PHD

Photonic Crystals for the Control of Light Extraction from III-Nitride Light-Emitting Diodes

Lewins, Christopher

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Photonic Crystals for the Control of Light Extraction from III-Nitride Light-Emitting Diodes

submitted by

Christopher J. Lewins

for the degree of Doctor of Philosophy

University of Bath

Department of Electronic and Electrical Engineering

October 2015

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Signed on behalf of the Department of Electronic and Electrical Engineering
Abstract

This thesis investigates the effect and exploitation of photonic crystals (PhCs) for light extraction in light-emitting diodes (LEDs). LEDs have come some way to meeting the requirements for several applications, but are limited in their suitability, particularly for étendue-limited applications requiring high directivity. Light extraction from LEDs presents a challenge, due to total internal reflection at the surface of the LED chip and current commercial light extraction techniques offer limited control over the direction of emission.

PhC LEDs can operate in either a weak regime, where the PhC acts principally as a diffraction grating, or in strong regime where the PhC introduces a significant periodic (Bloch) component to the optical modes supported in the device. Experimental LEDs incorporating a buried photonic quasi-crystal are investigated and their weak-regime behaviour described by a simple model, with a 2D part concerning the PhC tiling and a 1D part considering the slab waveguiding properties of the device when the PhC is considered as an effective medium. A transfer and scattering matrix model for arbitrary slab waveguides is developed, including a model for emission from an embedded source layer. Experimental devices are shown to operate in the strong regime, possibly for the first time, comprised of large-area periodic arrays of nanorods with embedded light emitters suitable for large area fabrication and electrical contacting. Through confinement of light by index guiding or Fresnel reflection to the periodic layers, Bloch modes can be formed. Exploitation of both the strong and weak regimes in device designs for highly directional LEDs are discussed, with a comparison made between the two approaches. The strong PhC operating regime enabled by this work may facilitate significant performance improvements for practical highly directional LEDs over alternative methods.
Acknowledgements

As with any research, the work undertaken for this thesis would not have been possible without the support and guidance of many people. I would like to thank all those who have provided that necessary assistance, whether it be through discussion, critique, advice, technical & administrative support or personal support, and I would like to explicitly mention a few of those people.

Firstly, I would like to thank my lead supervisor, Dr Duncan Allsopp, whose exceptional ability to inspire interest of a subject in students led to my decision to study for a PhD. Once he had captured me, his care and concern about my progress along with support and challenge to ideas have enabled this project to be undertaken to the best of my ability.

When I started, Dr Philip Shields was a postdoctoral researcher who was more than willing to provide his time and patience to introduce me to the world of academic study. Shortly after, he became a lecturer and appointed to my supervisory team where he has provided a solid voice of reason. I would like to thank Philip for always making time for discussion and providing a foundation for the project to build on.

I would like to thank Prof. Adrian Evans for his contribution as a supervisor at the start of the project, where he provided guidance on multidimensional data processing techniques. Beyond my supervisory team, there were postdoctoral researchers who have often gone out of their way to help. A particular mention is due to Drs Emmanuel Le Boulbar, Szymon Lis and Pierre-Marie Coulon for providing samples and simulation results with which to perform the research. In addition, I would like to thank Prof. Robert Martin and Dr Paul Edwards at the University of Strathclyde for performing cathodoluminescence measurements.

As is often the case in an academic institution, the support staff have been instrumental in enabling progress. I would specifically like to thank Dr Siva Sivaraya for his tireless efforts in the lab and clean room, Dr John Mitchell for his assistance and expertise in electron microscopy, Mr David Parker for his mechanical expertise in helping to construct the measurement system, and Dr Stephen Wedge, Mr Andy Matthews, Mr Neil Deacon and Ms Ursula Potter for their support roles.
Thanks are also due to all those in the III-nitride group and elsewhere at the University of Bath with whom I have shared time, office and/or lab space for their advice, company and consideration, Prof. Wang Wang, Drs Jay Sarma, Quanzhong Jiang, Margaret Hopkins and my fellow students, Katie Cavanagh, Sophie Fox, Paulo Ki, Simon O’Kane, Ionut Girgel, Yiding Zhuang, Chris Hotchen, Alex Sergejevs, Jules Hammond and Ben Metcalfe.
Declaration

This section sets out the extent to which this work has been done in conjunction with others and any work which has been incorporated from a submission for another degree.

Most of the fabrication of the experimental samples was carried out by others. The buried photonic crystal samples investigated in chapter 7 were fabricated by Dr P. Shields. Some of the quantum disc nanorod samples investigated in chapter 8 were fabricated by Dr P. Shields. The core-shell samples investigated in chapter 8 were fabricated by Dr E. Le Boulbar and Dr P-M. Coulon.

The FDTD simulations presented in chapter 8 were carried out by Dr S. Lis and the cathodoluminescence experiments were carried out at the University of Strathclyde by Dr P. Edwards.

The angular luminescence system and prototype data analysis software described in chapter 6 was constructed as part of a project which was submitted as work towards the degree of MEng(hons) Electrical and Electronic Engineering, awarded by the University of Bath in 2011.
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Abbreviations

AC - Alternating current
au - Arbitrary units
BOE - Buffered oxide etch
CCD - Charge-coupled device
CL - Cathodoluminescence
CLM - Cap layer mode
CRI - Colour rendering index
CTE - Coefficient of thermal expansion
DBR - Distributed Bragg reflector
DC - Direct current
DOS - Density of states
EBL - Electron beam lithography
EFS - Equifrequency surface
e-h - Electron-hole
EL - Electroluminescence
ELOG - Epitaxial lateral overgrowth
EQE - External quantum efficiency
FBZ - First Brillouin zone
FWHM - Full-width at half-maximum
HSQ - Hydrogen silsesquioxane
IBZ - Irreducible Brillouin zone
ICP - Inductively coupled plasma
IQE - Internal quantum efficiency
LED - Light-emitting diode
LT - Low-temperature
MBE - Molecular beam epitaxy
MCLED - Micro cavity light-emitting diode
MOVPE - Metalorganic vapour phase epitaxy
MQW - Multiple Quantum Well
NIL - Nanoimprint lithography
PhC - Photonic crystal
PL - Photoluminescence
PQC - Photonic quasi-crystal
QCSE - Quantum-confined Stark effect
QW - Quantum potential well
RCLED - Resonant cavity light-emitting diode
SEM - Scanning electron microscope
TIR - Total internal reflection
UV - Ultraviolet
WPE - Wallplug efficiency
Symbols

