DESIGN OF III-N ULTRAVIOLET VERTICAL-CAVITY SURFACE-EMITTING LASERS BY NUMERICAL SIMULATION

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Presented to
The Academic Faculty

by

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DESIGN OF III-N ULTRAVIOLET VERTICAL-CAVITY SURFACE-EMITTING LASERS BY NUMERICAL SIMULATION

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<th>Abbreviation</th>
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<tr>
<td>DBR</td>
<td>Distributed Bragg Reflector</td>
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<td>DDBR</td>
<td>Dielectric Distributed Bragg Reflector</td>
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<tr>
<td>EBL</td>
<td>Electron Blocking Layer</td>
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<tr>
<td>EIM</td>
<td>Effective Index Method</td>
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<tr>
<td>EL</td>
<td>Electroluminescence</td>
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<tr>
<td>ELOG</td>
<td>Epitaxial Lateral Overgrowth</td>
</tr>
<tr>
<td>ITO</td>
<td>Indium Tin Oxide</td>
</tr>
<tr>
<td>LD</td>
<td>Laser Diode</td>
</tr>
<tr>
<td>LED</td>
<td>Light-Emitting Diode</td>
</tr>
<tr>
<td>MD-SPSL</td>
<td>Modulation-Doped Short-Period Superlattice</td>
</tr>
<tr>
<td>MQW</td>
<td>Multiple Quantum Well</td>
</tr>
<tr>
<td>QB</td>
<td>Quantum Well Barrier</td>
</tr>
<tr>
<td>QCSE</td>
<td>Quantum-Confined Stark Effect</td>
</tr>
<tr>
<td>QNR</td>
<td>Quasi-Neutral Region</td>
</tr>
<tr>
<td>QW</td>
<td>Quantum Well</td>
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<tr>
<td>SPSL</td>
<td>Short-Period Superlattice</td>
</tr>
<tr>
<td>SRH</td>
<td>Shockley-Read-Hall</td>
</tr>
<tr>
<td>uid</td>
<td>Unintentionally Doped</td>
</tr>
<tr>
<td>UV</td>
<td>Ultraviolet</td>
</tr>
<tr>
<td>VCSEL</td>
<td>Vertical-Cavity Surface-Emitting Laser</td>
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**LIST OF SYMBOLS AND ABBREVIATIONS**
SUMMARY

This thesis describes the design of an ultraviolet (UV) vertical-cavity surface-emitting laser diode (VCSEL). The goal of the research presented in this thesis was to design a VCSEL with an emission wavelength $\lambda = 369.5$ nm for laser cooling in an Yb-based chip-scale atomic clock. Advanced semiconductor device simulation tools have been used for a theoretical study of III-N VCSELs by self-consistent electro-opto-thermal numerical simulations. Critical factors that limit device performance have been identified—such as resistive lateral hole current spreading layers with high optical loss, low reflectivity bottom distributed Bragg reflectors (DBRs), high thermal resistance, and electron leakage. Mitigation strategies for the abovementioned critical problems will be discussed in detail.

After introducing the device simulation techniques, this dissertation will discuss the primary problems faced in the design of UV-VCSELs. Critical components of this VCSEL—the bottom and top DBRs, the p-contact layer, spacer layers to align the optical mode’s anti-node with the active regions, and the electron blocking layers will be studied, and optimum designs will be presented for each of these layers.

The most critical bottleneck to the realization of III-N UV-VCSELs is in obtaining a bottom (n-side) DBR with suitably high reflectivity (>99.8%). Several options have been explored in this thesis, such as airgap DBRs, ternary DBRs (AlGaN and AlInN), as well as a novel hybrid metal-epitaxial DBR. This hybrid DBR uses a metal deposited underneath an epitaxial DBR stack to boost the reflectivity of the mirror, while also being able to achieve a higher yield than a dielectric bottom DBR, since the cavity length is set epitaxially and is hence relatively independent of the polishing thickness.
We find that ‘transparent’ oxides (like ITO) typically used in blue VCSELs are unsuitable for UV wavelengths, and hence an alternative hole current spreading structure is presented - a modulation-doped short-period superlattice (SPSL). This leads to greatly reduced optical loss while still maintaining suitably high lateral hole conductivity.

Electron leakage is a significant problem in all III-N light emitters, and this is a natural consequence of the large asymmetry in majority carrier conductivities in the p- and n-doped spacer layers ($\sigma_n \gg \sigma_p$). Furthermore, we find that the optimum design of the electron blocking layer (EBL) is strongly dependent on the devices operating current density. Hence, we find that LEDs, edge-emitting LDs and VCSELs all have different optimum EBL designs due to vastly different operating current densities of each of these devices.

VCSELs operate at very high current densities, making self-heating a significant problem, which ultimately serves as the upper limit for the maximum optical output power. Several different thermal management strategies (changing both the geometry and materials of certain layers) will be studied with self-consistent electro-opto-thermal simulations.

Lastly, microcavity LEDs (MCLEDs) that were grown and fabricated by our experimental collaborators were characterized at low temperatures under pulsed and continuous-wave operation (I-V and emission spectra). These results will be presented at the end of this thesis.
CHAPTER 1. INTRODUCTION

Over the past couple of decades, devices made of III-Nitride materials have been widely used as light sources from the ultraviolet (UV) to the visible portion of the electromagnetic spectrum, as well as for high-power electronic devices. For the development of blue LEDs, Shuji Nakamura, Isamu Akasaki and Hiroshi Amano were awarded the 2014 Nobel Prize in Physics. The primary breakthroughs which paved the way for the development of the blue laser diode (LD) and light emitting diode (LED) were the realization of p-doping in GaN [1] and the growth of high-quality InGaN active layers [2]. The first laser diode made with the III-N (AlInGaN) material system operating at room temperature was demonstrated by Nakamura et. al in 1996 [3]. Since then, further improvements in the III-N material system have enabled the development of ultraviolet (UV)-green light emitters. The III-N materials have a direct bandgap ranging from 0.74 eV for InN, to 6.2 eV for AlN. The wide bandgap of AlInGaN alloys makes this material useful for UV optoelectronic devices [4], as well as for high power devices due to its very high breakdown electric field [5].

Despite the many attractive properties of III-N materials, several issues are holding back device development with these materials, such as a high lattice mismatch between binary compounds [6], which leads to biaxial strain and produces defects which act as nonradiative recombination centers and reduce the device’s reliability. Another major problem associated with bipolar III-N devices is the difficulty in achieving p-doped material with high conductivity. This is because the acceptor species (Magnesium in this
case) has a very high activation energy, which further increases with the bandgap of AlGaN alloys [7], and due to the hole mobility being lower than that of electrons [8], [9].

The objective of the proposed research is to develop a narrow linewidth Vertical Cavity Surface Emitting Laser diode (VCSEL) operating at a wavelength of 369.5 nm for use in Yb-based atomic clocks. VCSELs have several advantages over edge-emitting laser diodes such as lower threshold currents, circular output beams, single longitudinal mode operation, wafer-scale testing and narrower beam divergence. VCSELs were first demonstrated by Soda et al. for infrared wavelength in 1979 [10]. VCSELs have various applications such as optical-fiber data transmission, pumping solid state lasers, optical scanners, etc.

The following chapters will contain a discussion of design techniques to solve some of the issues that plague UV and visible light emitting devices such as laser diodes (LDs) and light emitting diodes (LEDs) by numerical simulation. Advanced semiconductor device simulation tools have been used for a theoretical study of III-N VCSELs. Restrictions imposed by material properties and by current growth techniques have been identified by experimental collaborators, and practical solutions to critical problems faced in the development of UV laser diodes are proposed in full consideration thereof. The proposed work deals exclusively with device design rather than development of either numerical software or physical models. Existing simulation techniques used for this work are well established, and combine the principles of semiconductor physics, photonics and quantum mechanics to analyze critical factors influencing the performance of III-N VCSELs.
1.1 Key Objectives and Themes of this Dissertation

This dissertation has two themes— the obvious one is to design a UV-VCSEL for an Yb-ion atomic clock, but the more important overarching theme is to show the reader how to go about the daunting task of designing a laser diode.

The first step is to do a literature survey of the problem and try and understand why existing solutions don’t work for the problem at hand (Chapter 3). Understanding material properties and limitations is a part of this (Chapter 2). The next step is to think about what software tools will be needed to start. This requires a thorough understanding of the physics— to know what assumptions are valid and which equations need to be solved (Chapter 4). Now we move on to one of the most challenging steps— identifying the key factors affecting device design. This involves identifying the key problems (chapter 5)— be they thermal and/or optical and/or electrical problems or even just experimental limitations (e.g. strain and refractive index contrast). Once the key bottlenecks (sub-problems) have been identified, solutions must be thought of with the help of an imagination and numerical simulations. It is often not useful to run full electro-opto-thermal simulations right away. Initially, to get an understanding of the magnitude of the sub-problem, you may only need to run a much smaller, faster and more targeted simulation with better control of variables. That’s how the DBR design has been implemented— only if the reflectivity spectra simulations (takes less than 5 seconds) look promising does one need to bother with full laser simulations which can take from 45 minutes to over a day depending on the complexity of the geometry and/or physics.
The next step is the most complex— it involves understanding how certain design changes affect the electro-opto-thermal system, i.e. the coupling between electrical, optical and thermal equations being solved. An example of such a problem is the design of current spreading layer, because its thickness and material properties affect lateral current spreading (gain), Joule heating and the optical loss. Usually, the optical problem tends to be the most important, since having lower loss improves the laser in every single way. The thermal problem is usually the easiest and hence it is usually better to deal with it last. Chapters 6 to 9 provide solutions to the key problems identified in Chapter 5.
CHAPTER 2. CHALLENGES UNIQUE TO THE III-N MATERIAL SYSTEM

The III-Nitride material has some unique characteristics that make it harder to work with than conventional III-V materials (III-AsP material system), such as high lattice mismatch between binary compounds [6], spontaneous and piezoelectric polarization charges at heterojunctions [11], poor p-doping efficiency [7], [12] and optically lossy p-doped layers [13]. Each of these problems and their impact on the VCSEL’s performance will be briefly discussed in this chapter and will be followed by a more detailed discussion of solutions to these problems in later chapters of this thesis.

2.1 Lattice Mismatch Between Binary III-N Compounds

One of the primary advantages of the AlGaAs material system which led to its widespread use in highly efficient infrared VCSELs is the fact that GaAs and AlAs are almost perfectly lattice matched [14]. This seemingly simple fact has two big implications for a laser designer- better carrier and optical confinement with minimal defect generation caused by biaxial strain. Carrier confinement is achieved by growing adjacent layers with a large bandgap discontinuity, and optical confinement is achieved through a high refractive index contrast between adjacent layers. AlAs and GaAs have an index contrast of 20% at 900 nm [15], and bandgap discontinuities as high as 0.7 eV [16]!

The III-N material system, on the other hand, is highly strained with AlN grown on GaN experiencing tensile strain of 2.41% [6], and InN on GaN experiences compressive
strain of 11.16%. This is illustrated in Figure 1, which plots the bandgaps (and equivalent photon energies) and lattice constants of commonly used III-V semiconductors.

![Energy gap of the III-V as a function of lattice parameter](image)

**Figure 1 – Bandgap and emission wavelength vs lattice constants of III-V semiconductors. Image from Caro Bayo, M. A., Theory of elasticity and electric polarization, PhD Thesis, University College Cork (2013) [17].**

The biaxial tensile strain in AlGaN grown on GaN causes extended defects which can propagate vertically up to the active region. This greatly reduces the quantum well’s internal quantum efficiency (IQE) and the device’s reliability by acting as non-radiative recombination centers, which competes for bound carriers with radiative recombination. These defects introduce energetic states within the bandgap of the active region. The dominant non-radiative recombination mechanism due to extended defects is thought to be Shockley-Read-Hall recombination, and the effect of the dislocation density on an LED’s
IQE is described in [18], and its effect on the nonradiative recombination lifetime in bulk GaN is described in [19].

Thus, the strain severely limits the aluminum mole fraction in the electron blocking layer (EBL) and in the DBR. This leads to poor injection efficiency due to electron leakage and poor DBR reflectivity, since more aluminum incorporations allows us to increase the refractive index contrast, and hence the reflectivity. This will be discussed in more detail in the chapters pertaining to EBL and DBR design.

2.2 Spontaneous and Piezoelectric Polarization Charge

An ideal wurtzite crystal has a c/a ratio of $\sqrt{8/3}$ (which equals 1.633), but the ratios for AlN, GaN and InN are 1.601, 1.627 and 1.612 respectively [20]. This difference is due to the electronegativity differences between the group III and group V atoms that bond to one another. This generates a dipole, which leads to polarization charges at any interface between two different III-N alloys. This interfacial polarization charge has a great impact on the device’s optical and electrical properties. The polarization charge has two components- the piezoelectric polarization charge which arises due to the lattice mismatch, and spontaneous polarization charge which is caused by the abovementioned difference in the electronegativity. The total polarization charge is a sum of these two components. A detailed discussion on how to calculate the polarization charge in III-N materials can be found in [21].

Polarization charge has deleterious effects on the performance of III-N light emitting devices due to two primary reasons- reduction of the QW gain by reducing the overlap
between bound electron and hole wavefunctions and reducing the device’s injection efficiency by exacerbating electron leakage.

The built-in electric fields due to the abovementioned polarization charge at the two QW/QB interfaces separates electron and hole wavefunctions, thus reducing the overlap integral. As per Fermi’s Golden Rule, the rate of radiative recombination is proportional to the squared of the overlap integral of the electron and hole wavefunctions. The wavefunctions and eigenstates of a QW with and without the built-in electric field are shown in Figure 2 (from [11]).

![Figure 2](image.png)

**Figure 2** – Bound states in the conduction (top) and valence (bottom) bands of a QW without (left) and with (right) built-in electric fields due to polarization charge.

A common technique to mitigate the Quantum Confined Stark Effect (QCSE) and improve wavefunction overlap is to use narrow QWs (<3 nm). However, there are two downsides to this approach - a reduction in the optical confinement factor, and a greater volumetric carrier density in the QW. The increased volumetric carrier density is deleterious because it increases the carrier loss due to Auger recombination and it increases electron leakage, by shifting the electron quasi-Fermi energy up, and hence reducing the effective barrier height for electron escape. The polarization charge also bends the band edges near the interface to further increase carrier leakage. However, despite these disadvantages, the use of narrow QWs in c-plane material is still the best option.

In addition to reducing the gain, the polarization charge also severely affects electron leakage by trapping carriers at the interface, and hence changing the effective barrier height \((E_c-E_{fn})\) for electron leakage by thermionic emission. This will be discussed in much greater detail in the chapter regarding the design of the EBL.

Some other methods proposed and demonstrated to mitigate the QCSE is to use material grown on the nonpolar or semi-polar planes (a-plane [22] or m-plane [23], [24]). However, despite the advantages of lower built-in fields, semi-polar and non-polar lasers still have two to three times higher threshold current densities than the best c-plane laser diodes [24]. The reason for this is thought to be poorer crystal quality in non-c-plane material.

Another difficult technique to mitigate the QCSE involve the growth of quaternary AlInGaN alloys to enable polarization charge matching between the QW and QB [25], [26]. However, the growth of high-quality AlInN layers is extremely challenging due to
the different optimum growth temperatures of InN and AlN, and the composition inhomogeneity in AlInN which results from the large disparity in covalent bond lengths between the two binary compounds [27]. Another method to reduce the electric field in the QW is to reduce the mole fraction difference between the QW and QB, but this consequently reduces the energetic barrier for bound carriers, and thus enhances carrier leakage out of the QW.

2.3 Poor P-type Conductivity

The high resistivity of p-doped material (compared to n-doped material) has been a longstanding problem for researchers working on bipolar devices made with the III-N material system. In intrinsic material, electrons have 3-4 times higher mobilities than holes [28], and this difference is exacerbated in doped material, with electron mobilities in n-type material [8] being about 30-40 times higher than hole mobilities in p-type material [9]. Silicon, a donor, has an activation energy of about 20 meV [29], while magnesium, the acceptor of choice, has an activation energy of 166 meV in GaN [12], and this activation energy further increases with aluminum content in Al\textsubscript{x}Ga\textsubscript{1-x}N alloys [30]. 166 meV corresponds to an energy of 6 kT (at RT), making thermal ionization of the acceptor very inefficient. Thus, the poor free hole concentration and the low hole mobility makes p-Al\textsubscript{0.12}Ga\textsubscript{0.88}N more than 50 times more resistive than n-Al\textsubscript{0.12}Ga\textsubscript{0.88}N.

Assuming a Fermi-Dirac distribution, the electrically active acceptor concentration, or simply the free hole concentration is given by equation (1):
\[ N_A^- = \frac{N_A}{1 + g_A \exp \left( \frac{E_A - E_{F,p}}{kT} \right)} \]  

where \( N_A \) is the acceptor concentration, \( g_A \) is the degeneracy factor for the impurity levels, \( E_A \) is the acceptor activation/ionization energy, and \( E_{F,p} \) is the hole quasi-fermi energy level.

There are several important consequences of poor p-type conductivity, such as large potential drops in the p-quasi-neutral region (p-QNR), which increases the device’s operating bias, causes increased Joule heating which reduces the gain and enhances electron leakage. Poor p-doping efficiency increases electron leakage due to two primary reasons: it reduces the barrier for electron leakage at the QB/EBL interface, and enhances the bound carrier asymmetry by increasing the barrier to hole injection at the p-QNR/EBL interface. Both these points regarding electron leakage will be discussed in more detail in the chapter pertaining to EBL design.

2.4 Optical Loss in p-Doped III-N Material

p-doped AlGaN has an absorption coefficient that is over three times higher than n-AlGaN QNRs based on the model found in [13] and data in [31]. However, the loss in the p++ contact layer is of far greater importance than the QNR, and this point will be discussed in more detail in chapter 5. The reason for higher loss in p-materials may be explained by the fact that heavy magnesium doping (>1e18 cm\(^{-3}\)) creates optically active defects [32]. The high acceptor activation energy of Mg in AlGaN implies that a much higher
concentration of magnesium is required in order to achieve a suitably low resistivity. This further increases the concentration of the aforementioned optically active defects.
CHAPTER 3. CURRENT STATE-OF-THE-ART IN III-N VCSELs

Now that the reader is familiar with the problems that plague III-N light emitting devices, and the challenges involved with realizing UV-VCSELs, the current progress in developing III-N visible VCSELs will be reviewed in this section.

