunnel barrier. By taking advantage of the high density polarization sheet charge arose from sharp hetero-interfaces, abrupt tunnel junctions with thin tunnel barriers were proposed and simulated. Based on the simulations, low tunnel junction resistance of $\sim 10^4 \Omega \text{ cm}^2$ could be achieved for AlGaN tunnel junctions in a wide Al composition range. This makes it suitable for UV LED applications, and it motivated the studies on tunnel-injected UV LEDs.

The tunnel junction resistance as a function of the material bandgap energy is shown in Figure 58. The tunnel junction resistance followed an exponential trend as the material bandgap energy increased 0.6 eV to 3.4 eV. This is as expected from the tunneling theory, and is a result of the increased tunnel barrier height. However, through polarization
engineering and strongly degenerate doping, low resistance GaN tunnel junctions were achieved with tunnel junction resistance as low as $1 \times 10^{-4} \, \Omega \, \text{cm}^2$. As a first demonstration of AlGaN tunnel junctions, low resistances below $2 \times 10^{-3} \, \Omega \, \text{cm}^2$ have been experimentally extracted in this work. The success of non-equilibrium hole injection was confirmed through efficient light emission at 325 nm and 287 nm. Hole injection into ultra-wide bandgap AlGaN with Al composition as high as 75% was also achieved, as evidenced by light emission at 257 nm. Those studies demonstrated the feasibility of tunneling hole injection into ultra-wide bandgap AlGaN, and it pointed to a novel tunnel-injected UV LED structure toward the realization of high power UV emitters.

![Figure 58 Summary of tunnel junction resistances for different material systems](image)

The design considerations for tunnel-injected UV LEDs were also investigated experimentally based on MBE growths. The major effort of the device optimizations was focused on the optimization of the p-type layers to assist interband tunneling. Optimization
of AlGaN growth was first discussed in Chapter 3. It was found that the AlGaN growth using PA-MBE can be affected by the growth temperature, Ga flux and growth rate. Smooth surface morphologies were obtained in a substrate temperature range of 700 °C to 760 °C. Having liquid Ga coverage was also found to be critical in maintaining smooth surface morphology and reducing impurity incorporation. P-type doping of AlGaN using Mg was also investigated. While a significant reduction of the Mg doping concentration was observed as the growth temperature was increased, the p-type doping density can be as high as $1 \times 10^{19}$ cm$^{-3}$ at 730 °C. The ability to achieve effective p-type doping near optimized AlGaN growth temperatures ensured high material quality and low defect density in the p-type layers.

AlGaN interband tunnel junctions were further incorporated into UV LEDs. By substituting the conventional p-type contact layers, the tunnel junction contact could lead to an increase in both the light extraction efficiency and carrier injection efficiency. Successful demonstrations of tunneling hole injection was confirmed through efficient light emission from 326 nm to 257 nm. This paves the road toward the realization of high efficiency UV emitters employing interband tunnel junctions.

While hole injection was achieved for deep UV LEDs, it was realized that the current AlGaN tunnel junctions require excess reverse bias, therefore, the balance between effective hole injection by reverse biasing the tunnel junction layer and minimal electron overflow is critical during device operation. Therefore, the major research effort has been focusing on the optimization of the p-type layers, including p-AlGaN and the electron blocking layer. Through the use of a polarization graded p-AlGaN layer, high on-wafer
EQE and WPE of 3.37% and 1.62% have been achieved for UV-A LEDs. For UV-B LEDs, a combination of high p-type doping density and thick AlN electron blocking layer led to the demonstration of EQE of 2.8% and WPE of 1.1%. The obtained efficiency values were comparable to state-of-the-art results, even though they were underestimated by the on-wafer measurements.

In the last part of this thesis, the metal/semiconductor tunnel junctions designed for UV LEDs were demonstrated for the first time. The structure allowed for the use of reflective Al-based metal stack for top contact, and at the same time, it could be more compatible with other epitaxy methods, such as MOCVD.
6.2. Future work

6.2.1. Reducing excess voltage

![Graph showing the dependence of AlGaN tunnel junction resistance and the excess voltage drop on the bandgap of the AlGaN layer.](image)

Figure 59 The dependence of AlGaN tunnel junction resistance (extracted at 1 kA/cm²) and the excess voltage drop (extracted at 20 A/cm²) on the bandgap of the AlGaN layer.