\( a \) - the pitch of a crystal lattice  
\( A_{FF} \) - air filling fraction  
\( \Gamma \) - the origin of reciprocal space  
\( D \) - directivity  
\( D_{FF} \) - dielectric filling fraction  
\( \mathbf{E} \) - electric field vector  
\( \mathbf{E}^{' \prime} \) - Etendue  
\( \epsilon \) - relative electrical permittivity  
\( \mathbf{G} \) - reciprocal lattice vectors  
\( \eta_{EE} \) - external quantum efficiency  
\( \eta_{<\theta} \) - the proportion of power emitted within the half angle \( \theta \) of normal incidence  
\( \eta_{IQE} \) - internal quantum efficiency  
\( \eta_{WPE} \) - wall plug efficiency  
\( \mathbf{H} \) - magnetic field vector  
\( \theta \) - angle from normal incidence  
\( i \) - the positive square root of -1  
\( \mathbf{K, M} \) - the points at the edge of the irreducible Brillouin zone of a 2D lattice  
\( \mathbf{k} \) - wavevector  
\( k_{||} \) - component of the wavevector parallel to a slab waveguide  
\( k_0 \) - freespace wavevector or wavenumber  
\( \lambda \) - wavelength  
\( \mu \) - relative magnetic permeability  
\( \mu_{loss} \) - characteristic length of optical loss mechanisms  
\( \mu_{phC} \) - photonic crystal extraction length  
\( m_N \) - the magnitude of a diffraction order, normalised to the magnitude of the first order  
\( n \) - refractive index  
\( n_{eff} \) - effective refractive index of a guided mode  
\( P_{<\theta} \) - power emitted within the half angle \( \theta \) of normal incidence  
\( \mathbf{R} \) - spatial lattice vectors  
\( \mathbb{R} \) - real space  
\( \phi \) - angle of azimuth  
\( x \) - Cartesian direction aligned parallel to the plane of a slab, in-plane direction of propagation if applicable  
\( y \) - Cartesian direction aligned parallel to the plane of a slab  
\( z \) - Cartesian direction aligned perpendicular to the plane of a slab  
\( \omega \) - frequency

Set notation is used on a number of occasions:  
\{...\} - braces are used to denote the enclosed variables are elements of a set  
\|{...}\| - the cardinality (number of elements) of a set  
\( \in \) - element of  
\( \forall \) - for all  
\( \subset \) - subset of
Chapter 1

Light-emitting diodes (LEDs)

Light-emitting diodes (LEDs) are a promising light source for many lighting applications. They have been widely used as indicators on electronic equipment and for low bandwidth optical communications for a number of years. LED-based space lighting products are now becoming commonplace in the market as they begin to become cheap and efficient enough to compete with other lighting sources in a wide range of applications.

1.1 Lighting technology

Before electrical light sources and widespread installation of electrical services, flames were used to produce light. Although this technology became more sophisticated through inventions such as candles and oil lamps, the method of light generation had remained largely unchanged for thousands of years. The first commercial light bulb was invented in 1880 and it used a long-lasting carbon filament. An electrical current is passed through the filament to heat it, creating light via black-body radiation. The assembly is suspended in a vacuum or controlled atmosphere inside a bulb of glass to prevent the filament oxidising at a temperature of around 2700K, providing a viable and safer alternative to an open flame. Modern light bulbs use tungsten filaments due to its high melting point, but are typically limited to around 2.5% efficiency as so much of the electrical energy injected is converted to heat or emitted as invisible infra-red light. Halogen lamps use a halide atmosphere which allows the filament to be run hotter ($\approx 3300K$), and subsequently increases the efficiency to around 3.5% by increasing the proportion of visible light emitted.

Fluorescent tubes became available in c.1940 and more practically-sized compact fluorescent lamps (CFLs) in c.1980. These work by exciting electrons to higher energy states, commonly in a mercury vapour, which emit high energy ultra-violet (UV) photons. The UV photons are re-absorbed through the photoelectric effect by the mercury and other substances known as phosphors by exciting electrons, which fall in energy and then are re-emitted as lower-energy visible light. The light from the mercury has specific narrow
spectral peaks due to the quantised nature of the available energy states of electrons around the atoms, but phosphors can be designed to emit over a broad band. Typical phosphors are designed to emit in the green and red, whilst the mercury emits primarily in the violet-blue, creating what is perceived as a white-light source. A spectrum of a typical fluorescent lamp is shown in figure 1.1b.

As the spectrum from a fluorescent source has visible wavelengths with little or no light emission, some colours cannot be faithfully represented when illuminated. This effect is measured using the colour rendering index (CRI), which is given as a percentage of the total visible spectrum which can be represented by a light source. The lumen (lm) unit is used to quantify the perceived total light output, which is a measure of the total optical power emitted by a source weighted in colour by the eye’s sensitivity. The maximum possible efficiency is provided by a single wavelength green source at 555nm of 683lm per watt of optical energy, as the human eye is most sensitive to this wavelength. For an ideal daylight source, this upper limit to efficiency becomes around 250lm/W at 100% CRI for light with a spectrum of a black body radiator (at 5800K), but the value is quite sensitive.

Figure 1.1: Spectra of common light sources.
to the exact colour of the source. With careful consideration of the output spectrum, it should be possible to produce an acceptable light source with an efficiency of up to 350lm/W [4].

Whilst the first known reported light emission from the solid state was in 1907 [5], the first practical devices were observed in 1962 and emitted in the infrared from the pn junction formed between n and p-doped GaAs layers [6]. Red LEDs were developed using the GaAsP material systems throughout the 1960s [7] and then green in c.1970, giving a range of colours for indicating applications in electronic devices, but with too little brightness for useful illumination. In the 1980s, high brightness red and yellow LEDs were demonstrated using AlGaInP, but it was found that efficient green or blue LEDs could not be created with these materials. In the early 1990s, a breakthrough was made by Nakamura et al. who demonstrated high brightness blue LEDs in the InGaN material system [8]. The work resulted in the award of the 2014 Nobel prize for physics to Nakamura, Akasaki and Amano and enabled white light LEDs to be created by illuminating a phosphor with blue light. An example spectrum of the combination of a red-green phosphor and a blue light LED source is shown in figure 1.1c and is representative of most commercial white light LEDs, particularly for high-brightness lighting.