3.1 Literature Survey of III-N VCSELs

The VCSEL being designed in this project operates at a wavelength of 369.5 nm and will be used in chip-scale atomic clocks. The first electrically-pumped VCSEL based on the III-N material system was demonstrated in 2008 by Nichia [33], with a lasing wavelength of 414 nm, under room-temperature (RT) continuous-wave (CW) operation. It was grown on a sapphire substrate and used dielectric DBRs on both sides. To deposit a dielectric mirror on the bottom (n-side), the substrate removed by laser lift-off after bonding the p-side to a support substrate. Subsequently Nichia managed to increase the maximum output optical power under RT CW operation and reduce the threshold current by using a native GaN substrate [34], [35] which has a reduced dislocation density on the order of $10^6 \text{cm}^{-2}$. The GaN substrate could not be removed by laser lift-off, and hence had to be thinned by chemical mechanical polishing (CMP). This caused an increase in the variation of the VCSEL’s cavity length, leading to reduced yields compared to VCSELs grown on sapphire. A similar approach was used by Panasonic to fabricate a VCSEL emitting light with $\lambda=408 \text{ nm}$ [36] under RT CW operation. They too fabricated a device bonded upside down to a support substrate and thinned the substrate by CMP before depositing a dielectric DBR stack on the n-side. All these devices extracted heat from the p-side as a result of the flip-chip process. The primary disadvantages of this method are the
difficulty in precisely controlling the cavity length since polishing lacks the precision of epitaxy by MOCVD or MBE, and the necessity of obtaining a smooth surface after polishing in order to minimize scattering losses at the cavity and dielectric DBR interface.

An alternative approach to achieving VCSELs with double dielectric DBR stacks was demonstrated by Sony, who made use of epitaxial lateral overgrowth (ELOG) to overcome the drawbacks mentioned above. The ELOG method has been effectively used by Sony to obtain milliwatt class blue VCSELs [37], [38]. In this process, the SiO$_2$/SiN$_x$ bottom dielectric DBR stack is embedded in n-GaN grown by ELOG [38]. This method allows more precise cavity length control than that obtained by CMP, thus increasing the yield. GaN is highly absorptive in the UV spectrum, and hence a tensile strained AlGaN cavity (on a GaN substrate) is needed in UV VCSELs. ELOG is easier to realize with GaN than with AlGaN due a reduced lateral growth rate for AlGaN and because the AlGaN polycrystals tend to stick to the dielectric masks [39]. The advantages of using double dielectric DBRs over hybrid DBRs include higher reflectivity and wider stopbands obtained due to the increased refractive index contrast between the two dielectric materials. This leads to lower threshold currents (due to higher reflectivity), and the wider stopband improves the VCSEL’s robustness against fluctuations in material composition and thickness by ensuring that the lasing wavelength is always within the DBR’s stopband, while simultaneously extending the VCSEL’s operating temperature range.

The three groups discussed above (Nichia, Panasonic and Sony) all used double dielectric DBRs. Another class of VCSELs use hybrid DBRs, which means that the p-side DBR is a dielectric DBR, while the bottom n-side AlInGaN DBR is grown epitaxially. The use of epitaxial DBRs allows precise cavity length control and it reduces the complexity of
the fabrication process by eliminating the laser-liftoff and/or polishing steps. However, the primary challenge in achieving indium-free epitaxial DBRs is in managing the biaxial tensile strain when AlGaN is grown on GaN. The III-nitride material is highly strained, with AlN grown on GaN experiencing tensile strain of 2.41% [6]. This makes it challenging to grow crack-free AlGaN-based DBRs with a sufficient number of pairs to overcome the low refractive index contrast and achieve 99% reflectivity. The only report to date of an electrically-pumped VCSEL operating CW at RT which uses an indium-free AlGaN/GaN or AlGaN/AlGaN DBR is by Lu et al. at a wavelength of 412 nm [40], in which the bottom DBR consisted of 29 pairs of AlN/GaN [41]. They claim that the insertion of superlattice layers every 5.5 pairs helps to suppress crack generation.

Another class of epitaxial DBRs are made of lattice-matched AlGaN/AlInN, which solves the abovementioned problems associated with the high strain, such as cracking. These materials have high refractive index contrasts and are hence able to attain reflectivities exceeding 99%, at wavelengths extending from the UV to the visible portion of the electromagnetic spectrum by tuning the aluminum mole fraction. EPFL obtained DBRs whose reflectivity exceeded 99% at \(\lambda=340\) nm with as few as 35 pairs [42], and a reflectivity of 99.6% at \(\lambda=424\) with 42 pairs [43]. The only other groups to demonstrate lattice-matched AlInN/GaN DBRs are at Meijo University and Nagoya University [44]. In fact, they recently demonstrated blue VCSELs with a record high optical output power of 15.7 mW at 20\(^\circ\) C and 2.7 mW at 110\(^\circ\) C [45]. Using these mirrors, EPFL obtained an electrically-pumped VCSEL operating at RT in pulsed mode [46], while Nagoya University and Meijo University obtained a VCSEL which lased at RT under CW operation [47]. However, the growth of high-quality AlInN layers is challenging due to the
different optimum growth temperatures of InN and AlN, and the composition inhomogeneity in AlInN which results from the large disparity in covalent bond lengths between the two binary compounds [27]. In our experience, the ability to grow AlInN (with more than 6% indium) also strongly depends on the geometry of the MOCVD reactor. Thus, AlInN/AlGaN DBRs will not be discussed in this dissertation.

3.2 Why are all III-N VCSELs in the literature only at visible wavelengths and not UV?

All the VCSELs cited previously are at visible wavelengths (406 nm – 450 nm). This is because UV light-emitters have several drawbacks over their visible (violet-green) counterparts, such as poorer conductivity in p-layers, reduced internal quantum efficiency (IQE) of the quantum wells (QWs), high tensile strain of the AlGaN epitaxial layers on a GaN substrate, and higher optical losses at UV wavelengths. The activation energy for Mg (acceptor species) increases with the bandgap of Al$_x$Ga$_{1-x}$N [30], [48], [49]. Visible III-N light-emitters use GaN-based cavities, which have more conductive p-layers than the AlGaN-based cavities used in UV devices.

Furthermore, visible devices’ GaN-based cavities are essentially lattice-matched to FS-GaN substrates or GaN templates, but growing AlGaN-based cavities on GaN leads to large tensile strain (2.41% tensile strain for AlN on GaN [6]) which leads to cracks being formed on the wafer. Several groups have reported that InGaN quantum wells have the highest IQE for the violet-blue portion of the electromagnetic spectrum, and the SRH recombination lifetime reduces with the reduction in the indium content in the QWs used
in UV devices [50], [51]. This enables increased gain for visible LDs compared to UV laser diodes.

InGaN QWs show strong violet-blue light emission despite threading dislocation densities (TDDs) exceeding $10^9$ cm$^{-2}$. The prevailing explanation for this observation is indium fluctuations in the QW, which generates localized excitons in regions with higher indium, thus preventing those bound carriers from recombining non-radiatively at a defect site [52]–[54]. As the indium content reduces for UV light emitters, so does the potential barrier height due to reduced indium fluctuations, leading to increased non-radiative recombination at defects due to an increase in the effective diffusion length of bound carriers in the plane of QW. However, at this point, this theory of indium segregation increasing the IQE has no conclusive evidence.

Finally, materials commonly used in visible VCSELs are far more optically lossy at $\lambda = 370$ nm than at $\lambda = 420$ nm. Typically, the difference between the quasi-neutral region (QNR) material’s bandgap and the photon energy $h\nu$ is smaller for UV devices than for visible light-emitters. This is because the aluminum mole fraction is limited by the critical thickness of AlGaN grown on GaN. The absorption loss in ITO approximately doubles from 2900 cm$^{-1}$ to 5800 cm$^{-1}$ as the wavelength reduces from 410 nm to 370 nm [55], [56].

However, despite these drawbacks, UV edge-emitting laser diodes have been demonstrated by PARC [57], [58], Nichia [59] and Hamamatsu [60]–[62]. PARC got around the problem of growing a crack-free thick AlGaN cladding by using a 100 nm thick In$_{0.02}$Ga$_{0.98}$N compliance layer on top of the GaN substrate/template. Hamamatsu created an AlGaN template on a GaN substrate by hetero-facet controlled epitaxial lateral
overgrowth (hetero-FACELO) [63]–[65]. This relaxed AlGaN template allowed them to grow thick Al$_{x}$Ga$_{1-x}$N claddings with $x>0.2$. 
CHAPTER 4. SIMULATION TECHNIQUES AND MATERIAL PARAMETERS

4.1 VCSEL Simulation Model and Techniques

There are several commercial tools available for the simulation of laser diodes such as Crosslight’s PICS3D, Synopsys Sentaurus TCAD by Synopsys, RSoft’s LaserMOD, and Photon Design’s PICWave. All these essentially solve the same set of equations, which will be discussed in this chapter. Most of these tools are based on the Minilase-II program [66], [67] developed at the University of Illinois and the laser simulation tool developed at ETH Zurich [68], [69]. Among the reported proprietary simulations tools for III-N optical devices, two groups stand out- Witzigmann et al. have developed a tool to study the gain spectra of InGaN/GaN MQW light emitters [70], and Karbownik and Sarzala have created a tool to simulate ridge waveguide III-N lasers [71].

The equations solved by the laser simulation tools used in this dissertation are the (1) Poisson equation, (2) Charge carrier continuity equations, (3) Quantum well (QW) scattering equations to model the capture of carriers into the QW, (4) QW gain calculation using Fermi’s Golden Rule, (5) Photon rate equation, and (6) Helmholtz equation to compute the optical modes, and (7) Thermodynamic model (heat continuity equation) to calculate the lattice temperature due to self-heating. To consider the effects of self-heating in VCSELs, a lattice heat flow equation based on diffusive transport is solved. The complexity of a laser diode simulation and a visual aid to understand how the various equations are coupled to one another is illustrated in Figure 3.
4.1.1 Charge Transport Models

The Poisson equation, along with the carrier continuity equation are the fundamental equations to describe charge transport in the low-field regime. The Poisson equation (equation 2) calculates the electrostatic potential $\Phi$, while the continuity equations compute the hole (equation 3) and electron current densities (equation 4).

$$\nabla \cdot (\varepsilon \nabla \Phi) = -q(p - n + \mathcal{N}_D^+ - \mathcal{N}_A^-)$$  \hspace{1cm} (2)

where $\varepsilon$ is the permittivity of the semiconductor, $q$ is the electronic charge, $p$ and $\text{hole}$ are the hole and electron densities respectively, and $\mathcal{N}_D^+$ and $\mathcal{N}_A^-$ are the ionized donor and acceptor concentrations respectively.
\[-\nabla \cdot \vec{J}_P = q(R_{\text{net}} + \frac{\partial p}{\partial t})\]  \hspace{1cm} (3)

\[\nabla \cdot \vec{J}_N = q(R_{\text{net}} + \frac{\partial p}{\partial t})\]  \hspace{1cm} (4)

where \(\vec{J}_P\) and \(\vec{J}_N\) are the hole and electron current densities respectively, and \(R_{\text{net}}\) is the electron-hole recombination rate.

A thermionic emission boundary condition is used to describe charge transport across an abrupt heterojunction [72]. The thermionic emission current from a narrow bandgap material into a wide bandgap material is described in equation (5) [73]:

\[J_{\text{thermionic}} = AT^2 \left[ e^{\frac{(E_{fn}^W - E_{Cc}^W)}{kT}} - e^{\frac{(E_{fn}^N - E_{Cc}^N - |\Delta E_C|)}{kT}} \right] \]  \hspace{1cm} (5)

Where A is the effective Richardson constant, T is the carrier temperature (assumed equal to the lattice temperature in simulation results presented in this dissertation), k is the Boltzmann constant, \(\Delta E_C\) is the conduction band offset between the narrow and wide bandgap materials forming the heterointerface, while \(E_{Cc}^{NW}\) and \(E_{fn}^{NW}\) is the conduction band edge and electron quasi-fermi energy in the narrow bandgap (N) and wide bandgap (W) material. The thermionic emission current has an exponential dependence on the energetic barrier height and temperature.
4.1.2 Calculation of QW Gain

Carriers move by drift and diffusion in the bulk regions and are then injected into the QW by thermionic emission, where the carrier be either be scattered into a bound state or back into the bulk (carrier leakage) by thermionic emission. The net capture rate for carriers into 2D bound states from continuum 3D states by equation 6 [68]:

\[
C_{\text{cap}} = \left( 1 - e^{\frac{E_{F,n}^{2D} - E_{F,n}}{kT}} \right) \left( 1 - \frac{n^{2D}}{N^{2D}} \right) \frac{n^{3D}}{\tau_e} \tag{6}
\]

for electrons and similarly for holes (replace ‘n’ with ‘p’). \(E_{F,n}^{2D}\) and \(E_{F,n}\) are the electron-quasi Fermi energies for free and bound electrons respectively, \(n^{3D}\) and \(n^{2D}\) are the free and bound electron concentrations, \(N^{2D}\) is the sum of all bound states in the QW per unit volume, and \(\tau_e\) is effective electron capture time and it is meant to represent the time-scale for scattering processes due to carrier-carrier and carrier-phonon interactions to facilitate the transfer of electrons from continuum into bound states.

The carriers in bound states are spatially distributed in the QW as per the carrier wavefunctions that was calculated by a 1D Schrodinger Equation solver running through the MQW active region. The 1D Schrodinger Equation and the bound density of states are numerically solved by the k·p method with a 6x6 Hamiltonian for wurtzite materials [74].

The reduced density of states, quantized subband energies and spatially-dependent carrier densities are then fed into Fermi’s Golden Rule [75] to calculate the gain for each mode. The stimulated emission coefficient in the QW is calculated as per equation 7 [68]:
\[ r^{st}(E) = \sum_{ij} \int dE \, C_0 |M_{ij}|^2 \, D(E) \, (f_i^C(E) + f_j^Y(E) - 1) \, L(E) \] 

(7)

where \( C_0 = \frac{\pi e^2}{n c \varepsilon_0 m_0^2 \omega} \) 

(8)

where \( |M_{ij}|^2 \) is the optical matrix element, \( D(E) \) is the reduced density of states, \( L(E) \) is the gain-broadening function, \( n \) is the refractive index, \( m_0 \) is the free-electron mass, and \( \omega \) is the photon’s angular frequency.

4.1.3 Optical Model

Finding the optical modes in the cavity involves solving the Helmholtz equation (equation 9):

\[ \nabla^2 \psi + k_0^2 (n^2 - \varepsilon_{eff}) \psi \] 

(9)

where \( \psi \) could be the electric field vector or the magnetic field vector, \( n \) is the refractive index profile and \( \varepsilon_{eff} \) is the effective dielectric constant. Only the solution to the vector Helmholtz equation can account for diffraction losses at interfaces. The numerical method for solving the vector Helmholtz equation is described in [68]. The vectorial eigensolver takes longer to compute than the effective index method (EIM) [76]. The optimum method for our design optimization is thus to run the vectorial eigensolver just once, followed by the EIM to find the diffraction loss (difference between the losses computed by the vectorial solver and the EIM solver). This diffraction loss can then be added to future EIM
simulations. Thus, the judicious use of vectorial eigensolvers can greatly reduce the time need for VCSEL prototyping.

Finally, the electrical and optical simulations are coupled through the photon rate equation (equation 10):

$$\frac{dS_v(t)}{dt} = -2\omega'' v(t) S_v(t) + R_{sp}^v(t)$$

(10)

where $S_v$ is the electromagnetic energy in the $v^{th}$ mode, $\omega''$ is the eigenvalue, $R_{sp}^v$ is the rate of spontaneous emission into the $v^{th}$ mode. $2\omega''' v$ is also the net loss rate of photons.

### 4.1.4 Thermal Model

Current injection causes self-heating under current injection due to non-radiative recombination and Joule heating. This leads to an increase in the active region temperature, which exacerbates carrier leakage and reduces the modal gain. The steady-state thermal diffusion equation for the lattice temperature is given by equation 11:

$$-\nabla \cdot \kappa \nabla T = Q$$

(11)

$$Q = \frac{j_n^2}{\mu_n n q} + \frac{j_p^2}{\mu_p p q} + q R_{nr} (\phi_p - \phi_n + T(P_p - P_n)) - j_n \cdot T \nabla P_n - j_p \cdot T \nabla P_p$$

(12)

where $Q$, $T$ and $\kappa$ are the heat generation density, the lattice temperature and the thermal conductivity, respectively. $J$, $\mu$ and $n$ (or $p$) are the carrier densities, mobility and carrier concentration, $R_{nr}$ is the net rate of nonradiative recombination, $\phi_n$ and $\phi_p$ are the electron and hole quasi-fermi potentials, and $P$ is the thermoelectric power.
The first two terms in equation 12 are the Joule heating terms, the third term describes the heating effect due to nonradiative recombination throughout the device, and the last two terms account for Thomson and Peltier heat. A more detailed explanation of these heat generation terms may be found in [77].

4.2 Simulation of a DBR Reflectivity Spectrum

The DBR reflectivity spectra have been calculated by the 1D- Transmission Matrix Method (TMM) with complex impedances. A detailed explanation of the reflectivity calculation for DBRs using this method can be found in [78] and will be briefly discussed in this section. The use of complex impedances allows us to account for absorption losses in the reflectivity calculation. Including the absorption losses is essential for modelling DBRs in which the bandgap of one or both layers is close to the photon energy, or when the layers are heavily doped and free carrier absorption is significant. Wavelength dispersion of the real and imaginary part of the refractive index has been considered ($\varepsilon(\lambda)$). The strain dependence of the refractive indices is an important consideration since the strain determines the position (in wavelength or energy space) of the excitonic resonance peaks in the dielectric function.

Figure 4 shows a schematic of an m-layer DBR. Layer m+1 is the incident medium (can be air or the cavity), and layer 0 is the substrate. The complex impedance of the $i^{th}$ layer ($Z_i$) can be calculated by equation 13:

$$Z_i = \frac{\mu_0}{\sqrt{\varepsilon_{i,\text{real}} + j \varepsilon_{i,\text{imag}}}}$$ (13)
where $\mu_0$ is the magnetic permeability, and $\varepsilon_{i,\text{real}}$ and $\varepsilon_{i,\text{imag}}$ are the real and imaginary parts of the electric permittivity of the $i^{\text{th}}$ layer of the DBR stack, respectively.