Figure 59 summaries III-Nitride tunnel junction resistances (extracted at 1 kA/cm²) and excess voltage drop (extracted at 20 A/cm²) obtained from tunnel-injected III-Nitride LEDs. Low tunnel junction resistances below $2 \times 10^{-3} \Omega \text{cm}^2$ have been achieved for ultra-wide bandgap AlGaN with Al composition up to 75%. This makes it promising in the applications of tunnel-injected laser diodes. However, a substantial increase in the extra voltage drop is observed as the AlGaN bandgap increases in the tunnel junction structure. Even though polarization engineering has been utilized to shrink the tunnel barrier through the insertion of an ultra-thin InGaN layer between $p^+$- and $n^+$-AlGaN layers, the large
Conduction band and valence band offsets at the hetero-interfaces lead to extended depletion barriers as discussed in Chapter 2. As the Al content increases in the AlGaN layers, higher depletion barriers and reduced tunneling probability are resulted. Therefore, further optimizations in the tunnel junction layer are necessary to reduce the extra voltage drop. The approaches can be adopted to further improve the tunneling probability include the optimization of the polarization grading layers in the tunnel junction region, and the optimization of the InGaN interband barrier layer.

The growth of polarization-engineered tunnel junctions requires larger lattice constant InGaN growth on top of smaller lattice constant AlGaN. The in-plane lattice constant of AlN, GaN and InN are 3.112, 3.189 and 3.545 angstroms. Linear interpolation could give the ternary compound lattice constants. For example, Al$_{0.7}$Ga$_{0.3}$N has an in-plane lattice constant of $a=3.135$ angstrom, while $a=3.456$ angstrom for In$_{0.25}$Ga$_{0.75}$N, leading to a lattice mismatch of 10%. A rough estimation of the critical thickness is given by $t_{cr}=a(AlGaN)^2/(a(InGaN)-a(AlGaN))$, which yields 3 nm. Even though the critical thickness could depend on the growth methods, this estimate shows that the InGaN layer is subject to easy relaxation if grown on highly lattice mismatched AlGaN layers. Since piezoelectric polarization, which arises from the strain status of the layers, is a dominant part of total polarization, strain relaxation would lead to great reduction in the polarization charge. In this case, the interband tunneling barrier will increase and extend to AlGaN layers, making it impossible to maintain the benefit of polarization engineering. Realization of strained uniform InGaN layers on AlGaN as a function of growth conditions would be a major work for future research.
Background impurity incorporation is another problem that could limit the tunnel junction performance. During AlGaN growth, impurities in the growth chamber, such as oxygen and carbon, can incorporate into the epitaxial layers. The impurities show up as deep donor states, which could compensate the p-type doping. In addition, nitrogen vacancies could behave as intrinsic compensating defects in Mg-doped AlGaN alloys. High Al composition AlGaN growth is even favorable for impurity incorporation, making it even challenging to have hole current flow in the p-AlGaN layers during device operation. Both growth optimization and design of the p-AlGaN side in the tunnel junction structure will require further research effort. Conductivity of p-doped AlGaN and polarization graded p-doped AlGaN should be further explored targeting for improved tunneling probability in the tunnel junction structure.

6.2.2. Deep UV emitters

As discussed in Chapter 4, tunnel junctions could play more important role for deep UV emitters, including UV LEDs and laser diodes, which requires high Al composition AlGaN materials. Due to the high acceptor activation energy, the thermally activated hole density could be even less than 1/10,000 of the acceptor doping density, leading to very poor injection efficiency. Tunneling injected UV LEDs is expected to achieve much better hole injection, and at the same time enable UV-transparent n-AlGaN contacts. As a result, the operation voltage is expected to be greatly lowered, and the emission efficiency enhanced compare to conventional UV LEDs. The wall-plug efficiency of conventional UV LEDs has been limited to be less than 1% for the emission wavelength below 250 nm. Apart from
the high radiative efficiency for those deep UV LED, both the electrical efficiency and light extraction efficiency could be greatly enhanced using tunneling hole injection. It is expected to surpass the state-of-the-art values using tunnel-injected UV LED structures.

The challenges include the optimization of the conductivity of the bottom contact layer, control of the dislocation density and defect density in the structure, and optimization of the active region for high radiative efficiency.

For the bottom contact layer, thick n-AlGaN have been widely used to reduce current crowding effect[124]. A more effective method that is specially enabled by tunnel-injected UV LED is to form backside vertical contact using UV reflective metal, and collect light from the top side. In this case, the problem related to bottom current spreading could be solved. The high spreading resistance and respective Joule heating can both be avoided, leading to enhance wall-plug efficiency and extended device lifetime. Development of substrate removal techniques, such as laser liftoff[125] and photoelectrochemical etching[126,127], for vertical contact formation could lead to dramatic increase in device performance.

Even though tunneling injection could solve many fundamental problems, there is still a severe limitation on the light extraction efficiency coming from the material side, which is the transition of the light polarization states. As the Al composition increases in AlGaN, the crystal field split-off energy changes from positive to negative, leading to a change of transverse electric (TE) mode to transverse magnetic (TM) mode for emitted light from GaN to AlN.[26] TE mode light corresponds to surface emission, while TM polarized light shows side emission. The switching point from TE dominated polarized light to TM
dominated polarized light could change with strain status of the material and the quantum confinement in the quantum well, but it typically varies around $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$ to $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$, corresponding to emission wavelength near 320 to 330 nm.[128] Any shorter emission wavelength has to suffer from dominating side emission, which leads to poor light extraction.