1.2 LED operation

LEDs produce light through spontaneous emission of photons from a semiconductor. An electron in the conduction band recombines with a hole in the valance band and loses a discrete quantity of energy as a single emitted photon, approximately equal to the band gap of the semiconductor. The recombination process can be radiative, where a photon is produced, or non-radiative, where the energy is released in other ways such as as thermal energy through lattice vibrations. The electron and hole (e-h) pair must have approximately the same momentum to recombine readily, which is the case only in a semiconductor with a direct band gap and additionally, the excited e-h pair must be close enough together in space. A localised e-h pair can be created using a source of photons with energy greater than the band gap, which is absorbed via the photoelectric effect. The excited electron will typically fall in energy to the low-energy edge of the conduction band through non-radiative processes and then recombine with the hole to produce photon luminescence. This method is frequently used in research with a laser as the source and is termed photoluminescence (PL). Excited electrons can also be directly injected through an electron beam, known as cathodoluminescence (CL). Although these methods of producing light are used in select applications, such as cathode ray tube (CRT) displays, neither method is usually useful for LED emission outside of research.
Instead of relying on either of these processes, the e-h pairs can coincide in space at a semiconductor pn junction, with the electron and holes injected as electrical current into the n and p-type layers respectively in a process known as *electroluminescence* (EL). The electrons and holes are given enough energy to flow in the semiconductor by forward biasing the junction above the band gap voltage. This requires the semiconductor forming the device to be doped – the difficulties doping GaN as p-type was a significant obstacle to the development of high-brightness blue LEDs. Using a pn junction, a practical device can be realised which allows a small DC voltage and current to be directly converted to light with, in principle, 100% efficiency. Localising e-h pairs for efficient operation is a challenge affected by many factors and is discussed in chapter 2. If the junction is reverse biased, it can be used to convert light into a detectable current as e-h pairs generated by incident light can be separated in space before they can recombine, creating a photodiode.

### 1.3 LED applications

As LED technology has improved, new applications have opened up for their exploitation. The largest market for white LEDs is backlighting for thin-film displays in laptops, smart phones, televisions and similar consumer devices due to their commoditisation. Domestic and commercial space illumination is an expected application for high-brightness LEDs, where the LED must be as efficient as possible at high output power, be priced appropriately for the market and have a suitable colour. Indeed, commercial lighting products based on LEDs have become readily available in the last decade. Less typical applications coming to market after significant research effort include horticultural lighting for growing plants where sunlight is not available, UV sources for curing materials and other illumination applications such as torches. LEDs may make excellent sources for headlights and projectors, enabling miniaturisation, but at present their usefulness is restricted by their relatively low maximum brightness compared to other sources such as arc lamps. High brightness UVA and UVB LEDs are the focus of much attention due to their potential for surface and water sterilisation, medical and sensing applications.

These different applications require different characteristics and for uptake, it is important that a new product for each application provide suitable cost savings or performance enhancements over the alternatives. In battery powered devices, the most important figure of merit is the efficiency as the energy required to light e.g. a display is usually a significant limitation to battery life. The CRI is important for good reproduction of colours and weight may be a factor for the smart phone market. For space lighting, the concern of the market is the cost of running and replacing fixtures over time for a given lighting level and colour quality. For example, an expensive device with a long lifespan and low energy consumption may work out more economical than a cheap device with high energy usage.
and short lifespan, or an art gallery or restaurant may require excellent CRI. In torch, headlight and projection applications, the cost becomes less of a concern and is primarily replaced by the need for high efficiency and brightness, and specific applications may require compact and/or lightweight devices. For horticultural applications, high brightness is required and the colour must be carefully chosen to match with the plant’s requirements.

1.4 Étendue-limited applications

LEDs have the potential to provide ultra-efficient light sources close to theoretical maximum performance with suitable device design and are becoming widely used for many applications requiring long life span and high efficiency, such as space lighting. However, the low-cost devices suitable for the space lighting market are limiting for étendue-limited applications due to their low overall brightness compared to alternative sources. The polar emission pattern of sources is also critical as not all the light emitted can be used in these applications. For example, in a projection system only the light scattered from the screen is of use to the viewer and car headlamps require the light to be directed on to the road in front of the vehicle. Any light from the source which cannot be sent to the intended place by the optical system is clearly wasted, leading to inefficiencies. When considering these and similar applications, the most straightforward measure for characterising performance is the perceived brightness or luminance, which is the luminous flux per unit area of source (in this case the illuminated road or screen) per unit solid angle. This quantity is restricted by many parts of the optical system, and those that apply to the illuminating light source at the start of optical system are its luminance and how much luminous flux can be collected and directed towards, for example, the road or screen. §9.1.1 provides a more detailed discussion of why directional and high-brightness sources are required for these applications.

Research-grade devices have been demonstrated which will produce slightly better performance than devices fabricated by widely-used commercial techniques, but their marginal increase in performance does not justify the increased complexity of fabrication. LEDs with more directional emission and higher brightness than those available at present are required for étendue-limited applications, and will enable higher performance and miniaturisation of optical systems such as projectors, torches and headlamps. The rest of this thesis investigates whether photonic crystal LEDs are suitable for increasing the performance of blue InGaN/GaN LEDs for étendue-limited applications.

The study is arranged as follows: Chapter 2 summarises the status of research into the concepts affecting LED efficiency and highlights the current challenges to performance. Chapter 3 describes the physics of photonic crystals and photonic crystal LEDs. Chapter
4 reviews research into the operation and performance photonic crystal LEDs for improved light extraction and device efficiency. Chapter 5 describes the development of a transfer matrix model for the emission from a light source embedded in a slab waveguide, used to simulate the behaviour of light trapped in an LED in the subsequent investigation. In chapters 7 and 8, experimental observations made using angular luminescence are analysed to understand and model the operation of photonic crystal LEDs, with the angular luminescence system described in chapter 6. Specifically, chapter 7 investigates buried photonic quasicrystals as a diffraction grating and their suitability for increasing the extraction efficiency and directivity of LEDs. Chapter 8 experimentally investigates nanorod and core-shell LEDs where the light is emitted inside the photonic crystal, and shows that it is possible to use the photonic crystal to change the behaviour of the light in the device so the periodicity dominates, operating in the Bloch regime. Chapter 9 consists of an investigation into the operation and performance limits for directional light emission from LEDs in both the diffractive and Bloch regime, showing the Bloch regime offers a pathway to highly directional emitters for étendue-limited applications.
Chapter 2

LED efficiency

The overall efficiency of an LED depends upon the efficiencies of the different stages of light production and energy transfer in the device, each of which are discussed in their own section below.