The total input impedance of the DBR is $Z_{\text{in},m}$, and $Z_{\text{inc}}$ is the impedance of the incident medium, which could be air or the AlGaN cavity. The reflectivity (%) is then calculated with equation 15:

$$R = \left( \frac{Z_{\text{in},m} - Z_{\text{inc}}}{Z_{\text{in},m} + Z_{\text{inc}}} \right)^2 \times 100$$  \hspace{1cm} (14)$$

This process is repeated over a range of wavelengths to get the reflectivity spectrum.
4.3 Material Parameters

4.3.1 Electrical and Gain Parameters

The majority carrier mobilities are taken from our experimental data, which closely match published data [8], [9], with $\mu_h = 11.25 \text{ cm}^2/(\text{V.s})$ in p- Al$_{0.12}$Ga$_{0.88}$N and $\mu_n = 338.5 \text{ cm}^2/(\text{V.s})$ in n- Al$_{0.12}$Ga$_{0.88}$N. The minority carrier mobilities and lifetimes are taken from [79]. The polarization charge at heterojunctions has been calculated according to [21], and adjusted to 50% of the full interfacial polarization charge to account for indium fluctuations in the quantum wells [80]. The band offset ratio $\Delta E_C:\Delta E_V$ used in these simulations is between 65:35 to 70:30 depending on the compositions of the materials used to form the heterojunctions [81].

The k-p band structure parameters can be found in [6]. The SRH recombination lifetime in the QWs emitting light at a center wavelength of 370 nm is $\tau_{\text{SRH}}=1.5 \text{ ns}$, which is lower than that for blue laser diodes, but is consistent with observations of reduced SRH lifetimes in quantum wells with reduced indium content [50], [51]. The Auger recombination coefficient reduces as the bandgap increases; accordingly, its impact is reduced for UV light emitters compared to visible light emitters. The Auger recombination coefficient used in these simulations is $10^{-32} \text{ cm}^6/\text{s}$, which is consistent with the values obtained from first principle calculations by Kioupakis et al. [82] and Bertazzi et al. [83] for the InGaN composition used in these simulations. Their calculations included indirect Auger processes caused by carrier-phonon scattering, and alloy disorder. The QWs in the blue laser diodes (wavelength of 415 nm) have an increased SRH lifetime of 10 ns, and an increased Auger recombination coefficient of $10^{-31} \text{ cm}^6/\text{s}$, which is consistent with the
references mentioned above. Blue QWs have different nonradiative recombination coefficients than QWs emitting light with a center wavelength of 370 nm due to increased indium content.

4.3.2 Thermal Conductivity

The thermal conductivity of Al\textsubscript{x}Ga\textsubscript{1-x}N alloys has been computed as per [84], and is 196 W/(K-m) for GaN. The thermal conductivity of AlInN lattice-matched to GaN is 4.87 W/(K-m) [85]. However, several studies suggest that the thermal conductivity of GaN depends on the growth conditions and defect concentrations, with values ranging from 130 W/(m-K) [86], [87] to 220 W/(m-K) [88], a range of over 40%! One of the most thorough studies of the thermal conductivity of GaN substrates as a function of dislocation density was reported in [89], where they found that the thermal conductivity remains at 230 W/(m-K) up to a dislocation density of 10\textsuperscript{6} cm\textsuperscript{-2}, and then logarithmically reduces to ~110 W/(m-K) at a dislocation density of 10\textsuperscript{10} cm\textsuperscript{-2}. Thus, the value of 196 W/(m-K) that we have picked for the thermal conductivity of GaN is reasonable.

4.3.3 Optical Parameters

The strain, wavelength and bandgap dependent real part of the refractive indices of AlInGaN alloys are calculated according to [90], while the doping, strain, wavelength and bandgap dependent imaginary part of the refractive indices are calculated according to a modified version of [13]. The modification to [13] was done to match the absorption losses of our own material, and to that of commercial substrate vendors.
CHAPTER 5. PRIMARY CHALLENGES INVOLVED IN THE DESIGN OF UV-A VCSELS

Chapter 2 described the problems associated with creating optoelectronics devices made of III-N materials, and this chapter will focus on device (UV-VCSEL) design challenges, which are intimately linked to material properties. Three primary challenges have been identified, and they are: (1) optical loss (primarily in p++ contact layer and if present, ITO, and the n-side DBR), (2) carrier leakage, and (3) high thermal resistance. The optical loss increases the operating current, which reduces the peak output optical power and the wall plug efficiency. Electron leakage reduces the injection efficiency, and high thermal resistance limits the peak output optical power by determining the current at which thermal rollover occurs (slope efficiency drops to zero). Each of these issues will be discussed in more detail in subsequent chapters.

5.1 How to Design a Better Laser Diode

Figure 5 shows a typical plot of the modal gain vs input current (current aperture is 8 μm). The details of the laser in Figure 5 is not important at this time, and the shape of the gain vs J curve is similar for all laser diodes. Note that d(gain)/dI keeps dropping as the operating current increases. This means that reducing the loss can lead to super-linear reductions in the threshold current. Furthermore, a lower threshold current means that the maximum optical output power increases before thermal rollover. Thus, reducing the loss would allow the threshold current to fall into region 1 in Figure 5, which is far preferable
to operating in region 2. This reduces self-heating (more gain) and electron leakage (better injection efficiency) due a greater energetic barrier height at low currents.

In the worst case, the optical loss can be the difference between obtaining a laser or a microcavity LED, and in the best case the laser’s performance degrades if the loss is high.

![Figure 5 – Modal gain (left axis, solid line) and temperature in the active region (right axis, dotted line) vs input current solid lines)](image)

**5.2 Reducing the Optical Loss**

In edge-emitting laser diodes, light propagates in the plane of the active region, thus enabling high round-trip gains. VCSELs, on the other hand, have a much smaller round-
trip gain due to the fact that the light propagates perpendicular to the active region, and hence only sees the gain region in 2-3% of the optical cavity. Therefore, VCSELs must have very high reflectivity mirrors (>99% reflectance) at the ends of the cavity and a low internal loss, while edge-emitting LDs can achieve lasing even with antireflective coatings on one end, or simple facet cleaves on either end which act as mirrors with 20-30% reflectivity.

This makes it crucial to minimize the mirror loss and absorption loss within the cavity in order to achieve RT CW lasing operation in VCSELs. Our prototypical VCSEL is shown in Table 1, with a DBR reflectivity of 99.8%, and we have identified the main sources of optical loss in Table 2.

Assuming 10 pairs of HfO$_2$/SiO$_2$ as the top and bottom DBRs, calculations suggest that about 40% of the loss can be attributed to the mirrors, while 50% of the total loss can be attributed to the p-contact layers (a 15 nm thick ITO current spreading layer and a 20 nm thick p++ AlGaN cap layer). Strategies to reduce the optical loss in the contact layers are discussed in Chapter 6, where a modulation-doped short-period superlattice has been proposed as a lateral hole current spreading layer instead of ITO for UV-VCSELs. Alternative strategies to obtain a high reflectivity bottom DBR is discussed in Chapter 7, where a hybrid epitaxial and metal mirror is proposed— an epitaxial DBR to provide a reflectivity of >90% and a planar metal mirror underneath provides the remaining 90% reflectivity.
Table 1 – Layers in a prototypical UV VCSEL.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top DBR</td>
<td>10x HfO$_2$/SiO$_2$</td>
<td>10x 42 / 63</td>
</tr>
<tr>
<td>Spacer</td>
<td>HfO$_2$</td>
<td>32</td>
</tr>
<tr>
<td>ITO</td>
<td>ITO</td>
<td>15</td>
</tr>
<tr>
<td>p++ AlGaN</td>
<td>Al$<em>{0.06}$Ga$</em>{0.94}$N</td>
<td>20</td>
</tr>
<tr>
<td>p-QNR</td>
<td>Al$<em>{0.12}$Ga$</em>{0.88}$N</td>
<td>114</td>
</tr>
<tr>
<td></td>
<td>Inverse Taper Al$<em>{0.2}$Ga$</em>{0.8}$N-</td>
<td></td>
</tr>
<tr>
<td>Taper</td>
<td>Al$<em>{0.12}$Ga$</em>{0.88}$N along c-axis</td>
<td>10</td>
</tr>
<tr>
<td>EBL</td>
<td>Al$<em>{0.2}$Ga$</em>{0.8}$N</td>
<td>5</td>
</tr>
<tr>
<td>MQW</td>
<td>6x Al$<em>{0.15}$Ga$</em>{0.88}$N /5x In$<em>{0.045}$Ga$</em>{0.955}$N</td>
<td>6/2.5</td>
</tr>
<tr>
<td>n-QNR</td>
<td>Al$<em>{0.12}$Ga$</em>{0.88}$N</td>
<td>291</td>
</tr>
<tr>
<td>Bottom DBR</td>
<td>10x HfO$_2$/SiO$_2$</td>
<td>10x 42 / 63</td>
</tr>
</tbody>
</table>
### Table 2 – Contributors to optical loss in a typical VCSEL

<table>
<thead>
<tr>
<th>Layer</th>
<th>Optical Loss (cm(^{-1}))</th>
<th>% of Total Loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>ITO</td>
<td>6.1</td>
<td>10.9</td>
</tr>
<tr>
<td>p++ AlGaN</td>
<td>21.3</td>
<td>38.2</td>
</tr>
<tr>
<td>p-AlGaN</td>
<td>5.9</td>
<td>10.6</td>
</tr>
<tr>
<td>Mirrors</td>
<td>22.5</td>
<td>40.3</td>
</tr>
</tbody>
</table>

#### 5.3 Dealing with Electron Leakage

Electron leakage reduces the injection efficiency of the laser and leads to poor thermal stability (high T\(_0\)). Vezellesi et al. demonstrated by numerical simulation that when p-type conductivity is lower than n-type conductivity, holes are not supplied to the active region at the same rate as electrons, causing electrons to leak out of the active region and recombine non-radiatively in the p-QNR and at the anode, resulting in efficiency droop in LEDs and reduced gain in LDs; however, by making the electron and hole conductivities equal, electron leakage was reduced and efficiency droop was suppressed [91].

We find that the optimum EBL design strongly depends on the device’s intended operating current density, and thus we find different optimum EBL designs for LEDs, edge-
emitting LDs and VCSELs. Chapter 8 takes a detailed look at design techniques to stem electron leakage, and suggests guidelines on optimum EBL design for a III-N light emitting device.

### 5.4 Thermal Resistance

The thermal resistance ultimately limits the maximum optical power output of a VCSEL due to self-heating under current injection. Self-heating degrades the performance for three reasons: (1) increased carrier leakage by thermionic emission, (2) reduction in the maximum gain due to gain-broadening by carrier-carrier and carrier-phonon scattering, and (3) increased non-radiative recombination effects. The simulations in this thesis only account for point (1), which is a good first-order approximation as that is the largest contributor to gain reduction at high temperatures [92], [93].

Chapter 9 compares the most common heatsinking techniques employed by various groups in academia and industry working on III-N VCSELs—ELOG VCSELs (Sony [37]), flip-chip double dielectric DBR VCSELs (Nichia [35]) and hybrid DBR VCSELs (Nagoya University [47]), and optimum designs are suggested based on self-consistent electro-opto-thermal simulations of VCSELs in each of these categories.
CHAPTER 6. HOLES CURRENT SPREADING LAYER AND P-CONTACT AND P-CAP LAYERS

The ITO is the p-contact layer and serves as a lateral hole current spreading layer. To achieve sufficient reflectivity (>99%) for a VCSEL, insulating dielectric DBRs must be deposited on the top (p-side). This necessitates a lateral current injection scheme for hole injection. To achieve efficient hole injection, a highly conductive current spreading layer is needed to pump the optical mode and minimize current crowding near the aperture. All III-N VCSELs reported to date use ITO as the p-contact layer.

Table 2 shows that the loss due to p++ cap layer is more than that in the ITO. The loss coefficient of ITO is higher than the p++ Al$_{0.06}$Ga$_{0.94}$N cap layer at $\lambda = 370$ nm but the ITO is better ‘hidden’ in the node of the optical mode, and hence has a lower contribution to the overall loss than the p++ AlGaN layer. The optical loss is calculated by weighing the layer’s absorption coefficient with its overlap with the optical mode.

6.1 Why is ITO unsuitable for UV-VCSELs?

6.1.1 High Loss Coefficient of ITO

GaN-based VCSELs and resonant cavity light emitting diodes (RCLEDs) traditionally use indium tin oxide (ITO) as the current spreading layer on the p-side [35], [37], [46], [47], [94], due to its high electrical conductivity and optical transparency in the visible spectrum. However, ITO is unsuitable in the UV spectrum due to extremely high optical absorption losses. The typical absorption coefficient at $\lambda=450$ nm is between 1300-2000 cm$^{-1}$, while it sharply increases to $\alpha = 5900-6800$ cm$^{-1}$ at $\lambda=370$ nm according to our own
measurements, which is consistent with more extensive published data shown in Figure 6 [55], [56].

Figure 6 – Absorption coefficient vs wavelength for an ITO film measured by Lai et al. [56] and Konig et al. [55].

6.1.2 Optical Loss is Extremely Sensitive to Thickness Fluctuations

The use of ITO in the VCSEL may be acceptable if it is placed perfectly at the node, but any thickness fluctuations during growth can shift the ITO out of the node of the standing wave profile. For the VCSEL shown in Table 3, the spacer and p-QNR thickness has been varied to simulate the effects of a 5 nm misalignment of the ITO. The excess p-QNR thickness is denoted as $\Delta_{\text{ITO}}$. The increase in the optical loss for $\Delta_{\text{ITO}} = 0, 5$ and 10 nm is tabulated in Table 4. The consequences of this increase in the loss can be the difference between lasing or not, as shown in Figure 7.
## Table 3 – Epitaxial structure of a VCSEL

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top DBR</td>
<td>10x HfO$_2$/SiO$_2$</td>
<td>10x 42 / 63</td>
</tr>
<tr>
<td>Spacer</td>
<td>HfO$_2$</td>
<td>34 / 29</td>
</tr>
<tr>
<td>ITO</td>
<td>ITO</td>
<td>12</td>
</tr>
<tr>
<td>p++ AlGaN</td>
<td>Al$<em>{0.06}$Ga$</em>{0.94}$N</td>
<td>20</td>
</tr>
<tr>
<td>p-QNR</td>
<td>Al$<em>{0.12}$Ga$</em>{0.88}$N</td>
<td>110 / 115</td>
</tr>
<tr>
<td>Taper</td>
<td>Inverse Taper Al$<em>{0.25}$Ga$</em>{0.75}$N-Al$<em>{0.12}$Ga$</em>{0.88}$N along c-axis</td>
<td>15</td>
</tr>
<tr>
<td>EBL</td>
<td>Al$<em>{0.25}$Ga$</em>{0.75}$N</td>
<td>5</td>
</tr>
<tr>
<td>MQW</td>
<td>6x Al$<em>{0.12}$Ga$</em>{0.88}$N/5x In$<em>{0.045}$Ga$</em>{0.955}$N</td>
<td>6/2.5</td>
</tr>
<tr>
<td>n-QNR</td>
<td>Al$<em>{0.12}$Ga$</em>{0.88}$N</td>
<td>291</td>
</tr>
<tr>
<td>Bottom DBR</td>
<td>30x Al$<em>{0.04}$Ga$</em>{0.96}$N/Al$<em>{0.3}$Ga$</em>{0.7}$N</td>
<td>30x 34.1 / 36.7</td>
</tr>
<tr>
<td>Silver</td>
<td>Silver</td>
<td>40 nm</td>
</tr>
</tbody>
</table>
Table 4 – Effect of thickness fluctuations on the modal loss due to ITO misalignment

<table>
<thead>
<tr>
<th>$\Delta_{\text{ITO}}$ (nm)</th>
<th>Modal Loss (cm$^{-1}$)</th>
<th>% increase in loss compared to $\Delta_{\text{ITO}} = 0$ nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>49</td>
<td>–</td>
</tr>
<tr>
<td>5</td>
<td>57</td>
<td>16.3%</td>
</tr>
<tr>
<td>10</td>
<td>79</td>
<td>61.2</td>
</tr>
</tbody>
</table>

Figure 7 – Optical power (solid line, left axis) and active region temperature (dotted line, right axis) vs input current for various heatsink temperatures and $\Delta_{\text{ITO}}$. 
6.2 Optical Loss in p++ Contact Layer

Among epitaxial material in the optical cavity, the p++ cap layer is the most optically lossy. This thin layer must have degenerate doping to facilitate the formation of an ohmic p-contact to ITO. As discussed in section 2.4, the optical loss increases with doping concentration and reducing bandgap. For an assumed Mg concentration of $10^{20}$ cm$^{-3}$, the optical absorption coefficient and difference between the bandgap and photon energy is plotted in Figure 8.

![Absorption coefficient and difference between the bandgap and photon energy (λ = 370 nm) for AlGaN alloys used as p++ cap layer.](image)

The right axis of Figure 8 helps understand another reason why visible VCSELs have been achieved, but not UV VCSELs. In visible VCSELs, GaN is used as the material for
the QNR, and this is lattice matched to the substrate. At $\lambda = 420$ nm, GaN’s band-edge is 0.44 eV above the photon energy. To get the same difference at $\lambda = 370$ nm, we require Al$_{0.2}$Ga$_{0.8}$N, which is highly tensile strained when grown on GaN and is hence susceptible to cracking. Hence, we must use lossier material for the p-cap layer and the QNRs in UV-VCSELs compared to what is used in visible VCSELs.

6.3 Modulation-Doped Short-Period Superlattices

6.3.1 Introduction

To avoid the high optical losses in UV VCSELs caused by ITO, a modulation doped short-period superlattice (MD-SPSL) has been proposed. This allows the p++ AlGaN cap layer to occupy the node of the optical mode (which was previously occupied by the ITO), and makes the modal loss less sensitive to thickness fluctuations. An MD-SPSL has two advantages: (1) holes in the unintentionally doped (uid) narrow bandgap material suffer less ionized impurity scattering, and (2) absorption loss in the narrow bandgap material is reduced due to lower acceptor concentrations. The p-doped material has a wider bandgap, thus minimizing the absorption loss (compared to p-doping the narrow bandgap material).