One solution to this is to utilize GaN quantum dots as recombination centers in the active region.[73-76] The direct benefit of using GaN quantum dots is that the active region maintains GaN valence band ordering, and the light emission is completely TE mode. This will lead to enhanced light extraction efficiency. Controlling the sizes of GaN quantum dots will result in the change of the spacing between ground state energy levels, leading to a change of the effective energy bandgap for light emission. If the quantum dot is treated as a simple quantum box with height of $L$, then the ground state quantization energy is $E_0=\frac{\pi^2\hbar^2}{2m^*L^2}$. The effective energy bangap is then expressed by $E_g^* = E_g + E_0^c + E_0^v$.

Decrease of the quantum dot size $L$ could lead to huge increase in the effective energy bandgap. For $L$ of 1 nm, $E_g^*$ could be $3.4 \text{ eV} + 1.9 \text{ eV} + 0.25 \text{ eV} = 5.55 \text{ eV}$, which corresponds to emission at 223 nm. However, detailed analysis including the actual barrier height and strain state is necessary for the understanding of the effective energy bandgap. Experimental demonstrations with emission wavelength lower than 230 nm has been achieved using GaN quantum dots.[73] However, challenges lie in the precise control of the GaN quantum dot sizes. Monolayer change of the quantum dot size could lead to substantial variation of the emission wavelength as shown from the effective bandgap expression. Another challenge is related to the possible confinement states in the quantum
dots. The 1D density of state is \( g(E) = 2\delta(E - E_c) \), where \( E_c \) is the discrete states in the box. There are two confinement states in the ground state. The total available confinement states in the active region simply depends on the number of quantum dots \( N \), leading to a total state of \( G_{\text{total}} = 2N \). Therefore, the quantum dot growth could highly impact carrier confinement.

In summary, the development of deep UV LEDs to take advantage of non-equilibrium hole injection could form an important aspect of future work following this dissertation.

### 6.2.3. Hybrid MOCVD/MBE growths for tunnel-injected UV LEDs

MOCVD has been used as the major growth technique for commercial UV LEDs. The ability for high growth temperature above 1000 °C makes it especially favorable for AlGaN growth. In comparison, the growth temperature in the MBE system is significantly limited by the ability to achieve liquid Ga coverage on the surface. As discussed in Chapter 3, the optimized growth temperature in a standard MBE system is below 800 °C. As a result, the Al adatoms on the sample surface suffer from low diffusion length, which could lead to compositional fluctuations and introduction of native defects. This further affects the radiative efficiency of the active region. Another constriction in the epitaxy growth of UV LEDs using MBE is the low growth rate, which is typically ~ 400 nm/hour, while the growth rate using the MOCVD systems could be 2-10 µm/hour. The high growth rate offered by the MOCVD systems is especially useful for the heteroepitaxy growth on non-native substrates, such as sapphire or SiC, where microns-thick buffer layers are necessary to ensure optimized material quality. However, there are significant challenges associated
with the realization of tunnel-injected UV LEDs using MOCVD as discussed in Chapter 5. The challenge in achieving p-type activation when embedded in n-type layers, and the severe memory effect of dopant impurities could both contribute to the poor device performance. The hybrid growth method employing both MOCVD and MBE growth techniques could solve the aforementioned issues.

The hybrid growth method employing both MOCVD and MBE growth techniques could solve the aforementioned issues.

![Figure 60 Hybrid growth method for tunnel-injected UV LEDs](image)

Figure 60 Hybrid growth method for tunnel-injected UV LEDs

The epitaxial stack growth using the hybrid method is shown in Figure 60. The material nucleation and the active region are grown using MOCVD to take advantage of the high material quality. This can be followed by the growth of the tunnel junction layer and the n-AlGaN top contact layer using MBE to exploit the high doping concentrations and the sharp heterointerfaces. This provides a promising approach for the realization of high power and high efficiency UV emitters.

6.2.4. Novel architectures to improve the light extraction efficiency

The tunnel-injected UV LED structure minimizes the internal light absorption loss, making it possible to substantially improve the light extraction efficiency. Epoxy and silicone have been widely used as encapsulation material for device packaging, however, both could
show high absorption rate to the UV light. Due to high photon energy emitted from the UV LEDs, it is challenging to find transparent encapsulation material with long operation lifetime. The tunnel-injected UV LED structure provides the feasibility in novel designs for light extractions and device packaging that are free from the widely used packaging materials, such as epoxy. A combination of high reflectivity metal stack based on aluminum and the shaping of the device mesa structure could be designed for enhanced light extraction efficiency.
Bibliography