- **Injection efficiency,** $(\eta_{\text{inj}})$ – The proportion of carriers supplied to the active region of the device that undergo recombination, both radiative and non-radiative\(^1\). For modern LED designs, most research considers $\eta_{\text{inj}} \approx 100\%$, and an effect not applicable to photoluminescent excitation as the carriers are created in the active region.

- **Internal quantum efficiency,** $(\eta_{\text{IQE}})$ – The ratio of carriers reaching the active region which undergo radiative recombination to the total number of carriers that undergo both radiative and non-radiative recombination. $\eta_{\text{IQE}}$ is a substantial limiting factor in the performance of InGaN/GaN LEDs for high brightness applications as it ‘droops’ with increasing current density.

- **Extraction efficiency,** $(\eta_{\text{ext}})$ – The proportion of photons which are emitted in the active region which leave the LED. Without applying light extraction techniques, this is $\approx 5\%$ for GaN LEDs. Conventional surface roughening and encapsulation techniques can achieve up to 90\%, but both the encapsulation and resulting Lambertian emission pattern reduce the extracted light available for use by an order of magnitude when considering étendue-limited applications.

- **External Quantum Efficiency,** $(\eta_{\text{EQE}} = \eta_{\text{inj}} \eta_{\text{IQE}} \eta_{\text{ext}})$ – The proportion of carriers entering the device which exit the device as photons after undergoing radiative recombination.

- **Wall plug efficiency,** $(\eta_{\text{WPE}})$ – The ratio of the total optical power output from the device to the electrical power supplied to the device. This takes into account resistive

\(^1\)Some literature refers to this as part of the internal quantum efficiency, due to the difficulties in experimentally separating $\eta_{\text{inj}}$ from $\eta_{\text{IQE}}$. 
losses where electrons lose energy and can include electrical conversion efficiency (e.g. AC-DC conversion) and the electrical power dissipated in surface currents. It may also include application specific effects, giving the ratio of the optical power which can be made use of to the electrical power supplied. OSRAM claim a laboratory $\eta_{WPE}$ of 205lm/W for a white LED with a CRI of 90, and Cree $\eta_{WPE}$ of 303lm/W for an unstated CRI.

The vast majority of published research considers the efficiency compared to a control sample without providing absolute values using a consistent method, only quantifying the improvement. Most studies address ways to improve on one problem causing performance limitations without considering its effect on other parameters, and so values quoted in the literature therefore can rarely be applied directly to calculating the best achievable device performance. As a result, it is only possible to describe most of the efforts and the problems which are approached qualitatively. The purpose of this chapter is therefore to provide information on the present challenges to efficiency performance, and identify the scope for improvement. In the subsequent sections, understanding of the source of and methods to enhance each efficiency limitation are discussed.

### 2.1 Injection efficiency

Some electrons pass straight through the active region in an LED in forward bias without recombining with holes. In the Shockley theory of the diode, this is known as the *diffusion current*\textsuperscript{2}, but some texts \cite{10} refer to this as the *leakage current*\textsuperscript{3}. LED emission was first observed at a homojunction at very low efficiency \cite{6,7}, where most of the injected electrons have sufficient energy to overflow the active area, as shown in figure 2.1a. Double heterostructures consisting of a semiconductor layer embedded in a wider band gap semiconductor form an electron potential well, as shown in figure 2.1b. The potential well can trap carriers more efficiently than at the homojunction formed at the interface between n and p-doped layers of the same semiconductor as carriers need to gain thermal energy to escape the potential well. Before carrier overflow, heterojunction LEDs perform at close to 100% injection efficiency, neglecting surface leakage effects. In the InGaN material system, LEDs are typically formed with bulk n and p-GaN sandwiching a thin (few nm) InGaN layer, which forms a *quantum well* (QW) for the electron energy states.

\textsuperscript{2}See for example Dimitrijev \cite{9}.

\textsuperscript{3}Here, leakage current refers to a separate phenomenon to that often referred to as leakage current in the study of electronic devices (the current which flows or ‘leaks’ through a device when under reverse bias).
Chapter 2. LED efficiency

2.1 Carrier distribution and overflow

The distribution of electrons in energy follows the Fermi-Dirac distribution function. As a result, some carriers will occupy an energy level greater than the confining ‘wall’ of the well, as shown in figure 2.1c, causing carriers to escape out of the active region by diffusion without recombining. As the injection current is increased, the Fermi level (shown as $E_{Fn}$ in figure 2.1c) increases slightly and so the proportion of the carrier distribution at a higher energy than the potential barriers becomes larger. When the carriers are injected into the device faster than they can recombine in the active region, the potential well can be said to become full. Carrier overflow now becomes a significant loss process compared to the intended recombination in the active region. As a result, the optical intensity saturates and cannot increase substantially for a higher injection current, leading to a reduction in efficiency for high brightness applications. The effect becomes more pronounced as the width (and therefore capacity of electron states) of the potential well becomes smaller and similarly, as the temperature is increased, the efficiency will decrease as it becomes more probable for electrons to occupy higher energy levels and diffuse out of the potential well.

To recapture carriers which have escaped the potential well before they have recombined, additional wells can be added to trap carriers which have escaped from previous wells. For example, a study by Hunt et al. presents a practical illustration of this effect, showing a >6-fold increase in the saturation level of light output for 8 QWs when compared to a single QW [11]. This provides a 6-fold enhancement to the light emission intensity of the device before carrier overflow causes the injection efficiency to decrease.
from near to 100%. An additional layer with a larger band gap can be added on the p-side of the active region – this creates a area of high potential which acts to block carriers escaping the potential wells. As a result, only electrons with very high energy can escape and leak through this electron-blocking layer [10], allowing the effect of carrier overflow on the efficiency to become insignificant, although some researchers consider it to be the cause of efficiency droop (discussed later). AlGaN is often used as an electron blocking layer in GaN LEDs.