This technique of using MD-SPSLs has been used before to improve the conductivity [95]–[97] by increasing hole mobilities (in the uid-layer) by a factor of three to six, and the improvements in the lateral conductivity has been studied theoretically in [98]. Modulation doped p-GaN/uid GaN has been studied both experimentally and theoretically in [99], where an improvement in the conductivity by a factor of 40 has been observed for the modulation doped nanostructure, compared to a uniformly doped p-GaN layer. This work is discussed in more detail in [100], and it shall be reviewed in this section.
The cross-section view of the VCSEL is shown in Figure 9. The current-confinement aperture is assumed to be created by nitrogen implantation, and has a diameter of 8 µm, and is 125 nm thick. Other groups have used boron [101] or aluminum implantation [102] to create a current aperture.

The MQW consists of 3 pairs of In$_{0.045}$Ga$_{0.955}$N QWs and Al$_{0.12}$Ga$_{0.88}$N QBs. Image from [100].

The free hole concentrations in the p-Al$_{0.12}$Ga$_{0.88}$N quasi-neutral region (QNR) and the electron blocking layer (EBL) is approximately 5.4x10$^{17}$ cm$^{-3}$. The mobility of p-doped Al$_{0.12}$Ga$_{0.88}$N and Al$_{0.08}$Ga$_{0.92}$N is 12 cm$^2$/V·s and 13 cm$^2$/V·s) respectively. Unintentionally doped (uid) Al$_{0.08}$Ga$_{0.92}$N has a hole mobility of 40-300 cm$^2$/V·s), with the wide range of hole mobilities in the uid- layer accounting for mobility degradation due to imperfect modulation doping. The n- Al$_{0.12}$Ga$_{0.88}$N QNR has a free electron
concentration of $1.8 \times 10^{18}$ cm$^{-3}$ (Si concentration of $3 \times 10^{18}$ cm$^{-3}$). The electron mobility in n-Al$_{0.12}$Ga$_{0.88}$N is 330 cm$^2$/V·s. These majority carrier mobilities and free carrier concentrations have been derived from Hall measurements of the material grown by our group. The minority carrier diffusion lengths as a function of doping concentration and type (Mg or Si) are taken from [79].

6.3.2 Types of Hole Current Spreading Layers

Three different types of AlGaN current spreading layers (CSLs) are shown in Figure 9. For comparison, the L-I-V characteristics of a reference VCSEL with 20 nm thick ITO has also been shown in Figure 10. 20 nm is the thinnest ITO contact layer reported to date [47], and hence this ITO thickness is used in the reference VCSEL.

Structure A is a modulation doped SPSL (MD-SPSL) and it consists of 25 pairs of Mg-doped Al$_{0.16}$Ga$_{0.84}$N (2.5 nm) and uid- Al$_{0.08}$Ga$_{0.92}$N (1.5 nm). 25 pairs of this SL add up to a total thickness of 100 nm for the current spreading layer. In this section, the mobility of the uid-AlGaN layer has been assumed to be 60 and 200 cm$^2$/V·s. The effect of varying the uid- Al$_{0.08}$Ga$_{0.92}$N layer’s mobility between 13-350 cm$^2$/V·s) will be described in the next section. Structure B is identical to structure A, except that even the 1.5 nm thick Al$_{0.08}$Ga$_{0.92}$N is Mg-doped and is hence a uniformly doped SPSL (p-SPSL). The optical absorption coefficient and carrier mobilities in the Al$_{0.08}$Ga$_{0.92}$N layers have been adjusted to reflect the change in the Mg concentration. Structure C employs 100 nm of bulk p-Al$_{0.12}$Ga$_{0.88}$N.
Figure 10 – Simulated optical power (solid lines) and voltage (dotted lines) vs current for laser diodes with different current spreading layers: MD-SPSL (red circles), uniformly doped p-SPSL (green squares), bulk AlGaN (blue triangles) and 20 nm thick ITO (magenta stars). Image from [100].

Figure 10 shows the corresponding L-I-V characteristics of VCSELs with different CSLs. Figure 11 is a plot of the vertical component of the hole current density vector in the p-QNR just before the EBL, at an input current of 3 mA. The current is primarily vertical in the p-QNR ($J_z > J_{radial}$) since p-AlGaN is approximately 70-80 times more resistive than n-AlGaN. Thus, $J_z$ in the p-QNR is essentially the hole current being injected into the active region. Figure 11 also shows the transverse mode pattern for the TE$_{01}$ superimposed on $J_z$ to illustrate the overlap between the optical mode and the current density. The greater the overlap, the lower the threshold current required to achieve lasing. Note that all the CSLs only pump the edge of the optical mode. Various optical modes were computed
(HE11, EH11, HE21, EH12, TE01 and TM01), and we found that the TE01 mode lased first.

Figure 11 – Vertical component of the hole current density vector (left axis) for different CSLs in the p- Al_{0.12}Ga_{0.88}N QNR near the EBL at an input current of 3 mA, and the radial profile of the TE01 mode (right axis). Image from [100].

Structure A has the lowest threshold current since it has minimum current crowding at the aperture (among the AlGaN CSLs) and lower optical losses than ITO, due to which the optical mode is pumped more efficiently. ITO has the best lateral current spreading, but still shows a high threshold current due to the high optical loss. Structure B (p-SPSL) has the poorest performance among AlGaN-based CSLs. We believe this is because Structure B has higher optical losses than Structure C due to Mg-doped Al_{0.08}Ga_{0.92}N,
which is optically lossier than Mg-doped Al$_{0.12}$Ga$_{0.88}$N. Also, the doped SPSL adds a series resistance at each heterointerface, while not significantly improving lateral current spreading (compared to bulk AlGaN), as evidenced by the I-V curves in Figure 10, since the mobility is degraded in both the low and high bandgap materials due to Mg-impurity scattering. Current across a heterojunction is limited by thermionic emission, which is not the case for bulk material.

![Graph showing hole density and bandgap](image)

**Figure 12 – Free hole carrier densities in the CSLs for an MD-SPSL (red crosses) and a uniformly doped p-SPSL (green squares). Image from [100].**

Figure 12 shows the hole concentrations in the uid-narrow bandgap material due to modulation doping in the p-SPSL and MD-SPSL. As expected, the hole concentration is greater for the uniformly doped p-SPSL by an amount equal to the activated acceptor concentration, but the degradation in mobility has a far bigger impact than the increase in the hole concentration- the vertical mobility reduces by a factor of 15, while the hole
concentration only increases by a factor of 1.3 for a uniformly doped SPSL compared to the MD-SPSL.

6.3.3 Sensitivity to the mobility of the uid narrow bandgap layers in the SPSL

Due to the Mg memory effect [103], [104] perfect modulation doping with sharp doping profiles is extremely challenging to realize with MOCVD. Thus, there will be residual Mg doping in the Al$_{0.08}$Ga$_{0.92}$N layer, leading to an increase in impurity scattering, causing mobility degradation. Remote ionized impurity scattering, alloy disorder and residual impurities are other mechanisms leading to mobility degradation in the Al$_{0.08}$Ga$_{0.92}$N layer. The relative contributions of these scattering mechanisms at low temperatures have been discussed in [105].

Previous attempts at p-type modulation doped superlattices unambiguously show an improvement in conductivity (3 to 6 times higher conductivity) over uniformly doped superlattices [95]–[97]. The biggest improvement in conductivity (40 times higher conductivity than bulk p-GaN) has been observed for a modulation doped structure with alternating layers of p-GaN/uid-GaN, in which the authors achieved mobilities of ~180 cm$^2/(V\cdot s)$ in the uid-layer [99]. The effect of mobility degradation on the threshold current and radial current spreading has been studied in this section. Intrinsic Al$_{0.08}$Ga$_{0.92}$N in the previous section had a hole mobility of 200 cm$^2/(V\cdot s)$ while p- Al$_{0.08}$Ga$_{0.92}$N had a hole mobility of 13 cm$^2/(V\cdot s)$. To account for mobility degradation due to the aforementioned scattering mechanisms, the hole mobility in the uid- narrow bandgap layer of the MD-SPSL has been varied between 13-300 cm$^2/(V\cdot s)$, and its effect on the threshold current and slope efficiency is shown in Figure 13.
Figure 13 – Threshold current and slope efficiencies of VCSELs with MD-SPSLs having different hole mobilities in the narrow bandgap uid- Al_{0.08}Ga_{0.92}N layer.

Image from [100].

Thus, even if the hole mobility in the uid-layer of the MD-SPSL is 60 cm²/(V·s)- a value that has been experimentally demonstrated [96], [99], leads to a 31% reduction in the threshold current, and an 82% increase in the slope efficiency compared to a bulk AlGaN CSL, and a 31% lower threshold current, and 170% improvement in the slope efficiency compared to the reference VCSEL with 20 nm of ITO.

6.3.4 How to Grow MD-SPSLs?

Modulation-doped SPSLs must be re-grown on top of the N-implanted aperture. MD-SPSLs are extremely challenging to grow by MOCVD due to the Mg memory effect [103], [104] and greater diffusion coefficients for magnesium in MOCVD-grown material
due to higher growth temperatures. This precludes us from obtaining the sharp doping profiles needed for modulation doping by MOCVD. However, molecular beam epitaxy (MBE) does not suffer from the memory effect. Also, crystal growth temperatures for MBE are $200^\circ\text{-}300^\circ\text{C}$ lower than MOCVD, thus reducing the diffusion of magnesium into the narrow bandgap layer. Magnesium has a higher diffusion coefficient at $\sim1000^\circ\text{C}$ (typical MOCVD growth temperatures), and it reduces by over an order of magnitude for a growth temperature of $700^\circ\text{-}800^\circ\text{C}$ (typical MBE growth temperature) \cite{106}–\cite{108}. High-quality MBE re-growths at lower temperatures have been demonstrated in laser diodes- Malinverni \textit{et al.} regrew a thick p-(Al)GaN layer with MBE on top of an MOCVD grown active region and n-(Al)GaN layers \cite{109}, \cite{110}, and obtained sharp magnesium doping profiles, as determined by SIMS measurements \cite{109}. In \cite{111}, a complete blue LD has been grown by MBE, with a threshold current density which is comparable to MOCVD-grown LDs. This shows that the higher point defect density in low-temperature growth by MBE is not catastrophic to lasing in terms of optical losses and material quality. The p-QNR and regrown CSL layers are not depleted, so additional non-radiative recombination centers due to the higher point defect density is not as deleterious as it would have been were it in the active region.

Hence, a promising approach is that the n- and p-QNRs, the EBL and the active region of the VCSEL can be grown by MOCVD. The 100 nm thick MD-SPSL could then be regrown by MBE after the current aperture definition by ion implantation.
6.3.5 Summary

In summary, MD-SPSLs can help create efficient UV-VCSELs and UV-RCLEDs, where ITO cannot be used due to its high absorption loss in the UV spectrum. Modulation doping helps create highly conductive channels for lateral hole currents, which allows the optical mode to be more efficiently pumped by reducing current crowding near the aperture edge. Some passages and figures in section 6.3 have been reproduced from [100].

Thus, the use of MD-SPSLs allows us to avoid all the drawbacks associated with ITO, which were discussed in section 6.1.
CHAPTER 7. BOTTOM (N-SIDE) MIRROR

As shown in Table 2, the bottom mirror loss is a dominant contributor to the overall optical loss, and the sensitivity of the total modal loss to the mirror reflectivity is further emphasized in Figure 14. The top mirror is assumed to be 10 pairs of λ/4-thick HfO$_2$ and SiO$_2$ with a reflectivity of 99.93%.

![Graph showing the total modal loss for the VCSEL as a function of the bottom mirror reflectivity.](image)

**Figure 14 – Total modal loss ($\alpha_i + \alpha_m$) for the VCSEL as a function of the bottom mirror reflectivity.**

Thus, the total loss almost doubles if the bottom mirror reflectivity drops from 100% to 99.5%. Realizing a suitable bottom mirror has been the most challenging part of this project. In this chapter, techniques to obtain suitable dielectric bottom DBRs and
epitaxial DBRs will be discussed, with the final section describing a novel epitaxial DBR/metal mirror. This novel mirror mitigates the primary drawbacks of both the previously mentioned techniques—cavity length control for a bottom dielectric DBR and the low reflectivity of epitaxial DBRs. Several paragraphs and figures in this chapter have been copied from [112].

7.1 Dielectric Bottom DBR

Dielectric DBRs have very high reflectivities due to the large index contrast between the deposited oxides. An oxide deposition is also easier and faster than an epitaxial growth. p-material is usually grown last to ensure high material quality in the active region. Thus, n-material is grown first, followed by the active region and then finally the p-material. The p-side mirror is always a high reflectivity dielectric DBR stack of Ta$_2$O$_5$/SiO$_2$ [113] or Nb$_2$O$_5$/SiO$_2$ [33], [37], [47] or ZrO$_2$/SiO$_2$ [94] for blue VCSELs and HfO$_2$/SiO$_2$ [114], [115] for UV light emitters. There have been two main approaches to obtaining high reflectivity bottom mirrors: epitaxial AlInGaN DBRs and dielectric DBRs.

We were able to achieve a reflectance greater than 99.95% for the p-side dielectric DBR at $\lambda = 370$ nm. This DBR comprised of 10 pairs quarter-wavelength layers of HfO$_2$ and SiO$_2$. The reflectivity spectrum is shown in Figure 15.
VCSELs grown on GaN substrates with a dielectric DBR on the bottom can be realized primarily by two methods: substrate thinning by chemical mechanical polishing (CMP) [34]–[36], [116], [117] or by epitaxial lateral overgrowth (ELOG) [37], [38]. After bonding the VCSEL to a Si support substrate, CMP can be used to thin the substrate, followed by a dielectric DBR deposition. The primary disadvantages of this method are the difficulty in precisely controlling the cavity length since polishing lacks the precision of epitaxy by MOCVD or MBE, and the necessity of obtaining a smooth surface after polishing in order to minimize scattering losses at the cavity and dielectric DBR interface.

The ELOG method has been effectively used by Sony to obtain milliwatt class blue VCSELs [37], [38]. In this process, the SiO$_2$/Si$_N$$_x$ bottom dielectric DBR stack is
embedded in n-GaN grown by ELOG [118]. This method allows more precise cavity length control than that obtained by CMP, thus increasing the yield. The advantages of using double dielectric DBRs over hybrid DBRs include higher reflectivity and wider stopbands obtained due to the increased refractive index contrast between the two dielectric materials. This leads to lower threshold currents (due to higher reflectivity), and the wider stopband improves the VCSEL’s robustness against fluctuations in material composition and thickness by ensuring that the lasing wavelength is always within the DBR’s stopband, while simultaneously extending the VCSEL’s operating temperature range.

However, we were unable to precisely control the back-side etching or polishing process, which made the cavity resonance wavelength uncontrollable.

ELOG is easier to realize with GaN than with AlGaN due to a reduced lateral growth rate for AlGaN and because the AlGaN polycrystals tend to stick to the dielectric masks [39]. Since GaN is absorbing in the UV-A spectrum, we had to try ELOG with AlGaN and we were unsuccessful. For these reasons, we wanted to find suitable alternatives to a dielectric DBR on the n-side.

7.2 Epitaxial Bottom DBR

A DBR consists of alternating layers of high and low refractive index materials that are each quarter-wavelength thick. Higher reflectivity can be obtained by using more pairs and/or by increasing the refractive index contrast between the two materials. Increasing the number of GaN/AlGaN mirror pairs increases the strain and the likelihood of the wafer cracking as the DBR stack’s thickness approaches the critical thickness of AlGaN on GaN. Increasing the refractive index contrast involves further reducing the low index material’s
refractive index which can be accomplished by increasing the aluminum mole fraction in the AlGaN or AlInN alloy. However, this leads to a reduction in the critical thickness (if grown on GaN) and hence approaches the limit of cracking with fewer pairs.

However, we can use certain techniques to increase the refractive index contrast between the alternating high and low index materials. We can utilize excitonic resonances to increase the refractive index (section 7.2.1) and use heavy doping to reduce the refractive index (section 7.2.2) of the AlGaN alloy. These techniques increase the refractive index contrast without increasing the tensile strain. The use of epitaxial DBRs allows precise cavity length control and it reduces the complexity of the fabrication process by eliminating the laser-liftoff and/or polishing steps. This can potentially greatly improve the yield compared to alternate methods.

7.2.1 Exploiting near band edge excitonic resonances to enhance the refractive index

$\text{Al}_x\text{Ga}_{1-x}\text{N}$ ternary semiconductors have a direct bandgap over the entire alloy composition range, and thus exhibit pronounced absorption in the vicinity of the bandgap, which leads to a sharp increase in the real and imaginary parts of the refractive index near the band edge, as shown in Figure 16 (a,b). Near band edge excitonic resonances influence the real part of AlGaN’s dielectric function, and this can be exploited to sharply increase the high index material’s refractive index, enabling higher reflectivities (by increasing the refractive index contrast) through judicious choice of the DBR materials. Depending on the desired center wavelength, the aluminum composition of the high refractive index material is chosen to find the optimum trade-off between increasing the refractive index contrast and increased absorption loss, which allows us to maximize the DBR’s reflectivity.
Figure 16 – Real (left axis, solid lines) and imaginary (right axis, dotted lines) parts of the refractive indices of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ for: (a) $0 \leq x \leq 0.3$ on GaN and (b) $0.7 \leq x \leq 1$ on AlN. The refractive index contrast between (c) $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ($0 \leq x \leq 0.3$) and GaN, and (d) $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ($0.7 \leq x \leq 1$) and AlN [112].

Using numerical simulation, we have investigated the trade-off between increased refractive index contrast and increased absorption losses as the photon energy approaches
the bandgap, along with its impact on peak reflectivity and stopband width, for both UV-C and UV-A DBRs, as shown in Figure 17.

Three DBRs have been grown by our group, so our simulations in this section will be restricted to these DBRs: (1) 40-pair GaN/Al$_{0.12}$Ga$_{0.88}$N DBR with a peak reflectivity at 368 nm (DBR A), (2) 45-pair Al$_{0.04}$Ga$_{0.96}$N/ Al$_{0.3}$Ga$_{0.7}$N DBR with a peak reflectivity at 368 nm (DBR B), and (3) 30-pair AlN/ Al$_{0.865}$Ga$_{0.135}$N DBR with a peak reflectivity at 226 nm (DBR C). In Figure 17, the dotted lines show the experimental data, with the solid lines representing simulation results. As shown in Figure 17, as the center wavelength shifts to shorter and longer wavelengths than designed, the peak reflectivity reduces. The reflectivity on the short wavelength side reduces due to increased absorption loss in the narrow bandgap material, and the reflectivity reduces on the longer wavelength side due to reduced refractive index contrast, as indicated by Figure 17 (c, d).