2.1.2 Surface leakage

Non-radiative current paths can be formed by defects created in the crystal lattice at the interface with the surfaces and edges of the device. This surface leakage causes an additional loss mechanism, which can be included in injection efficiency – attributed to the surface of the sidewalls of a device mesa in e.g. [12, 13] or damage during laser lift off in vertical LEDs [14]. The quantitative significance of this effect on overall device efficiency is not reported in any published work known to the author, but some effort has been focussed towards reducing the leakage currents. For example, Kim et al. report that a device with photoresist passivated sidewalls to control the crystalline properties at the surfaces reduced the -5V reverse leakage from 400nA to 4nA. The influence of this effect depends upon the device design, and is usually managed by passivation and avoiding excessive sidewall area. Difficulties in mitigating this loss path are created as the mesa design is key to many device performance considerations, such as current spreading and contacting (discussed later).

2.1.3 Summary

The electronic band structure of the LED affects the carrier overflow and the device layout affects the surface leakage. Injection efficiency and surface leakage losses are rarely cited as significant limiting factors to efficiency beyond the need for electron blocking layers and heterostructures. Commercial LED manufacturers will have optimised their designs to minimise these effects, possibly through exhaustive parameter scans. Surface leakage is significantly greater in device designs with much larger surface areas such as nanorod LEDs, discussed in §4.3.
2.2 Internal quantum efficiency

The internal quantum efficiency (IQE) is the ratio of carriers in the active region which recombine radiatively to those which do not and is very often referred to as a figure-of-merit for device performance. The usual way to consider the recombination in the device is through the rates of the different processes, i.e. the time required for a given proportion of the carriers to recombine. Figure 2.2 summarises the recombination mechanisms commonly thought to occur in III-nitride quantum wells. The IQE can be determined from the relative rates of radiative and non-radiative recombination, once the carrier density dependence of the rates is taken into account. The obvious effect the IQE has on the device performance means it is the subject of intense research and accompanying debate, but it is beyond the scope of this thesis to present more than an informative overview.

As the emission wavelength is increased in InGaN QWs from blue (450nm) to green (570nm) by increasing the indium content, the IQE is observed to decrease substantially down to <10%. When the emission wavelength is decreased from the red into the green in the InAlGaP material system, the IQE also drops to <10%, leading to the green gap. Figure 2.3 graphically illustrates the wavelength range (≈520-580nm) where high efficiency LEDs are challenging to produce [15].

The primary causes of recombination inefficiencies in InGaN LEDs are charge separation in quantum wells and non-radiative recombination (which usually includes light not emitted at the intended wavelength) [16]. Additionally, droop of the efficiency with at the high current densities due to an effect not agreed upon in the literature is a significant limiting factor.

2.2.1 Non-radiative recombination

Crystallographic defects are extensively cited as a significant cause of non-radiative recombination. They can take the form of one of or a combination of single defects of two types: misalignments in the crystal structure referred to as dislocations (sometimes extended defects), or faults in the atomic structure referred to as native or point defects, such as additional (interstitial), missing (vacant) or impurity atoms. Defects have different electron and hole energy levels locally which often create energy levels in the band gap of the semiconductor. These can form very efficient recombination centres [17,18] via the deep level recombination process shown in figure 2.2. Some deep level recombination is radiative and can be observed using PL studies through emission of lower energy yellow wavelengths termed defect luminescence, and the effect is temperature and excitation intensity dependent [17].
Figure 2.2: Recombination mechanisms (a) deep level (b) Auger (c) radiative – from [10].

Figure 2.3: Illustration of the green gap, where $V(\lambda)$ shows the luminosity function. Reproduced from [15] ©2007 IEEE.
The LED structure must be grown on a supporting substrate material, which ideally has a matching lattice constant to produce high quality crystals free from cracks and defects. The ideal substrate for GaN growth is GaN itself as it is perfectly lattice matched, but high-quality native substrates are highly expensive and difficult to manufacture in sizes suitable for cost-effective mass production. Although the availability of GaN substrates is improving, alternative substrates are still most often used. When selecting a substrate, both the match between the lattice constants and the coefficient of thermal expansion (CTE) need to be considered to control the strain and prevent cracking during cooling after growth. For GaN devices, sapphire ($\text{Al}_2\text{O}_3$) has a reasonable lattice and CTE match and is often used as a substrate both commercially and for research due to its relatively low cost and high transparency. Silicon carbide is transparent and conducting with a reasonable lattice and CTE match, but Cree Inc. have concentrated on commercialising LED devices grown on SiC with many patents and so literature on the subject is limited. More recently, there have been successful efforts to produce GaN LEDs from silicon substrates due to the very low cost and high availability of large wafers, partially driven by semiconductor companies to put to use redundant silicon processing lines. Silicon is optically absorptive and does not have a good CTE match, but is a better thermal conductor than sapphire and is electrically conductive. Other properties of the substrate, such as transparency, electrical and thermal conductivity are potentially desirable, depending upon the overall design of the device. A good review of the properties of substrates used for producing GaN is presented by Kukushkin et al. [19].

There is disagreement upon which types of defects contribute most significantly to the non-radiative processes and therefore where optimisation efforts should focus to reduce losses through this channel [20]. Dislocations are created in strained epitaxial layers grown on a material with a lattice and/or CTE mismatch. The mismatches causes strain to build up during material growth or subsequent cooling, which is released through cracks and dislocations once of sufficiently high magnitude. Strain also degrades the IQE through charge separation, and is discussed in the next section. In the 1980s, Yoshida et al. and Amando et al. both reported using an AlN layer with a similar CTE to GaN to improve the crystal quality when grown by molecular beam epitaxy (MBE) on a sapphire substrate [21,22], for example increasing the Hall mobility (an indicator of the semiconductor defect density) from $\approx 10\text{cm}^2/\text{Vsec}$ without the AlN layer to $\approx 35\text{cm}^2/\text{Vsec}$ in [21]. In 1991, Nakamura found that growing a GaN buffer layer by the much faster metalorganic vapour phase epitaxy (MOVPE) method at lower temperature before growing a GaN film substantially improved the crystal quality of the film [23], giving $600\text{cm}^2/\text{Vsec}$ mobility. Low-temperature (LT) GaN buffer layers are now very frequently used in modern LED structures and helped enable the first practical blue-emitting devices to be made [8], with
an EQE of 0.18%. Iwaya et al. and Amano et al. reported further improvement in crystal quality using an additional LT buffer layer after growth of a GaN film on top of an initial LT layer [24], which was extended to study several LT interlayers shortly after [25]. These methods leading into the 21st century all primarily control strain relaxation to decrease the number of dislocations created during growth and enabled widespread commercialisation of blue LEDs.

An alternative technique was presented by Nam et al., who found that lateral overgrowth with a very low defect density could occur over a SiO$_2$ growth mask [27]. They exploit this finding by creating thin parallel stripes of SiO$_2$ on top of a GaN film, allowing vertical growth in between the stripes. After sufficient vertical growth, the conditions are changed to favour lateral growth of ‘wings’ until the material from adjacent stripes coalesces to form a low defect density film. This method is often referred to as epitaxial lateral overgrowth (ELOG) and is illustrated in figure 2.4. By interrupting the growth and changing its direction, dislocations are ‘blocked’ by the growth mask, giving the wings very low defect densities. The low defect density in the wings contributed to enabling blue laser diodes to be manufactured at a good yield and performance, allowing higher density optical storage through DVDs to become commercially feasible in the late 1990s. Further improvements to defect density were seen by Kidoguchi et al. by shaping and masking much larger regions to create an air gap between the overgrown GaN and the mask in a technique they called air-bridged lateral epitaxial overgrowth [28]. ELOG can be extended into 2D and the nano-scale, using nano-scale patterning to produce the growth mask [29], termed nanoheteroepitaxy or nano-ELOG, which provides low defect density over a large

Figure 2.4: Epitaxial lateral overgrowth. Reprinted from [26] with the permission of AIP Publishing.
area. Bougiroua et al. created very low defect density GaN using dislocation-free nanopillar GaN seeds grown by MBE [30]. Both self-ordered and regular arrays of nanocolumns have been used to produce low defect density material [31–33] and this technique continues to be explored for GaN growth in various crystallographic orientations. Table 2.1 summarises the defect densities reported from the different growth techniques.

<table>
<thead>
<tr>
<th>Technique</th>
<th>Defect density (cm$^{-2}$)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single LT GaN buffer layer</td>
<td>$4 \times 10^9$</td>
<td>[25]</td>
</tr>
<tr>
<td>Single LT AlN buffer layer</td>
<td>$2 \times 10^9$</td>
<td>[25]</td>
</tr>
<tr>
<td>6x LT GaN buffer layer</td>
<td>$5 \times 10^7$</td>
<td>[25]</td>
</tr>
<tr>
<td>Air-bridged ELOG</td>
<td>$1 \times 10^6$ in wing, $9 \times 10^8$ in seed</td>
<td>[28]</td>
</tr>
<tr>
<td>NanoELOG</td>
<td>$&lt; 1 \times 10^8$</td>
<td>[30]</td>
</tr>
<tr>
<td>Nanocolumn overgrowth</td>
<td>$3.9 \times 10^7$</td>
<td>[32]</td>
</tr>
</tbody>
</table>

Table 2.1: Defect densities of GaN reported.

During Auger recombination (see figure 2.2), the energy from an e-h pair is lost by elevating another electron in the conduction band to a high energy level instead of through emission of a photon. The magnitude of the effect is dependent upon the cube of the carrier concentration and occurs with lower probability as bandgap energy increases, so is often considered negligible at lower injection currents and for wider band gap materials. It is not understood why, but Auger recombination is reported to be much higher in III-nitrides than expected from analysis of other III-V semiconductors [34]. However, there is debate over whether the assumptions of the model most commonly used to calculate the Auger coefficient are valid as the effects of electron leakage are neglected [34]. Indeed, Li et al. have shown that models for both Auger recombination and carrier leakage could explain experimental observations, particularly from PL measurements [35]. Some groups have even reported a reduction or absence of the Auger recombination coefficient in nanowire LEDs grown by plasma assisted MBE [36,37]. The role of Auger recombination in efficiency droop (see §2.2.3) provides heated debate between research groups.

As the band structure of a semiconductor depends upon the periodicity of the crystal lattice, the band structure will become different at surfaces due to the termination of the periodicity. Furthermore, dangling bonds or slightly modified atomic structures where atoms do not have another to bond to are common at surfaces and will also distort the band structure. This distortion of the band structure can introduce deep levels and is thought to be the cause of surface recombination which also causes heating at surfaces. To reduce the effect of surface recombination, the concentration of carriers at surfaces at or near the active regions can be controlled by good design of the contacts and current flow in the device. Careful device design is required to keep the surface area available for...
recombination to a minimum, but will be a trade-off with other device parameters \([10]\). Surface recombination is often considered as contributing to surface leakage currents, and is caused by the same effect.

### 2.2.2 Charge separation

III-nitride semiconductors are strongly polar materials, exhibiting both piezoelectric and spontaneous polarisation in their Wurtzite crystal form. Figure 2.5 shows the conventional labelling of the crystal axes and the various planes of the Wurtzite structure. The polarisation is along the \(c\)-axis, due to the alternating layers of Ga and N in the \(c\)-plane forming dipoles \([38–40]\). The dipoles create an electric field along the \(c\)-axis when under strain, such as in the QWs due to the lattice mismatch between the wide bandgap barrier layers and narrow bandgap potential wells. The difference in the spontaneous polarisation constants between the two materials in the QWs creates an additional electric field, which superposes on the piezoelectric field to give the total polarisation. In conventional GaN LEDs grown with the QWs parallel to the \(c\)-plane, the polarisation-induced electric field causes distortion of the intended band structure as in figure 2.6a. For an InGaN/GaN interface, the primary polarisation effect is caused by the strain on the InGaN layer as there is a large lattice mismatch, whereas for an AlGaN/GaN the effect is primarily caused by the large difference in spontaneous polarisation \([41]\).