As clearly seen in Figure 17, the DBRs at wavelengths of 368 nm and 226 nm are grown with the optimum materials to take maximum advantage of the increased refractive index contrast created by the excitonic resonance. Details regarding the growth conditions and growth techniques of DBRs A, B, and C can be found in [119]–[121], respectively. Shifting the center wavelength from 368 nm to 390 nm (redshift of 190 meV) led to a 14.9% and 2.5% drop in the reflectivity of DBR A and DBR B, respectively, as seen in Figure 17 (a, b). A similar drop in the reflectivity is also seen in the deep-UV DBR C in Figure 17 (c). The simulated reflectivity spectra assume that the incident medium is air, since that is the incident medium in our experimental apparatus.
Figure 17 – Simulated (solid lines) and experimental (dotted lines) reflectivity spectra of: (a) DBR A (experimental data from [119]), (b) DBR B (experimental data from [120]), and (c) DBR C (experimental data from [121]). Image from [112].
The index contrast can also be increased by reducing the refractive index of the low index layer through heavy n-type doping (5x10^{19} – 10^{20} cm^{-3}). This technique was first used in III-nitride laser diodes by Perlin et al. who used the reduction in the refractive index due to n++ doping to reduce the leakage of the optical mode into the substrate in an edge-emitting blue laser diode [122]. Growing a thick AlGaN cladding layer on GaN forms cracks due to the high tensile strain which degrades the quality of the active region and reduces the device’s lifetime. Hence this second cladding layer of plasmonic GaN (2% index contrast for n++ GaN compared to n-GaN) underneath a relatively thin 0.6 µm n-Al_{0.08}Ga_{0.92}N cladding layer allowed them to grow high quality material while also improving the optical confinement, due to which they could achieve a 54% reduction in the threshold current density.

Heavy doping affects the dielectric function, and hence the refractive index, by modifying the plasmonic frequency through free carrier concentration. The modified dielectric constant is given by equations 15 and 16:

\[ \varepsilon(\omega) = \varepsilon_\infty \left(1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}\right) \]  

(15)

\[ \omega_p^2 = \frac{ne^2}{\varepsilon_\infty \varepsilon_0 m^*} \]  

(16)

where \( \varepsilon_\infty \) is the dielectric constant, \( \omega_p \) is the plasma frequency, \( \gamma \) is the electron damping constant, \( e \) is the electronic charge, \( n \) is the carrier concentration, and \( m^* \) is the free carrier effective mass. Further details regarding GaN’s plasmonic frequency as a function of the
doping concentration can be found in [123], and a similar reduction in the refractive index for heavily doped indium phosphide has also been reported [124]. Another reason for the reduction in heavily doped GaN’s refractive index is due to band filling (Burstein-Moss effect) [125], [126].

To model DBRs incorporating n++ AlGaN, we have calibrated our model with our own experimental data, as shown in Figure 18, and we have obtained values that are within the range of those reported in [122]. Heavy doping also increases the free carrier absorption loss, so we have modified the loss coefficients used in our simulations as per [127], based on the difference between the bandgap of AlGaN and the photon energy. As per our experimental data shown in Figure 18 (a,b), we obtained a refractive index contrast of 2% at $\lambda=370$ nm between moderately doped $\text{Al}_{0.05}\text{Ga}_{0.95}\text{N}$ and n++ $\text{Al}_{0.05}\text{Ga}_{0.95}\text{N}$ with $N_{D,n^{++}} = 1 \times 10^{20}$ cm$^{-3}$, and a contrast of 1.5% for $N_{D,n^{++}} = 2 \times 10^{19}$ cm$^{-3}$, which explains why the DBR with higher doping in the n++ layer exhibits a higher peak reflectivity. This is within the range of index contrast obtained in [122]. Figure 18 (a, b) shows an increase in the reflectivity at 368-375 nm for n- $\text{Al}_{0.05}\text{Ga}_{0.95}\text{N} / \text{n}^{++} \text{Al}_{0.05}\text{Ga}_{0.95}\text{N}$ as the doping concentration increases.

Figure 18 shows the reflectance spectrum of a 40-pair DBR of $\text{Al}_{0.02}\text{Ga}_{0.98}\text{N} / \text{n}^{++} \text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$, which should theoretically have a peak reflectivity of 98.4%, assuming perfect interfaces, and no fluctuations in layer thicknesses or alloy compositions. However, the dotted lines show the experimental reflectivity spectrum, with a peak reflectivity of 94.5% at a wavelength of 369 nm.
Figure 18 – Simulated (solid lines) and experimental (dotted lines) reflectivity spectra of: (a) 20 x Al$_{0.05}$Ga$_{0.95}$N/n++Al$_{0.05}$Ga$_{0.95}$N with N$_{D,n^{++}}$=2x10$^{19}$ cm$^{-3}$, (b) N$_{D,n^{++}}$=10$^{20}$ cm$^{-3}$, (c) 40 x Al$_{0.02}$Ga$_{0.98}$N/n++Al$_{0.15}$Ga$_{0.85}$N, and (d) comparison of 40 x Al$_{0.02}$Ga$_{0.98}$N/Al$_{0.15}$Ga$_{0.85}$N DBRs with and without n++doping in the Al$_{0.15}$Ga$_{0.85}$N layers [112].
The photon energy associated with a wavelength of 369 nm is further from the band-edge of Al$_{0.15}$Ga$_{0.85}$N than for Al$_{0.05}$Ga$_{0.95}$N, and thus we find the contrast between n++ and unintentionally doped (uid) Al$_{0.15}$Ga$_{0.85}$N to be 1.5% rather than 2%, as seen for Al$_{0.05}$Ga$_{0.95}$N. The reduced index contrast obtained by heavy doping as the photon energy shifts away from the bandgap of AlGaN is consistent with experimental results obtained by Perlin et al. [122].

Figure 18 (d) compares the reflectivity spectrum of 40-pairs of Al$_{0.02}$Ga$_{0.98}$N/Al$_{0.15}$Ga$_{0.85}$N, both with and without heavy doping in the wider bandgap material. Heavily doping the Al$_{0.15}$Ga$_{0.85}$N layer increases the reflectivity from 97.3% (uid- Al$_{0.15}$Ga$_{0.85}$N) to 98.4%. A 1.1% improvement in the reflectivity is very significant for VCSELs, and it leads to a 41% reduction in the optical loss through the mirror (assuming the other mirror to be perfectly reflective)! The improved index contrast also slightly increases the width of the reflectivity spectrum’s stopband.

7.3 Use of Metal Mirrors

Metals exhibit very low indices of refraction (n<0.1) in a certain range of wavelengths, where the real part of the dielectric function is negative [128], [129]. The complex refractive index of silver is shown in Figure 19 (a). In the UV-A to infrared portion of the spectrum the reflectivity at the AlGaN/Ag interface exceeds 90%. For the UV-C to UV-A portion of the spectrum (180-350 nm), aluminum is preferable to silver. The choice of metal depends on the wavelength of interest, but for the rest of this paper we will use silver as an example. For wavelengths shorter than 360 nm, silver can be replaced by
aluminum. The reflectivity for light incident normal to this interface can be calculated through the Fresnel reflection coefficient and is approximately given by:

\[
R_0 = \frac{(n_{AlGaN} - n_{Ag})^2 + k_{Ag}^2}{(n_{AlGaN} - n_{Ag})^2 + k_{Ag}^2}
\]

(17)

Figure 19 – (a) Real (left axis, solid lines) and imaginary (right axis, dotted lines) parts of the refractive indices of silver as per Babar and Weaver [128] and McPeak et al. [129], and (b) measured reflectance as a function of rms roughness at a wavelength of 450 nm, reproduced from [130]. Image from [112].
At λ=370nm, as per [128], [129], \( n_{\text{Ag}} = 0.56 - 0.69 \), \( k_{\text{Ag}} = 1.72 \) and for \( \text{Al}_{0.1}\text{Ga}_{0.9}\text{N} \), \( n_{\text{AlGaN}} = 2.6 \), yielding a reflection coefficient of \( \sim 94\% \) at the AlGaN/Ag interface for normally incident light on a perfectly smooth interface. PARC has used this concept in edge-emitting laser diodes [131], [132] to replace the p-AlGaN cladding layer with silver. This greatly relieves the tensile strain compared to conventional thick AlGaN claddings, improves the confinement factor, and reduces the series resistance associated with thick poorly conducting p-AlGaN layers.

A rough metal surface will cause additional optical losses due to diffraction and increased absorption due to the excitation of surface-plasmon-polaritons (SPPs) [130]. The reduction in the reflection coefficient due to a rough sapphire/metal (silver and aluminum) interface has been shown experimentally and by 3D Finite-Difference Time-Domain (FDTD) at a wavelength of 450 nm in [130], for rms roughness values of 1, 7 and 13 nm. The experimental results have been reproduced in Figure 19 (b). The data shows that photons with a wavelength of 450 nm excite more SPPs in silver than in aluminum. We don’t expect the results at a \( \lambda = 370 \) nm to be radically different, since the real part of the dielectric function of silver and aluminum is negative at both wavelengths- 450 nm and 370 nm.

### 7.4 Epitaxial/Metal Hybrid Mirror

As seen in section 7.2, we cannot achieve a high enough reflectivity for a VCSEL using only epitaxial DBRs due to the low refractive index contrast and high tensile strain. But we have been able to demonstrate a DBR whose reflectivity exceeds >94%. Thus, situating a
planar silver mirror underneath the epitaxial DBR stack will yield a mirror that has an overall reflectivity that exceeds 99%. We call this a hybrid epitaxial/metal mirror [112].

In the best-case scenario (where absorption loss in the DBR is minimal), the number of pairs needed to achieve a reflectance of 99% is roughly twice the number of pairs required to obtain 90% reflectance. For example, if a 25 pair DBR is needed to obtain a reflectivity of 90%, then 50 pairs would be needed to obtain 99%. Most of the DBRs mentioned in section 1 consist of over 40 pairs. The reflectivity at an AlGaN/Ag interface is approximately 94% at 370 nm, which is clearly insufficient for a VCSEL. However, if we deposit an Ag film underneath an epitaxial DBR stack with a reflectivity of 90%, we can obtain a reflectivity exceeding 99%. This is because the DBR stack reflects 90% of the light, so now the Ag mirror only absorbs less than 1% of the total incident radiation. A similar concept has been used for GaAs based VCSELs in the past [133], [134]. AlAs and GaAs are almost lattice matched and have a high refractive index contrast, due to which obtaining a crack-free conducting epitaxial DBR with a reflectivity exceeding 99% is far less challenging for the III-As material system than for the III-N material system. Thus, this hybrid semiconductor/metal DBR is more important for III-nitride VCSELs.

Figure 20 shows a comparison of the reflectivity spectra of a 55-pair \( \text{Al}_{0.02}\text{Ga}_{0.98}\text{N}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{N} \) DBR on top of a GaN substrate and a 25-pair \( \text{Al}_{0.02}\text{Ga}_{0.98}\text{N}/\text{Al}_{0.2}\text{Ga}_{0.8}\text{N} \) DBR with silver underneath it. These simulations assume the incident medium to be \( \text{Al}_{0.1}\text{Ga}_{0.9}\text{N} \). Note how they have the same peak reflectivity, but the silver-backed epitaxial mirror has a wider stopband and 30 fewer pairs, due to which it is \( \sim 2\mu\text{m} \) thinner.
Figure 20 – Simulated reflectivity spectra of a 55 x Al\textsubscript{0.02}Ga\textsubscript{0.98}N/n++Al\textsubscript{0.2}Ga\textsubscript{0.8}N DBR with GaN underneath it (black), and a 25 x Al\textsubscript{0.02}Ga\textsubscript{0.98}N/n++Al\textsubscript{0.2}Ga\textsubscript{0.8}N DBR with silver underneath it (red). The inset shows a zoomed in image of the peak of the reflectivity spectra. The incident medium is Al\textsubscript{0.1}Ga\textsubscript{0.9}N. Image from [112].

By using this technique, the epitaxial stack can be made thinner (since only a reflectance of 90% is required) which reduces the crack density and hence improves the material quality. This leads to lower thermal resistance, and mitigates the deleterious effects of self-heating, while simultaneously increasing the stopband width, thus making the VCSEL more robust against temperature and layer thickness fluctuations. Like VCSELs with double dielectric DBRs, this method still requires complicated etching, polishing and lapping steps, but this semiconductor-metal hybrid DBR has one major
advantage over a dielectric DBR stack - the cavity length is independent of the polishing precision. One of the biggest drawbacks of VCSELs with double dielectric DBRs is the low yield since the cavity length must be an exact multiple of $\lambda/2$ to achieve lasing action at the wavelength that the quantum wells are optimized for.

Figure 21 – (a) Schematic of hybrid semiconductor/Ag DBR. (b) Simulated reflectivity spectra of 25 x Al$_{0.02}$Ga$_{0.98}$N/n++Al$_{0.2}$Ga$_{0.8}$N DBR with Ag underneath the DBR, with $t= 3 \, \mu m$ (black), $t= 1 \, \mu m$ (red), $t= 0 \, \mu m$ (green), and $t= -0.427 \, \mu m$ (blue). Image from [112].
However, with the hybrid semiconductor/metal DBR, the precisely controllable epitaxial DBR sets the cavity length, rather than the polishing precision. We believe that this would increase the VCSEL yield. This hybrid mirror is schematically shown in Figure 21 (a). As shown in Figure 21 (b), even leaving some of the substrate (positive ‘t’) or removing a part of the DBR (negative ‘t’) does not strongly impact the peak reflectivity. A reduction in the DBR thickness by $t = -0.427 \, \mu m$ corresponds to a reduction of 6 pairs, leaving only 19 pairs instead of 25 pairs, which leads to a reduction in the reflectivity from 99.25% to 99%. Leaving more than a micrometer ($7\lambda$) of the substrate/template between the epitaxial DBR and the Ag film (positive ‘t’) leads to a reduction in the stopband width, due to the formation of a second cavity between silver and the epitaxial DBR, which causes the transmission peaks seen in Figure 21 (b). A negative ‘t’ causes a reduction in the reflectivity, and the extent of the reduction depends on how many pairs of the epitaxial DBR are removed. Thickness control by CMP is on the order of a few hundred nanometers at best [135], but more accurate methods exist, such as a conductivity selective electrochemical etch, which can remove a highly doped GaN substrate but leave behind the undoped AlGaN DBR [136], or a bandgap selective photoelectrochemical (PEC) etch, in which the AlGaN DBR stack is grown on InGaN on a GaN substrate [137], [138]. The PEC etch removes the InGaN layer and would thus detach the cavity from the substrate. These methods can work for devices grown on FS-GaN, but if sapphire is used, then laser-liftoff followed by CMP is another reliable method to achieve better control over the thickness of the removed material [33], [139].
7.5 Summary

In summary, we have presented a strategy to obtain a high reflectivity bottom mirror with the hybrid epitaxial/metal mirror. For the epitaxial DBR, we can increase the refractive index contrast by exploiting excitonic resonances near AlGaN’s bandgap, in tandem with heavily doping the low index material to further reduce its refractive index. Finally, using a silver mirror underneath the epitaxial DBR stack has three advantages- (1) it mitigates the problem of cracking by reducing the epitaxial mirror’s thickness by $\sim 2 \, \mu m$, (2) reducing the thermal resistance (no substrate), and increasing the device yield compared to VCSELs with double dielectric mirrors, since now the cavity length is set by the epitaxial mirrors and not the precision of the polishing process.

This approach solves the problems associated with epitaxial DBRs (low reflectivity) and with dielectric bottom DBRs (poor cavity length control) with an elegant and simple solution.
CHAPTER 8. DESIGN OF ELECTRON BLOCKING LAYERS FOR III-N LIGHT EMITTING DEVICES

If there is anything the reader should take away from this chapter, it is that designing the optimum electron blocking layer (EBL) for your device is far easier if the fundamental physics of charge transport in the vicinity of EBL is understood. Thus, emphasis has been placed on trying to develop a physical intuition. This chapter largely derives from our previously published work [140].

8.1 Why does Electron Leakage Occur in III-N Light Emitting Devices?

Electron leakage is known to greatly reduce the injection efficiency of these laser diodes (LDs) and LEDs [93], [141], [142]. The overflow of electrons out of the active region into the adjacent p-type quasi-neutral region (QNR) is enhanced by the spontaneous and piezoelectric polarization charge at the quantum well (QW)/quantum barrier (QB) and last QB/EBL interfaces, and by the asymmetry between the majority carrier conductivities in n- and p-doped materials [143], [144]. In intrinsic III-N materials, electrons have 3-4 times higher mobilities than holes [28], and this difference is exacerbated in doped material, with electron mobilities in n-type material [8] being about 30-40 times higher than hole mobilities in p-type material [9]. Silicon, a donor, has an activation energy of about 20 meV [29], while magnesium, an acceptor, has an activation energy of 166 meV in GaN [12], and this activation energy further increases with aluminium content in Al_xGa_1-xN alloys [30]. Together, these factors imply far superior conductivity for n-type material than for p-type material.
In a perfectly symmetric LED structure (with no EBL), Vezellesi et al. demonstrated by numerical simulation that when p-type conductivity is lower than n-type conductivity, holes are not supplied to the active region at the same rate as electrons, causing electrons to leak out of the active region and recombine non-radiatively in the p-QNR and at the anode, resulting in efficiency droop; however, by making the electron and hole conductivities equal, electron leakage was reduced and efficiency droop was suppressed [91]. Fundamentally, carrier leakage is a natural consequence of asymmetric majority carrier conductivities in the quasi-neutral regions.

8.2 Consequences of Electron Leakage and a Literature Review of Various EBL Designs

Section 8.1 shows that an EBL is necessary to obtain efficient III-N light emitters, but it does not necessarily imply that the most commonly used rectangular EBL (a thin layer of wide bandgap material between the last QB and the p-QNR) is optimal. In fact, the rectangular EBL used in the first electrically pumped blue laser diode in 1996 [3] is still the most common type of EBL used in cutting edge vertical-cavity surface-emitting lasers (VCSELs) [36], [46], [47], [94], [145]–[147] and edge-emitting LDs [148]–[150]. However, this EBL has several drawbacks caused by the interfacial sheet polarization charges at the last QB/EBL and p-QNR/EBL interfaces that will be discussed in more detail in the following section of this chapter.