The distortion of the band structure forces the wavefunctions of electrons and holes trapped in the QWs to be physically separated to opposite sides of the QW, shown in figure 2.6b. The rate of radiative recombination is proportional to the overlap of the wavefunctions of the electron and hole states in consideration integrated over all space. Spatial separation of the electron and hole induced by a polarisation field will cause the radiative recombination rate and therefore IQE to decrease compared to the situation when there is no field \([42]\). A further effect is to narrow the effective bandgap and red-shift the emission, as illustrated in figure 2.6a. This effect is termed the *quantum-confined Stark effect* (QCSE) and was first reported by Miller et al. in AlGaAs/GaAs QWs \([44]\), observed by a red-shift in the emission wavelength from structures with a higher polarisation. In strained InGaN QWs, the QCSE was first reported by Takeuchi et al. who observed a blue shift with increasing carrier density \([45]\), as the field from a higher charge density acts to screen the polarisation-induced field.

Efforts to reduce the QCSE have mostly been reported by growing LEDs in the semipolar (e.g. \(r\)-plane) or non-polar \(a\) or \(m\)-plane orientations of InGaN/GaN where there is a reduced or zero polarisation field, discussed in detail by Park et al. \([46, 47]\). This is a simple solution, but these orientations cannot easily be grown on practical substrates.
Figure 2.5: Crystal planes and axes in the wurtzite structure, from [42], ©2009 IEEE.

(a) Effect of polarisation field on band structure, (above) with no field, (below) with field. From [43].

(b) Wavefunctions in QW (left) with no field, (right) with polarisation field. From [42], ©2009 IEEE.

Figure 2.6: The quantum-confined Stark effect (QCSE) – the influence of a polarisation-induced electric field on the band structure.
with a high enough crystal quality to produce efficient LEDs and is the subject of much research [48, 49]. Non-polar GaN devices have been grown which show little or no blue shift with increasing excitation indicating a reduced QCSE [50–53], which were grown on bulk c-plane GaN substrates sliced at an angle to produce a- or m-face GaN substrates. The growth conditions were found to be much harder to control than for the c-plane and initially very low EQEs were reported for photon emission in the 455nm [50] (≈0.5%) and 435nm [51] (≈3%) regions. Later attempts [52] and violet (407nm) [53] LEDs have produced better results (17% EQE). Device-quality non-polar GaN has also been grown recently on more commercially viable non-native substrates by exploiting the strong growth in the c-axis direction using selective ELOG [49]. The useable non-polar GaN is ‘built’ from a high defect density non-polar GaN film on a mismatched substrate. Stripes are etched away back down to the substrate and then the growth conditions are set to regrow the areas etched away through low-defect lateral growth in the c-axis direction. This growth is continued once the etched gaps are filled to produce upward and then once again lateral high quality growth [54], producing a smooth surface suitable for LED fabrication.

Several studies have been undertaken into the use of a deliberately strained layer designed to reduce the QCSE by managing strain in the active region. Huang et al. reported results using an InGaN layer below the active area with a lower indium content to pre-strain the device [55]. This actually resulted in increased QCSE, but the method does assist the high indium incorporation required to produce long-wavelength emitters. Ryou et al. investigated devices with a p-InGaN layer grown above the active layer and report that the polarisation field was reduced compared to a conventional device, giving a higher light output intensity than devices without the p-InGaN layer [56]. Reed et al. report a similar technique and result, but using an n-InGaN layer on a p-GaN p-side down device [57]. Schubert et al. have used AlInGaN interlayers between the InGaN QWs to reduce the polarisation mismatch, primarily in an attempt to reduce the leakage from polarisation effects [58] and report improved efficiency with less blue shift (and so reduced QCSE) at high injection currents in the droop regime when compared with a control sample. Etching planar LEDs with strained QWs into arrays of nanorods has been shown to relax the strain of the InGaN layer and reduce the QCSE [59–62] and has recently resulted in high performance devices [63].

Screening of the polarisation field by doping the active region with donors has also been shown to be successful in reducing the QCSE [64,65]. Zhao et al. directly approached the problem and showed a doubling in efficiency for ‘staggered’ QWs by creating layers with different indium composition to engineer the spatial wavefunction overlap to be larger compared to an unstaggered control sample [16].
2.2.3 Efficiency droop

As the injection current is increased in III-nitride LEDs, the IQE is observed to increase at low injection currents, then decrease in a phenomenon known as *efficiency droop*, illustrated in figure 2.7. The cause of efficiency droop is not known, but is the subject of much research as it is a major limiting factor in the performance of high brightness devices [34]. Researchers from UCSB claim to have ‘solved’ droop, arguing that their experimental observations are confirmation that phonon or defect-assisted Auger recombination is the cause [66]. However, a few mechanisms have been proposed to be the cause of droop and the literature is not in agreement. Indeed, droop may be due a combination of effects [67]. Several groups agree that phonon-assisted Auger recombination, which increases with increasing current density, has an influence [66,68–70], and that it is unlikely to be direct Auger recombination [71]. Droop is also regularly attributed to increasing carrier leakage with increasing injection current [72–74].

![Figure 2.7: Typical efficiency droop of InGaN LEDs, from [75], ©2013 Wiley-VCH.](image)

Many of the arguments for carrier leakage as the cause of droop are founded on whether droop is observed for PL excitation, which is in principle not subject to injection efficiency effects. When this assumption is made, the carrier leakage is often neglected from the recombination models used to analyse PL experiments, which can be interpreted to suggest Auger recombination is the cause of droop, for example in [76, 77]. However, some work concludes that droop is present in PL experiments at high excitation density [68, 76], whereas other work refutes this [72]. Schubert *et al.* argue that carrier leakage at high PL intensity cannot be ignored due to escape of photo-generated carriers from quantum wells,
and that this is the cause of droop observed in PL experiments [78]. Auger recombination could therefore be coupled to carrier leakage as it creates carriers with energies high enough to leak out of the quantum wells and over the EBL, which may explain the disagreement about the origin of droop as different interpretations of the same results [34]. To support the conclusion that droop is the result of Auger recombination-induced carrier leakage, research has reported decreased droop using both enhanced electron blocking techniques to mitigate carrier overflow [79, 80], and thicker or staggered active regions intended to reduce Auger effects [16,77,81,82].