It has been shown by numerical simulation that this problem can be alleviated by using a polarization-matched quaternary AlInGaN EBL with judiciously chosen aluminium and indium mole fractions [151], [152]. However, growing AlInGaN...
compounds with high indium content is challenging due to the difference in optimum growth temperatures and pressure conditions for InN and AlN, and it is for this reason that the EBLs discussed in this paper are restricted to AlGaN alloys. Superlattice EBLs have also been shown to block electrons more effectively than conventional rectangular EBLs in edge-emitting LDs [153] and VCSELs [154]. As will be discussed in later in this chapter, our group has used tapered EBLs to reduce the threshold current in edge-emitting LDs [155], [156], and this improvement has also been explained by numerical simulation [157], [158]. It will also be shown that the inverse tapered EBL appears to work best for VCSELs, and a similar concept has also been used by our group for deep UV LEDs and edge-emitting LDs, where the inverse taper can help improve p-AlGaN’s conductivity [159]–[161] through volumetric redistribution of polarization charge.

Considerable theoretical and experimental work has been reported on EBLs designed for LEDs, which operate at far lower current densities than laser diodes. Graded and step-graded EBLs [162]–[168], superlattice EBLs [169]–[171] and AlInGaN or AlInN EBLs [172]–[174] have been used in UV and visible LEDs to mitigate droop. The primary purpose of this chapter is to understand the physics and principles behind EBL design, such as the effects of the EBL on hole and electron transport, parasitic inversion layers caused primarily by the interfacial polarization charges, and on bound carrier densities in the active region.

8.3 Epitaxial Description and Geometry of the VCSEL

The cross section of the VCSEL is shown in Figure 22. It uses 10 pairs of dielectric distributed Bragg reflectors (DBRs) of alternating quarter wavelength thick HfO$_2$ and SiO$_2$,
on both the top and the bottom sides. The dielectric DBR on the bottom can be realized either by chemical-mechanical polishing [35], [36], or by epitaxial lateral overgrowth [37]. The p- and n-QNRs are made of Al$_{0.12}$Ga$_{0.88}$N, and are 170 nm and 304 nm thick, respectively. These values slightly change depending on the EBL used. The active region has three 2 nm thick In$_{0.045}$Ga$_{0.055}$N QWs that are strained with respect to GaN, and 6 nm thick Al$_{0.12}$Ga$_{0.88}$N QBs.

![Figure 22 – Prototypical VCSEL structure. Image from [140].](image)

The different types of EBLs being studied are illustrated in Figure 22. The rectangular EBL comprises of 20 nm thick Al$_x$Ga$_{1-x}$N (0.12<x<0.4). The inverse tapered EBL is graded from Al$_x$Ga$_{1-x}$N (0.2<x<0.4) down to Al$_{0.12}$Ga$_{0.88}$N in the growth direction. The inverse tapered step graded EBL is similar to the inverse-tapered EBL, except that instead of an abrupt increase in the aluminium mole fraction from the QB to widest bandgap material in the EBL, it is done in a series of steps. The current spreading layer
consists of 10 pairs of modulation doped Al$_{0.12}$Ga$_{0.88}$N (6 nm)/ Al$_{0.04}$Ga$_{0.96}$N (4 nm) [100]. ITO has very high optical absorption losses at 370 nm [175] due to which an AlGaN-based current spreading layer is preferable in UV VCSELs. The 8 µm current aperture can be defined by nitrogen [176] or boron implantation [101].

Figure 23 – Types of EBLs studied: (top) Rectangular EBL, (middle) Inverse Tapered EBL and (bottom) Inverse Tapered Step Graded EBL. Image from [140].

These simulations consider the incomplete ionization of each dopant species. The free electron concentration in the n-QNR is about 1.8x10$^{18}$ cm$^{-3}$, and the free hole concentration in the p-regions is 5-5.4 x 10$^{17}$ cm$^{-3}$ at room temperature, which is consistent with our Hall data. The EBLs are all p-doped with ionized acceptor concentrations of 3-5
\(x \times 10^{17}\) cm\(^3\), depending on the Al mole fraction. All other parameters and their references have been discussed in chapter 4.3.

### 8.4 Types of EBLs: Results and Discussion

Our hypothesis is that the quantum efficiencies of LEDs and LDs benefit from different EBL designs because they operate at very different peak current densities. Evidence for this claim will be provided in this section. LEDs operate at current densities of a few hundred A/cm\(^2\) (limited due to droop), edge-emitting LDs operate at current densities of 1.5-5 kA/cm\(^2\) [57], [59], [177], while VCSELs can go over 20 kA/cm\(^2\) at the aperture edge [37]. VCSELs operate at higher current densities than edge-emitting LDs because of the lateral current injection scheme (discussed in chapter 6). Our simulations show that this causes severe current crowding near the aperture edge and the current density rapidly decays towards the centre of the VCSEL along the radial direction, as evidenced by Figure 24.

Various optical modes were computed (HE11, EH11, HE21, EH12, TE01 and TM01), and we found that the TE01 mode lased first. The mode profile is shown in Figure 24. In VCSELs, we find that the maximum electron leakage occurs at a radial distance between 3.4 to 4 \(\mu m\) (the aperture is at a radial distance of 4 \(\mu m\)), and hence all band diagrams for VCSELs have been shown along a vertical cutline at a radial distance of 3.5 \(\mu m\) from the centre.

Edge-emitting LDs have a vertical current injection scheme, which makes the current density more uniform, leading to lower peak current densities. This wide spread in peak
current densities for different light-emitting devices presents an incentive to investigate the efficacy of different EBL designs as a function of operating current density.

Figure 24 – Radial and vertical current density profiles (left axis) at 3.4 mA superimposed on the TE01 optical mode (right axis). This figure shows the current crowding at the aperture in a VCSEL. Negative $J_r$ implies current flows in the $r$ direction. Image from [140].

The drawbacks of the typical rectangular EBL will first be discussed, followed by the inverse tapered EBL (IT-EBL) and the Inverse Tapered Step Graded EBL (ITSG-EBL). The applicability of the last two types of EBLs will be discussed for various regimes of operating current densities.
8.4.1 *The Rectangular EBL and its Drawbacks*

The rectangular EBL is the most commonly used EBL in III-N light emitters, and it is a thin layer of wide-bandgap material between the active region and the p-QNR that inhibits electrons from leaking out of the active region into the p-type QNR.

However, this type of EBL has several problems associated with it that can be understood by looking closely at Figure 25 (a). The simulation reveals an accumulation of holes at the p-QNR/EBL interface, and a parasitic inversion layer formed by the pileup of electrons at the EBL/QB interface. This is due primarily to the discontinuities in the conduction and valence band energies and is exacerbated by the polarization sheet charges at the top and bottom EBL interfaces. This adversely affects the injection efficiency because the accumulation of positively charged holes above the EBL electrostatically facilitates the leakage of negatively charged electrons from the active region over the EBL. Thermionic emission current exhibits an inverse exponential dependence on barrier height ($|E_v - E_c|$), making the hole injection current very sensitive to the valence band offset at the p-QNR/EBL interface.

The increasingly poor injection of holes into the active region in combination with the blocked holes’ electrostatic assistance of electron leakage over the EBL contribute significantly to the monotonic degradation of the I-V characteristics in Figure 26 as the aluminum mole fraction in the EBL increases.
Figure 25 – Band diagram at 3.4 mA for a VCSEL with (a) a rectangular Al$_{0.3}$Ga$_{0.7}$N EBL, and (b) a rectangular Al$_{0.4}$Ga$_{0.6}$N EBL. Bound carrier concentrations in the QWs are not position dependent. Image from [140]. Image from [140].
The positive sheet charge associated with interfacial polarization has two more effects that are deleterious: severe band bending in the last QB due to high polarization-charge-induced electric fields that enhances electron escape, and it also causes an electrostatic redistribution of bound charge carriers in the QWs, particularly the QW on the p-side, as evidenced in Figure 27. The p-side QW has far more electrons than holes. This may be explained by the Coulombic force exerted by the positive sheet charge at the QB/EBL interface. When the number of bound electrons greatly exceed the number of bound holes, the excess electrons cannot recombine radiatively and hence leads to a reduction in the injection efficiency. Figure 27 shows that as the aluminium mole fraction in the EBL increases, the carrier mismatch in the p-side QW is exacerbated due to an increase in the sheet charge density at the QB/EBL interface. The middle and n-side QWs have much

Figure 26 – L-I-V characteristics of VCSELs with rectangular EBLs with different AlGaN compositions. Image from [140].
lower carrier mismatch than the p-side QWs. This is due to the p-side QW’s bound electrons screening the other two QWs from the sheet charge at the QB/EBL interface. The VCSEL with no EBL has the least carrier mismatch, but it has highest electron leakage current, which explains the three- to fourfold increase in the threshold current, as shown in Figure 26 and Figure 28. The L-I characteristics keep improving as the aluminium mole fraction in the EBL increases (up to Al$_{0.35}$Ga$_{0.65}$N). This improvement is shown in Figure 26, and can be explained by Figure 28, which suggests that the benefit of reduced electron leakage current due to an increased conduction band offset by increasing the aluminium mole fraction in the EBL outweighs the drawbacks such as increasing the bound carrier mismatch, forming deeper parasitic inversion layers and increasing the barrier to hole injection. Eventually, however, this trend reverses once the aluminium content exceeds a certain threshold, as explained in the following section.

Figure 27 – Carrier mismatch in the three QWs for VCSELs with different AlGaN rectangular EBLs. $n_{\text{QW}}$ is the bound electron density in that QW, and $p_{\text{QW}}$ is the bound hole density. Image from [140].
8.4.1.1 Why do depleted EBLs (too much Al%) lead to poor device performance?

The L-I characteristics of the Al$_{0.4}$Ga$_{0.6}$N rectangular EBL (Figure 26) reverses the trend of more aluminium leading to lower threshold currents and higher slope efficiencies. Simulation results suggest that there are two reasons for this: (1) the increased barrier to hole diffusion leads to the depletion of the EBL (Figure 25 (b)), and (2) more electron leakage than Al$_{0.3}$Ga$_{0.7}$N and Al$_{0.35}$Ga$_{0.65}$N EBLs (Figure 28). Figure 25 (b) shows that most of the applied bias is dropped across the depleted EBL, leading to high electric fields across it (electric field is proportional to d$E$/d$x$). This electric field causes a depletion of free holes in the depleted EBL- the depleted EBL in Figure 25 (b) has two orders of magnitude fewer holes in the EBL. For the undepleted EBL in Figure 25 (a), most of the
potential is dropped across the active region (the bands in the EBL are relatively flat). The increased electric field across the depleted EBL, and the reduced hole current density enhances electron leakage. At 3.6 mA, the 2-D integration over the p-QNR of the SRH recombination rate increases by a factor of 6.4 in the case of the depleted EBL, to $1.8 \times 10^{17} \text{s}^{-1}\text{cm}^{-1}$ for the depleted Al$_{0.4}$Ga$_{0.6}$N EBL, and only $2.8 \times 10^{16} \text{s}^{-1}\text{cm}^{-1}$ for the undepleted Al$_{0.3}$Ga$_{0.7}$N EBL. A higher integrated SRH recombination rate in the p-QNR is clearly indicative of more electrons spilling out of the active region into the p-QNR.

However, from Figure 29, we can infer that the increased barrier height for hole diffusion from the p-QNR to the QWs is the primary reason for greatly degraded L-I-V characteristics of the VCSEL with a depleted EBL. Figure 29 shows that the vertical hole current density calculated just 0.5 μm away from the aperture edge drops by 35% (from 8 kA/cm$^2$ down to 5.2 kA/cm$^2$) for the depleted Al$_{0.4}$Ga$_{0.6}$N EBL compared to an undepleted rectangular Al$_{0.3}$Ga$_{0.7}$N EBL. This argument is also corroborated by the observation that a rectangular EBL with Al$_{0.4}$Ga$_{0.6}$N has lesser electron leakage than a Al$_{0.2}$Ga$_{0.8}$N EBL, but it still has far worse L-I characteristics, so the enhanced electron leakage alone is not a sufficient reason to explain the Al$_{0.4}$Ga$_{0.6}$N EBL’s inferior performance compared to devices with undepleted Al$_{0.3}$Ga$_{0.7}$N and Al$_{0.35}$Ga$_{0.65}$N EBLs. The device with a depleted EBL may have a lower threshold current than one without an EBL due to reduced electron leakage (Figure 26), but it has a much smaller slope efficiency which can be attributed to the low hole current density. Thus, the depletion of the rectangular EBL further enhances the asymmetry between hole and electron current densities that further reduces the injection efficiency.
Figure 29 – Vertical hole current densities 0.5 µm away from the aperture edge 
(r=3.5 µm) at an input current of 3.4 mA, for a rectangular Al$_{0.3}$Ga$_{0.7}$N EBL (red), a 
rectangular Al$_{0.4}$Ga$_{0.6}$N EBL (green) and an inverse-tapered (IT) Al$_{0.3}$Ga$_{0.7}$N EBL 
(black). Right y-axis is a plot of the bandgap (black dotted line) vs vertical position.
Image from [140].

8.4.2 Inverse-Tapered EBL (IT EBL)

The inverse-tapered (IT) EBL substantially reduces the barrier to hole injection by 
employing compositionally graded material at the p-QNR/EBL interface instead of an 
abrupt heterojunction, hence increasing the hole current density. The band diagram is 
shown in Figure 30. Note the smooth band profile at the p-QNR/EBL interface. 
Compositional grading also makes it more difficult to deplete the EBL by removing the 
barrier to hole diffusion at the p-QNR/EBL interface, thus allowing holes to be injected 
even for an Al$_{0.4}$Ga$_{0.6}$N IT EBL, as shown in Figure 31.
Figure 30 – Band diagram at an input current of 3.4 mA for a VCSEL with an Al$_{0.3}$Ga$_{0.7}$N inverse-tapered EBL. Bound carrier concentrations are not position dependent. Image from [140].

The negative sheet charge density is volumetrically redistributed along the taper, and the simulations show that the free-hole concentration in the tapered region is actually three times higher than that in the p-QNR, as made evident by Figure 25 (a) and Figure 30. This is because the negative charge makes it energetically favourable for holes to enter the tapered region from the p-QNR. However, the parasitic inversion layer due to the positive sheet charge at the QB/EBL interface still exists. A similar concept has been used by our group in the past for deep-UV laser diodes to enable efficient hole injection. This is done by pulling holes from the more efficiently Mg-doped narrow-bandgap layers through the taper into the active region [160]. This was done because achieving high p-conductivity in Al$_x$Ga$_{1-x}$N alloys with x>0.5 is very difficult due to high Mg activation energies [30].
Figure 31 – L-I-V characteristics of VCSELs with inverse-tapered and rectangular EBLs. Image from [140].

Figure 31 shows that an inverse-tapered EBL always has better L-I-V characteristics than a rectangular EBL with the same aluminium composition. This is because holes can be easily injected into the active region without having to overcome a large valence band offset in the device with an inverse-tapered EBL (Figure 30). Figure 31 shows that the inverse-tapered EBL has higher slope efficiencies than a rectangular EBL with the same peak aluminium mole fraction, which we believe can be attributed to reduced electron leakage and increased hole current density, as shown in Figure 32 and Figure 29 respectively.
Figure 32 – (a) Percentage of electron leakage current in VCSELs with different rectangular and inverse-tapered EBLs as a function of current, and (b) electron leakage current in the p-QNR as a function of radial position at 3.4 mA. Image from [140].

An inverse tapered EBL has lower electron leakage than a rectangular EBL because: (1) Figure 29 shows that it has 16% higher hole current densities in the region of higher gain (closer to the peak of the optical mode), which enhances the rate of stimulated recombination, thus resulting in increased slope efficiencies, and (2) the reduced electric field across the EBL which reduces downward band-bending, thus resulting in an increased barrier height for electrons in the EBL-167 meV for the Al$_{0.3}$Ga$_{0.7}$N rectangular EBL and 209 meV for the Al$_{0.3}$Ga$_{0.7}$N inverse tapered EBL at 3.4 mA. This leads to the five-fold reduction in electron leakage for the inverse-tapered EBL as compared to a rectangular EBL of the same peak AlGaN composition, as seen in Figure 32. Figure 32 (b) shows the
total electron current density along a radial cutline just 10 nm above the EBL in the p-QNR. This inverse-tapered EBL has also been used to improve the injection efficiency and reduce droop in LEDs [163], [167], [168].

8.4.3 *Inverse-Tapered Step-Graded EBL (ITSG EBL)*

This EBL is similar to the inverse-tapered EBL, except that now instead of abruptly increasing the aluminium mole fraction from the QB to the EBL, the transition is made in a series of steps. The idea behind using this type of EBL is to suppress the parasitic inversion layer at the EBL/QB interface (reduced electron accumulation), and thus increase the effective barrier height $\Phi_B$ difference between the conduction band edge $E_C$ and the electron quasi-fermi energy $E_{fn}$) for electrons at the QB/EBL interface, which reduces electron leakage. However, it will be shown in this section that whether the above-mentioned advantages are realized or not strongly depends on the operating current density, since that affects $E_{fn}$. To illustrate this point, we shall study the efficacy of the Inverse-Tapered Step-Graded (ITSG) EBL for VCSELs (higher operating current density) and edge-emitting laser diodes (lower operating current density).
Figure 33 – Band diagram for a VCSEL with a 40/20/16 inverse-tapered step-graded (ITSG) EBL. Image from [140].

8.4.3.1 VCSELs

A 40/20/16 ITSG-EBL means the AlGaN steps consist of Al$_{0.16}$Ga$_{0.84}$N, Al$_{0.2}$Ga$_{0.8}$N and Al$_{0.4}$Ga$_{0.6}$N along the growth direction, and the band diagram is shown in Figure 33. Each step is 4 nm thick. A variety of compositions was simulated, with both 2 and 3 steps. They were all inferior to the inverse-tapered EBL, and for the sake of clarity, only the two best L-I-V curves have been compared to the IT-EBL in Figure 34. The ITSG-EBL does not show any improved over the IT-EBL. The sum of the electron concentrations in the ‘steps’ is roughly the same as the electron concentration in the abrupt EBL in Figure 25 (a)
and Figure 30. Hence, the problem of electron accumulation in the parasitic inversion layer has not been solved. This is further seen in Figure 33 and Figure 30, where the effective barrier height $\Phi_B$ at the EBL/QB interface is almost the same for ITSG-EBL and the IT-EBL. Nearly identical L-I curves for VCSELs with IT- and ITSG-EBLs in Figure 34 corroborates this analysis.

![L-I-V characteristics of VCSELs with an inverse-tapered step-graded (ITSG) EBLs. Image from [140].](image)

**Figure 34 – L-I-V characteristics of VCSELs with an inverse-tapered step-graded (ITSG) EBLs. Image from [140].**

8.4.3.2  **Edge-Emitting Fabry-Perot Laser Diode**

Our experimental and simulation results for blue (415 nm) edge-emitting LDs with rectangular (A) and step-graded EBLs (B) are shown in Figure 35 (b). The types of EBLs simulated for this edge-emitting laser diode are shown in Figure 35 (a). Both simulation
and experiment shows that a step-graded EBL can reduce the threshold current density by as much as 36% [155], [156] in edge-emitting LDs, and this also been explained through numerical simulation in [157], [158]. By grading the p-QNREBL interface (EBL (C)), along with step grading the EBL/QB interface, the threshold current density can be further reduced by 14%, as shown in Figure 35 (b).

Thus, simulation and experiment show that step grading the EBL/QB interface has a significant impact on edge-emitting laser diodes. The reason for this is clearly seen in Figure 36. The step grading reduces the accumulation of electrons in the parasitic inversion layer by over an order of magnitude. In the device with EBL A, the parasitic inversion layer is formed since $E_{fn}$ rises above $E_C$, which reduces the energetic barrier for electrons leaking out of the active region.

On the other hand, Figure 36 (b,c) shows that EBLs (B) and (C) always have $E_C$ above $E_{fn}$ in the QB and EBL, which is why no parasitic inversion layer is observed. The barrier to electrons presented by the EBL at the EBL/QB interface is 208 meV, 307 meV and 319 meV for EBLs (A), (B), and (C) respectively. This increased barrier height ($\Phi_B$) for EBLs (B) and (C) leads to a reduction in electron leakage and explains the dramatic reduction of the threshold current density by 54%, as seen in Figure 35 (b).

This is a very impressive simulation result—the fact that it can catch a reduction in the threshold current density by >50% when only one layer has been changed.
Figure 35 – (a) Types of EBLs for edge-emitting blue laser diodes. (b) Experimental (dotted) and simulated (solid) L-I characteristics of edge-emitting laser diodes with a rectangular EBL (red), step-graded EBL (blue) and inverse-tapered step-graded (ITSG) EBL (black). Experimental data is from [156]. Image from [140].
Figure 36 – Conduction band (solid black line, left axis), electron quasi-fermi energy (dotted black line, left axis) and electron concentration (solid red line, right axis) at a current density of 4.23 kA/cm$^2$ for blue edge-emitting laser diodes with (a) rectangular EBL (A), (b) step-graded EBL (B) and (c) ITSG-EBL (C) [140].
8.4.4 Application of These Theories to Various Optical Devices to Design Optimum EBLs

There is a big difference between the current injection profile for edge-emitting LDs and VCSELs. As previously shown in Figure 24, VCSELs suffer from severe current crowding at the current aperture, so only the edge of the optical mode is pumped. This causes very high peak current densities near the aperture, often above 10 kA/cm² at threshold. At this increased current density, $E_{fn}$ is pushed above $E_C$ near the EBL/QB interface, and this leads to the formation of parasitic inversion layers, in both abrupt and step graded EBLs in the case of VCSELs.

Edge-emitting LDs, on the other hand, have very uniform current profiles, and hence much lower peak threshold current densities. As Figure 28 and Figure 32 show, the percentage of electron leakage current increases monotonically with the input current density, making VCSELs leakier than edge-emitting laser diodes at threshold. For example, an input current of 4 mA corresponds to a uniform current density of 7.95 kA/cm² across an 8 µm aperture. However, in our VCSEL simulation, the current density at 4 mA is 13 kA/cm² just 0.5 µm away from the aperture edge! Thus, the improvement obtained with a step-graded EBL in edge-emitting LDs does not translate to VCSELs.

Step-graded EBLs have been shown to work well for LEDs too [164], [166]. LEDs operate at far lower current densities than LDs, where electron leakage is less of a concern. Due to a reduced fraction of electron leakage current, the parasitic inversion layer formed at the two EBL heterojunctions has a far bigger impact on the injection efficiency in LEDs than in LDs. Smoothly grading the material between the QB and the peak bandgap of the
EBL greatly suppresses the parasitic inversion layer at the QB/EBL interface, and this technique has been utilized in [162] to obtain a four-fold improvement in output power.

8.5 Summary

In conclusion, several types of EBLs have been investigated by numerical simulation. An EBL consists of two critical junctions- the p-QNR/EBL interface and the EBL/QB interface.

The p-QNR/EBL interface should always be graded, for both LEDs and laser diodes. This grading aids hole transport into the active region by removing abrupt heterojunctions that serve as potential energy barriers to hole injection into the MQW active region and distributes negative polarization charge throughout the tapered volume which electrostatically draws in holes from the highly conductive p-Ohmic contact. Efficient injection of holes into the active region reduces electron leakage, prevents depletion of the EBL and improves quantum efficiency.

Designing the EBL/QB interface is subtler and the optimum design is strongly influenced by the intended operating current density of the laser. The high current densities that VCSELs operate at make suppressing the parasitic inversion layer infeasible. Hence, we need to increase the conduction-band offset at the EBL and last quantum barrier interface to minimize electron leakage currents by thermionic emission, and an inverse-tapered EBL is optimum. However, edge-emitters benefit from inverse-tapered step-graded EBL since they operate at lower current densities than VCSELs, and step grading the EBL/QB interface can suppress the electron concentration in the parasitic inversion layer by over an order of magnitude. This enables a reduction in the electron leakage current, which
allowed our laser diode to achieve a 54% reduction in the threshold current density! This is because devices with suppressed parasitic inversion layers present an increased potential barrier to electrons, thus stemming electron leakage out of the active region. This was demonstrated experimentally and explained by numerical simulation.

LEDs operate at far lower current densities, and hence benefit from more gradual steps, or even continuous grading to greatly suppress the parasitic inversion layer while simultaneously reducing the barrier to hole injection. Thus, the optimum design of the EBL/QB interface strongly depends on the intended operating current density.
CHAPTER 9. THERMAL DESIGN OF III-N VCSELS

Electrically-injected blue and violet VCSELS made of III-N materials have been developed by several groups [35], [37], [46], [47], [94]. However, these devices require much higher input power than VCSELS made of III-AsP materials. Due to the wider bandgap of III-N materials, the diode’s turn-on voltage is ~3-4 V, with threshold currents as low as 1.5-2.5 mA, to more than 16 mA. Furthermore, high optical losses in p-GaN and the indium-tin-oxide (ITO) layers increase the threshold current and further exacerbates the problem of self-heating. Several commonly used III-N VCSEL designs use a dielectric distributed Bragg reflector (DBR) in the thermal path, which increases the thermal resistance compared to III-AsP VCSELS which use more thermally conductive epitaxial DBRs. Thus, these VCSELS made of III-N materials have over three times the turn-on voltage, and between 7-70 times higher threshold currents than their III-AsP counterparts. All these factors conspire to make thermal management in III-N VCSELS a critical problem.

In VCSELS made of traditional III-V materials (III-As and III-P), the input power is much lower, since the operating voltage is less than 2V, and the operating current is usually under 5 mA, with several reports of GaAs-based VCSELS with sub-mA threshold currents, and threshold current densities less than 1 kA/cm² [178]–[181]. This low input electrical power (<1 mW at threshold) makes the problem of thermal management less pressing than III-N VCSELS.
The maximum output power of VCSELs is contingent on several factors such as absorption losses in the cavity (dominated by ITO and p++ GaN cap layer), mirror reflectivity (which affects the slope efficiency and threshold current), material quality, design of the epitaxial structure, and the thermal resistance. Thermal rollover (when the slope efficiency becomes zero) occurs primarily due to enhanced carrier leakage out of the active region due to elevated temperatures [182], [183], since $J_{\text{leakage}} \propto \exp(-\phi/kT)$, where $\phi$ is the energetic barrier height. In these simulations, thermal gain broadening has been neglected.

Elevated temperatures due to self-heating thus adversely affects the maximum optical power, threshold current, slope efficiency, wavelength stability (a change in the active region temperature detunes the peak gain wavelength from the cavity resonant wavelength) and the device lifetime.

9.1 Objectives and Limitations of Electro-Opto-Thermal Simulations

There have been several papers reporting the thermal characteristics of III-As VCSEL [184]–[187], but very few such studies exist for III-N VCSELs. Some notable thermal analysis on III-N VCSELs have been performed both by simulation and experimentally by Mei et al. [188]. Further theoretical studies of the thermal resistance of GaN VCSELs has been performed by FEM in [189]. However, both these studies neglect Joule heating, which is significant in the resistive p-GaN layers, and the thin ITO layers. Also, they assume uniform current spreading in the current aperture, while our simulations show severe current crowding near the edge of the aperture (see Chapter 6) which leads to
localized hotspots. Hence, we find that the most reliable method to model the thermal resistance is to use self-consistent electro-opto-thermal simulations.

Self-consistent electro-opto-thermal simulations have too many unknown and unreported parameters such as diameters of various layers, heatsink material, interface resistances etc. Hence, trying to make the simulation exactly match experimental data is a pointless activity. Instead, reasonable values should be used for the parameters, and they should be held constant for all simulations. This allows us to (1) extract and identify trends, and (2) identify key design parameters which have the largest influence on thermal resistance. This is the true value of numerical simulation in the design of semiconductor devices.

Modelling the DBR is computationally expensive, and hence we have replaced the DBR with a bulk material whose thermal conductivity is given by:

\[
\kappa_{DBR} = \frac{d_1 + d_2}{\frac{d_1}{\kappa_1} + \frac{d_2}{\kappa_2}}
\]  

where \(d_1\) and \(d_2\) are the layer thicknesses.

Since the optical power is much smaller than the electrical power, the thermal resistance is calculated as per equation 19:

\[
R_{thermal} = \frac{\Delta T}{VI}
\]  

where \(\Delta T\) is defined as the difference between the maximum active region temperature and the heatsink’s temperature (imposed as a Dirichlet boundary condition).
9.2 Device Epitaxial Structure and Geometry

Table 5 shows the epitaxial structure, along with the diameters, thermal conductivities and doping concentrations in the various layers. Figure 37 shows the structures of three typical VCSEL structures: (a) hybrid VCSEL with an epitaxial bottom (n-side) DBR and a dielectric top (p-side) DBR, (b) flip-chip VCSEL with a dielectric bottom (p-side) DBR and either an epitaxial or dielectric top (n-side) DBR, and (c) double dielectric VCSEL fabricated with the ELOG technique.

The epitaxial structure of [47] is a reference structure, and then only the DBR materials, n-GaN thickness, the bonding material for flip-chipped VCSELs and the substrate thickness have been modified. The active region, ITO thickness, p-GaN thickness and the electron blocking layer (EBL) have been kept constant to ensure an apples-to-apples comparison of various thermal designs. We find that through optimum thermal design we can achieve an increase in the maximum output power by well over 200% in some cases.

![Figure 37 - Schematics of three types of VCSELs: (a) hybrid DBR VCSEL, (b) flip-chip VCSEL and (c) ELOG VCSEL.](image-url)

Figure 37 – Schematics of three types of VCSELs: (a) hybrid DBR VCSEL, (b) flip-chip VCSEL and (c) ELOG VCSEL.
Table 5 – VCSEL epitaxial layers and parameters for reference structure

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Thickness nm</th>
<th>Thermal Conductivity W/(m-K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top DBR 1</td>
<td>8 x Nb$_2$O$_5$/SiO$_2$</td>
<td>40/69</td>
<td>1.4</td>
</tr>
<tr>
<td>Spacer</td>
<td>Nb$_2$O$_5$</td>
<td>22</td>
<td>1.4</td>
</tr>
<tr>
<td>CSL</td>
<td>ITO</td>
<td>20</td>
<td>3.95$^a$</td>
</tr>
<tr>
<td>p++ contact</td>
<td>p++ GaN</td>
<td>10</td>
<td>130</td>
</tr>
<tr>
<td>p-QNR</td>
<td>p-GaN</td>
<td>52</td>
<td>130</td>
</tr>
<tr>
<td>EBL</td>
<td>p-Al$<em>{0.2}$Ga$</em>{0.8}$N</td>
<td>20</td>
<td>17.9</td>
</tr>
<tr>
<td>QB</td>
<td>uid-GaN</td>
<td>6</td>
<td>130</td>
</tr>
<tr>
<td>MQW</td>
<td>5x uid-InGaN/GaN</td>
<td>3/6</td>
<td>13.2/130</td>
</tr>
<tr>
<td>n-GaN</td>
<td>n-GaN</td>
<td>54</td>
<td>130</td>
</tr>
<tr>
<td>Bottom DBR</td>
<td>46 x Al$<em>{0.18}$Ga$</em>{0.82}$N/GaN</td>
<td>43/40</td>
<td>4.87/130</td>
</tr>
<tr>
<td>Substrate</td>
<td>GaN</td>
<td>330</td>
<td>130</td>
</tr>
</tbody>
</table>

$^a$ Reference [190]

QNR: quasi-neutral region
uid: unintentionally doped

VCSELs of type (b) and (c) have different n-QNR thicknesses and bottom mirrors. Differences in materials and thicknesses from the reference VCSEL will be specified in the appropriate section.
VCSELs of type (a) with an AlInN/GaN bottom mirror have been demonstrated by EPFL [46], Nagoya and Meijo universities [47], [145]. NCTU demonstrated a hybrid DBR VCSEL with an AlN/GaN bottom mirror [113].

VCSELs of type (b) need to have the substrate thinned or removed, and this can be done in two ways- through chemical-mechanical polishing (CMP) or laser lift-off. The CMP approach has been demonstrated by Panasonic [36] and Nichia [34], while the laser lift-off technique to remove the substrate has been used by Nichia [33] and Xiamen University [139]. An epitaxial top mirror in a VCSEL of type (b) has been reported in [191].

The only group to demonstrate VCSELs of type (c) using epitaxial lateral overgrowth (ELOG) is Sony [37], [38].

The VCSEL design of choice (among the 3) is primarily determined by the technology available to a group to get a good n-side mirror, and the thermal resistance is a secondary design consideration. Hence, instead of comparing the three designs directly, this chapter will optimize each of them separately to minimize the thermal resistance. The VCSELs in this section (9.2) are visible ($\lambda = 406$ nm), but the design techniques are equally applicable to UV-VCSEL in the right circumstances.

All VCSELs in this section have a dielectric DBR diameter of 10 $\mu$m and a current aperture that is 8 $\mu$m in diameter.
In the following L-I-T plots, the dotted lines and right axis always corresponds to the maximum temperature in the active region. The left axis and solid lines denote the optical power.

9.2.1 Hybrid VCSEL

This VCSEL uses an epitaxial bottom mirror and is described by Table 5. The AlInN layers in the DBR are problematic due to its very low thermal conductivity, as shown in Figure 38. It is fairly obvious that the n-DBR diameter should we as wide as possible to minimize the thermal resistance. This is described in great detail in [188]. In this section, the effect of the substrate thickness on the L-I characteristics will be studied.

![Thermal conductivity of Al\textsubscript{n}Ga\textsubscript{1-x}N](image)

**Figure 38** – Thermal conductivity of Al\textsubscript{n}Ga\textsubscript{1-x}N as a function of Al mole fraction x [84]. The red dot is the thermal conductivity of Al\textsubscript{0.8}In\textsubscript{0.2}N lattice matched to GaN [85].
The thermal resistance is further degraded by the presence of a 300 μm thick substrate. Simulations have been with a device whose n-DBR has a diameter of 40 μm with substrate thicknesses of 100 μm, 200 μm and 300 μm respectively. The results are tabulated in Table 6.

There are a couple of interesting features to note in Figure 39. Thinning the substrate by 100 μm leads to an increase in the maximum output optical power by upwards of 50%! The reason for this is a drop in the thermal resistance, as shown in Figure 39 (b). Also, the $R_{\text{thermal}}$-I plot shows that $R_{\text{thermal}}$ keeps increasing with current and shows a kink at threshold.

Compared to the reference VCSEL with a 300 μm substrate, Table 6 shows that a hybrid VCSEL with a 200 μm and 100 μm substrate has 20% and 36% lower thermal resistance respectively. This is responsible for lower temperatures in the active region, which reduces electron leakage out of the region and hence increases the device’s injection efficiency.
Figure 39 – (a) L-I-T plots and (b) thermal resistance vs input current for the hybrid DBR VCSEL for different thicknesses of the GaN substrate.
The reason for the kink is that the rate of stimulated emission greatly increases at threshold, and hence locks the rate of non-radiative recombination in the active region. In other words, the internal quantum efficiency (IQE) keeps increasing with input current beyond threshold, with the sharpest change in IQE at the threshold current.

The reason that $R_{\text{thermal}}$ keeps increasing with current is because: (1) enhanced electron leakage leads to non-radiative recombination in the p-QNR, and (2) the resistance of the p-QNR due to poor p-doping efficiency and low hole mobility leads to significant potential drops across the “QNR” (which is now no longer quasi-neutral). These two factors increase temperature in the p-layers due to both SRH recombination and Joule heating.

Table 6 – Thermal resistance at the threshold current for hybrid VCSELs with various GaN substrate thicknesses.

<table>
<thead>
<tr>
<th>VCSEL ID</th>
<th>$t_{\text{substrate}}$ (μm)</th>
<th>Thermal Resistance at Threshold (K/W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid A</td>
<td>300</td>
<td>1142</td>
</tr>
<tr>
<td>Hybrid B</td>
<td>200</td>
<td>907</td>
</tr>
<tr>
<td>Hybrid C</td>
<td>100</td>
<td>731</td>
</tr>
</tbody>
</table>
9.2.2 Flip-Chip VCSEL with a Dielectric p-side DBR

Reducing the diameter of the p-side DBR is the obvious and easy way to reduce the thermal resistance. A p-DBR diameter of 10 μm has been assumed, and the current aperture diameter is 8 μm. In this section, the impact of radius of the heatsink and p-bonding metal/support substrate, the cavity thickness and the material of the support substrate will be explored in detail. The epitaxial stack is the same as that in Table 5, except that it is flip-chipped onto a heatsink (p-side down). All support substrates (both silicon and copper) are assumed to be 100 μm thick.

Table 7 Device description and thermal resistance of the various flip-chip VCSELs

<table>
<thead>
<tr>
<th>VCSEL ID</th>
<th>Cavity Length</th>
<th>Heatsink Diameter</th>
<th>Heatsink Material</th>
<th>Thermal Resistance at Threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>FC-1</td>
<td>0.229</td>
<td>20</td>
<td>Silicon</td>
<td>572</td>
</tr>
<tr>
<td>FC-2</td>
<td>0.229</td>
<td>30</td>
<td>Silicon</td>
<td>306</td>
</tr>
<tr>
<td>FC-3</td>
<td>0.229</td>
<td>40</td>
<td>Silicon</td>
<td>144</td>
</tr>
<tr>
<td>FC-4</td>
<td>0.229</td>
<td>30</td>
<td>Copper</td>
<td>178</td>
</tr>
<tr>
<td>FC-5</td>
<td>3.5</td>
<td>30</td>
<td>Silicon</td>
<td>153</td>
</tr>
</tbody>
</table>
Figure 40 – (a) L-I-T plots and (b) thermal resistance vs input current for the flip-chip Dielectric p-DBR VCSEL.
Figure 41 – (a) L-I-T plots and (b) thermal resistance vs input current for the flip-chip Dielectric p-DBR VCSEL with different cavity lengths.
As evident from Figure 40, the diameter of the heatsink plays a very important role in the overall thermal resistance. This is because heat must escape from around the dielectric DBR.

Furthermore, replacing the silicon bonding substrate with copper can also reduce the thermal resistance by 42% for a 30 μm diameter. Both Panasonic [36] and Nichia [34] bond their VCSELs to silicon support substrates.

Figure 41 shows that increasing the cavity length on the n-side can also greatly reduce the thermal resistance by as much as 50%, leading to an increase in the optical power by >200%. This is despite the fact that heat is extracted from the p-side. These VCSELs also have far lower thermal resistances than the hybrid VCSELs of section 9.2.1. This is because there is no AlInN layer in the thermal path.

9.2.3 ELOG VCSEL

The final type of VCSEL that will be studied is the ELOG VCSEL. This VCSEL design is best demonstrated by Sony [37], [38]. Reducing the radius of the dielectric DBR to improve the thermal resistance is once again obvious. In this section, the effect of the cavity length and the device diameter will be studied. The n-side DBR’s diameter is fixed at 10 μm.

The ELOG VCSELs are described in Table 8. It is readily apparent from Figure 42 that the diameter of the overgrown n-GaN makes the largest difference in the overall thermal resistance, followed by cavity length.
Table 8 – The device description and thermal resistance of the various ELOG VCSELs

<table>
<thead>
<tr>
<th>VCSEL ID</th>
<th>Cavity Length (μm)</th>
<th>n-GaN QNR Diameter (μm)</th>
<th>Thermal Resistance at Threshold (K/W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ELOG-A</td>
<td>1.8</td>
<td>20</td>
<td>705</td>
</tr>
<tr>
<td>ELOG-B</td>
<td>0.37</td>
<td>30</td>
<td>453</td>
</tr>
<tr>
<td>ELOG-C</td>
<td>1.8</td>
<td>30</td>
<td>371</td>
</tr>
<tr>
<td>ELOG-D</td>
<td>3</td>
<td>30</td>
<td>330</td>
</tr>
</tbody>
</table>
Figure 42 – (a) L-I-T plots and (b) thermal resistance vs input current for ELOG VCSELs.
9.3 Effect of Gap Between p-contact and Edge of Current Aperture and Heatsink Location

In this section, we shall return to UV-VCSELs that use an ITO current spreading layer and a hybrid epitaxial/metal mirror (section 7.4). The device’s epitaxial structure is described in Table 9 and a cross-section view of the VCSEL is shown in Figure 43.

![Cross-section view of UV-VCSEL. 'x' is the spacing between the end of the p-metal (in the lateral direction) and the end of the current aperture.](image)

Figure 43 – Cross-section view of UV-VCSEL. 'x' is the spacing between the end of the p-metal (in the lateral direction) and the end of the current aperture.

As ‘x’ increases, the device’s performance degrades. We speculate that the main reason for this performance hit is that a higher value of ‘x’ leads to higher electrical resistance through a thin 10 nm ITO layer (lateral hole current spreading). This increase in resistance is clearly seen in Figure 44 (b) and Figure 45 (b). This leads to increased Joule heating and all the downsides associated with operating the device at a higher temperature. Thus, thermal management is another reason why ITO is unsuitable for UV-devices. A thicker ITO layer will reduce self-heating but will increase the optical loss.
Table 9 – Epitaxial structure of UV-VCSEL with hybrid epitaxial/metal n-side DBR.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top DBR</td>
<td>10x HfO$_2$/SiO$_2$</td>
<td>42/63</td>
</tr>
<tr>
<td>Spacer</td>
<td>HfO$_2$</td>
<td>35</td>
</tr>
<tr>
<td>CSL</td>
<td>ITO</td>
<td>10</td>
</tr>
<tr>
<td>p++</td>
<td>GaN/Al$<em>{0.1}$Ga$</em>{0.9}$N</td>
<td>2/18</td>
</tr>
<tr>
<td>p-QNR</td>
<td>Al$<em>{0.1}$Ga$</em>{0.9}$N</td>
<td>111</td>
</tr>
<tr>
<td>Taper</td>
<td>Inverse Taper Al$<em>{0.25}$Ga$</em>{0.75}$N $\rightarrow$ p-QNR along c-axis</td>
<td>15</td>
</tr>
<tr>
<td>EBL</td>
<td>Al$<em>{0.25}$Ga$</em>{0.75}$N</td>
<td>5</td>
</tr>
<tr>
<td>MQW</td>
<td>6 x Al$<em>{0.12}$Ga$</em>{0.88}$N</td>
<td>6</td>
</tr>
<tr>
<td>n-QNR</td>
<td>5 x In$<em>{0.045}$Ga$</em>{0.955}$N</td>
<td>2</td>
</tr>
<tr>
<td>n-AlGaN</td>
<td>Al$<em>{0.1}$Ga$</em>{0.9}$N</td>
<td>291</td>
</tr>
<tr>
<td>Bottom DBR</td>
<td>30x Al$<em>{0.04}$Ga$</em>{0.96}$N / Al$<em>{0.3}$Ga$</em>{0.7}$N</td>
<td>34.1/36.7</td>
</tr>
<tr>
<td>Silver</td>
<td>Silver</td>
<td>40</td>
</tr>
</tbody>
</table>
In VCSELs with the above structure, there are two possible heatsink locations—on the p-side or the n-side. Both shall be compared in this section. For a device with a p (n)-side heatsink, the p (n)-metal serves a dual purpose as both an electrode and a thermode. As ‘x’ increases for devices with a p-side heatsink, so does the thermal resistance (as seen by the temperature in the active region with the dotted lines).

**Figure 44**—(a) L-I-T and (b) I-V plots of hybrid epitaxial/metal DBR with p-side heatsink.

Device characteristics (L-I-V-T) with a p-side and an n-side heatsink are shown in Figure 44 and Figure 45 respectively. Every parameter in the devices is kept constant, except ‘x’ and the heatsink position in order to ensure a meaningful comparison. As clearly seen, a device with a p-side heatsink is far superior to a device with an n-side heatsink for the same value of ‘x’. This is because a p-side heatsink is closer to the primary sources of heat generation—Joule heating in the ITO and p-QNR layers, and heating due to SRH recombination in the active region.
9.4 Summary

Hybrid DBR VCSELs can be improved by substrate thinning. An elongated VCSEL cavity (n-QNR), an increased heatsink (overgrown n-GaN) diameter, and the use of a metal support substrate can all greatly improve the performance of III-N flip-chip (ELOG) VCSELs. All of these improvements can lead to over 200% increases in the maximum output optical power before thermal rollover. These general findings and principles are equally applicable to UV-VCSELs despite the simulations in section 9.2 being of violet VCSELs.

Finally, the parameter ‘x’ is a crucial design parameter for VCSELs using thin ITO layers, and the heatsink should be as close to the sources of heat as possible to minimize the thermal resistance. This requires utilizing a flip-chip process to heatsink the p-side (rather than the n-side) of the device, as demonstrated by Panasonic [36] and Nichia [34].
CHAPTER 10. LOW TEMPERATURE I-V AND SPECTRAL CHARACTERIZATION OF MICROCAVITY LEDS

When designing novel lasers, it is easier to first achieve lasing at lower temperatures. This is because reducing the temperature improves the internal quantum efficiency of the device by suppressing non-radiative SRH recombination, and it also improves the injection efficiency due to reduced leakage currents by thermionic emission at lower temperatures. However, if the temperature gets too low, carrier freeze-out occurs (inability to thermally ionize dopant atoms to achieve efficient doping). Thus, as discussed in this chapter, we have found the optimum temperature in terms of electroluminescence (EL) intensity to be 180-200 K.

The cryogenic I-V and the EL emission spectra measurements were performed by the author on a Lakeshore TTPX cryogenic probe station. More details on the epitaxial structure, growth techniques, and a description of the equipment used can be found in [20].

This thesis focusses on theoretical design techniques for lasers, but some interesting features were observed when the author was measuring the devices, and those features shall be the focus of this chapter.

10.1 Cryogenic I-V and Spectral Measurements of ‘Good’ RCLEDs

These MCLEDs use 20 nm thick ITO as a current spreading layer, a dielectric DBR as the p-side DBR, a 40-pair GaN/Al$_{0.12}$Ga$_{0.88}$N epitaxial DBR on the n-side, and a current aperture formed by N-implantation [20]. A good LED is defined as one which can be driven
at high current densities (J>15 kA/cm² for through an aperture diameter of 8 μm) without dying right away.

10.1.1 I-V Characterization

As expected, the I-V characteristics degrade as the temperature reduces, and this is due to higher series resistance (low free hole concentration) and an increased bandgap. This is shown in Figure 46. It is clear that carrier freeze-out only becomes a problem once the temperature drops below 200 K.

![Figure 46 - I-V curves of the MCLEDs at different temperatures on a linear (left) and semilog (right) plots. This data was collected with the assistance of Dr. S.C. Shen, Hoon Jeong, and Jialin Wang.](image)

10.1.2 EL Spectral Measurements

The emission spectrum was measured with an Ocean Optics spectrometer (HR2000CG-UV-NIR). The temperature and current dependent EL emission spectrum is shown in Figure 47.
Figure 47 – EL emission spectra of the MCLED at different temperatures and injection currents. (Image created by Dr. Liu [20]). This data was collected with the assistance of Dr. S.C. Shen, Hoon Jeong, and Jialin Wang.

The optical fiber was unmoved between measurements, so it is a fair assumption that the relative intensity ratios correspond to the relative external quantum efficiency of the MCLED. Between 180-300 K, the peak emission wavelength gradually blue shifts, which is most likely due to the refractive index reducing with temperature. The thermo-optical coefficient is [192].

$$\lim_{\lambda \to 370 \text{ nm}} \frac{dn}{dT} = 1.6 \times 10^{-4} / K$$ (20)
Figure 48 – EL emission wavelength and normalized intensity vs temperature for an
injection current of 5 mA. This data was collected with the assistance of Dr. S.C.
Shen, Hoon Jeong, and Jialin Wang.

As seen in Figure 48, there is an abrupt drop-off in intensity and the center emission
wavelength as the temperature reduces from 180 K to 150 K. This same trend is observed
at all three levels of current injection.

One possible explanation for this observation could be the detuning of the MQW’s
gain spectrum and the cavity mode. The n-DBR has a very narrow stopband due to a low
index contrast and can hence only support one longitudinal mode (free spectral range is
>10 nm). The n-DBR’s reflectivity rapidly tails of near 150 K, as seen in Figure 49. There
is a strong correlation between the temperature at which the emission wavelength abruptly
changes and the temperature at which the n-DBR’s reflectivity sharply drops. The overall
reflectivity depends on the index contrast as well as the absorption loss, as shown in Figure 49.

Figure 49 – Reflectivity for $\lambda = 370$ nm (blue, left axis) and index contrast $n_1 - n_2$ (red, right axis) of the n-DBR as a function of temperature.

At high temperatures, the absorption loss increases (due to bandgap narrowing and increased free-carrier absorption), and this limits the overall peak reflectivity.

At low temperatures, the index contrast gets too small, and hence the overall reflectivity drops despite the DBR contributing a relatively low absorption loss.

10.2 Room-Temperature I-V Measurements of ‘Bad’ Devices (Hysteresis)

A few batches of devices with new sidewall etch recipes had very poor performance (high turn-on voltage, low current-drive capability, short device lifetime etc.). It may be possible to screen bad wafers by observing the I-V hysteresis curves. ‘Good’ devices
showed practically no hysteresis while the ‘bad’ devices had very different curves for voltage sweeps in opposite directions. We suspect this is due to charge trapping effects at exposed sidewalls.

Figure 50 – Hysteresis sweeps on a ‘good’ LED in (a) reverse and (b) forward bias.

This data was collected with the assistance of Dr. S.C. Shen, Hoon Jeong, and Jialin Wang.

Figure 51 – Hysteresis sweeps on a ‘bad’ LED in (a) reverse and (b) forward bias.

This data was collected with the assistance of Dr. S.C. Shen, Hoon Jeong, and Jialin Wang.
Figure 50 shows I-V sweeps of ‘good’ devices under both forward and reverse bias. Note the lack of hysteresis in the I-V curves when sweeping from and to 0 V.

Figure 51, on the other hand, is a bad device and shows significant hysteresis in the I-V plots, which, as mentioned earlier, might be due to charge trapping.
CHAPTER 11. CONCLUSION

11.1 Summary

The design methodology and results shall be summarized to give an overview of the problem and to review the design techniques to overcome these challenges. Chapter 2 discussed some challenges with the III-N material system such as the high lattice mismatch between binary compounds (limits refractive index contrast and band offsets), poor p-conductivity (affect the injection efficiency), and high optical loss. Chapter 3 then reviewed the state-of-the-art III-N VCSELs, and it had examples of the three most common III-N VCSEL types (hybrid DBR, flip-chip double dielectric DBR and a double dielectric DBR obtained through ELOG), and why these are more challenging to implement for UV-VCSELs than for blue VCSELs. Chapter 4 described the simulation methods, the key equations that need to be solved and the material parameters.

The most crucial impediments to realizing a UV-VCSEL were identified in chapter 5, and these included high optical loss due to an ITO current spreading layer, high optical loss in the n-side DBR, poor injection efficiency due to electron leakage and to design a thermal management strategy for the most common type of III-N VCSELs.

The use of a modulation-doped short-period superlattice hole current spreading layer was suggested in chapter 6 as a far superior alternative to the commonly used ITO (ITO is much less lossy for visible wavelengths than for UV wavelengths).

Chapter 7 described techniques to increases the refractive index contrast between AlGaN alloys without introducing any additional tensile strain. This is done by exploiting
near band-edge excitonic resonance to increase the refractive index of the high index layer. Simultaneously, the low index layer’s refractive index can be reduced through heavy n-type doping. This reduces the refractive index by increasing the material’s plasma frequency and ‘effective’ bandgap (Burstein-Moss effect due to band-filling). These techniques can boost the reflectivity of an epitaxial DBR if the material compositions and doping concentrations are judiciously selected. Still, epitaxial AlGaN (indium-free) DBRs struggle to achieve reflectivities >99% due to the tensile strain. Thus, we propose substrate thinning and then depositing a planar metallic mirror underneath an epitaxial stack to boost the overall reflectivity. To get 99% reflectivity, the epitaxial stack only needs a reflectivity of 90%, and the remaining 9% is provided by the metallic mirror. This is a high yield process since the cavity length is set by precisely controllable epitaxy, and this mirror’s reflectivity spectrum is robust against fluctuations in substrate thickness due to imprecision in the polishing process.

Chapter 8 discusses the topic of electron leakage in III-N light emitting devices. It is found that the most commonly used type of EBL (rectangular EBL) has several disadvantages and there is no reason to use it except for reasons pertaining to easier growth. We find that the optimum EBL design strongly depends on the device’s intended operating current density. VCSELs need an Inverse-Tapered EBL (highest J operation), while edge-emitting LDs greatly benefit from an Inverse-Tapered Step-Graded EBL. This was experimentally and theoretically shown to reduce the threshold current by ~50% due to suppression of the parasitic electron inversion layer at the EBL/QB interface.

Chapter 9 dealt with thermal design of the VCSEL, and electro-opto-thermal simulations were performed for the three most common III-N VCSEL designs (hybrid
DBR, flip-chip double dielectric DBR and a double dielectric DBR obtained through ELOG). Since the design choice is primarily determined by the technology options available to the group, optimum thermal strategies (and key thermal design parameters) for all three types have been identified and discussed. Self-heating limits the maximum optical power output of the LD, and the thermal resistance is hence a very important consideration for achieving continuous-wave laser operation.

Finally, chapter 10 described some interesting observation when performing EL spectral characterization and I-V curves over a range of temperatures (150 K to 300 K). There was an abrupt change in the center emission wavelength and intensity when the temperature changed from 180 K to 150 K. Simulations suggest that the reflectivity of the n-DBR also abruptly reduced in that temperature range. Finally, poor quality devices tended to show hysteresis when the voltage was swept to and from 0 V in either direction, which might be due charge trapping at defect-rich sidewalls.

11.2 Future Research Directions

At this point, the key factors precluding a demonstration of UV-VCSELs is to find a reliable method for substrate removal (allows either a dielectric n-side DBR or an epitaxial/metal hybrid mirror) and the growth of high quality AlGaN templates to allow the incorporation of more aluminum in the EBL and the DBR, and to possibly realize UV-B laser diodes.

Finally, another exciting possibility for a designer is the use of both MBE and MOCVD in a single device. They each have certain advantages over the other. MOCVD grows higher quality material and active regions, but MBE can obtain sharp Mg doping
profiles (no Mg memory effect due to lower growth temperatures), MBE can also grow Ga-free alloys like AlInN (though some horizontal MOCVD reactors can do this too), and tunnel diodes (higher free-hole concentration than MOCVD-grown p-material). Thus, it might be possible to grow an AlGaN/AlInN DBR with MBE, and then go a regrowth of the rest of the cavity by MOCVD. This would solve the problem of the n-side DBR. Also, perhaps the cavity could be grown by MOCVD, and then the MD-SPSL, or a tunnel diode could be re-grown with MBE right at the end to act as the hole current spreading layer. Thus, having access to both MBE and MOCVD can potentially open up exciting options for UV laser designers in the future.
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