An alternative theory gaining in popularity suggests droop could be caused by localisation of carriers in the QWs suppressing defect-assisted non-radiative recombination at lower QW carrier densities. Work by Hsueh et al. reports an increase in efficiency when carriers are deliberately localised by creating indium-rich areas [83] and Badcock et al. correlate temperature and excitation power dependent PL measurements with the localisation of carriers [84]. Localised regions with higher indium concentration in the QWs create efficient radiative recombination centres which trap carriers due to the slightly lower bandgap energy, keeping the carriers away from non-radiative defect recombination centres and providing a high IQE. When the QW carrier density is increased, these local potential wells overflow, allowing the carriers to recombine at the non-radiative sites and thus causing droop of the IQE.

Given that several independent research groups support each possible cause, it seems likely that it can be caused by an interacting combination of multiple factors, likely by Auger recombination-induced carrier leakage and by carrier localisation through indium clustering. Both these effects are intrinsic to the material and do not have a clear mitigation path, so techniques to reduce droop will need to focus on reducing the operating current density.

### 2.2.4 Summary

The primary causes of internal quantum inefficiencies are crystallographic defects, which produce non-radiative recombination channels, and poor electron-hole wavefunction overlap due to the QCSE, leading to a reduction of the radiative recombination rate. With increasing emission wavelength, the indium content of the quantum wells is increased, leading to increased QCSE and strain, reducing the IQE. As a result, green emitters typically have a lower IQE than blue emitters. The peak IQE values which could be found in the available literature were reported by Sano et al. [85] and are summarised in table 2.2.

The efficiency also depends upon the current density, with ‘droop’ in the IQE at increasing injection currents. A typical relationship between IQE and current is shown in figure 2.7, showing that a high-current LED may operate at less than half its peak effi-
efficiency. Whilst progress has been made towards improving efficiency droop, it is still not well understood and remains a significant challenge for high brightness devices as at high current the IQE is often much lower than for optimal current. If droop is inherent to material effects in InGaN LEDs and cannot be mitigated, then the designed device operating current density must be reduced to coincide with the peak IQE for most efficient operation. This requires an increase in the active area of a device, which is available in core-shell structures and discussed in §4.3.

### 2.3 Extraction efficiency

GaN has a refractive index \( n \) of \( \approx 2.5 \) for blue light. Total internal reflection (TIR) will occur for any light travelling inside a GaN LED at an angle greater than the critical angle of \( 23.6^\circ \) from surface normal for an interface with air. Light which is propagating at an angle less than the critical angle can escape and is said to be inside the extraction cone or air cone as in figure 2.8, but will be subject to further Fresnel reflection where part of the optical power is reflected back into the LED. When sapphire \( (n \approx 1.8) \) is used as a substrate, it has a critical angle for GaN of \( 46^\circ \). Light rays can be in the air cone, trapped by TIR in the sapphire and GaN or trapped by TIR in just the GaN, depending upon their angle of travel. The problem of light extraction becomes much greater for optically absorbent substrates such as silicon \( (n \approx 4.5 \) at 450nm) as a substantial proportion of the light directed towards the substrate will pass into the silicon and be absorbed. Without taking into account Fresnel reflection inside the air cone, only \( \approx 4\% \) of the light emitted inside a bulk GaN will be extracted directly from the top surface [86], giving an extraction efficiency of 24\% if all six sides are extracted.

Light trapped in the LED will propagate to the sidewalls of the device, where it may again undergo TIR or exit through the extraction cone at this vertical interface. Light unable to escape the LED will eventually be absorbed by metal contact layers, in the GaN or substrate by free carrier absorption or impurities or re-absorbed by the QW structure. In the case of re-absorption by the QW, the e-h pair created may radiatively recombine again in a process termed photon-recycling, but any enhancement to \( \eta_{\text{ext}} \) from this process
Figure 2.8: Light rays emitted by an LED. Red: Light extracted. Blue: Light trapped in the GaN. Green: Light trapped in GaN and sapphire.

will be negligible if the IQE is not close to unity [15].

Light rays within the extraction cone but which are partially reflected through Fresnel reflection at the interface will interfere with earlier and later Fresnel reflections of the same light ray, often called Fabry-Pérot interference. This effect creates a series of resonances or Fabry-Pérot modes which are extracted from the device over the course of a few reflections. They are observed as a series of interference or Fabry-Pérot fringes in light emission intensity both spectrally and spatially, as shown in figure 2.9 for an example LED. The interference depends upon the width of the GaN cavity relative to the wavelength of the light and so the periodicity of the fringes can be used to measure the size of the optical cavity. Light which is travelling in Fabry-Pérot modes will propagate in the device for a time before being extracted, so a proportion of the optical power will be absorbed even though it is in the extraction cone. Fabry-Pérot modes can be observed easily with EL and PL techniques and so the fringes can offer a good probe into the strength of light guiding present within a device.

Figure 2.9: Fabry-Pérot fringes in a planar InGaN LED grown on sapphire, data obtained during the current work.
It is important to consider how much of the optical power radiated from the device can be used for the application the LED is chosen for as part of the complete optical system. When the optical system is étendue limited, such as projection or car headlamps, a more directional light source will allow higher performance due to increased luminance for angles near normal incidence [87]. As a result, the efficiency of a lighting system using an LED may be increased considerably by modifying the direction of emission of the optical power from the LED. Chapter 9 of this thesis considers the restrictions that an étendue limited system places on the source, the benefits of directional emitters and presents results towards ultra-directional LEDs.

The rest of this section discusses the most common approaches to improving the extraction efficiency and their performance. Most research reporting on extraction efficiency techniques compares the performance of the investigated approach with a control sample from the same wafer or growth run (and therefore comparable IQE), with few studies measuring the IQE of the samples to determine the extraction efficiency in isolation, rather stating the EQE if at all.

2.3.1 Encapsulation

A simple enhancement of $\eta_{\text{ext}}$ can be achieved by using a transparent epoxy encapsulation ($n \approx 1.4$) around the LED which is shaped as part of the packaging process. Increasing the refractive index at the LED surface increases the effective size of the extraction cone to this medium. The shape of the encapsulant-air is defined so light escaping to the encapsulation layer meets the epoxy-air interface approximately perpendicularly to minimise reflective losses, allowing most of the light in the encapsulant to exit to air. However, this presents no advantage to étendue limited applications, as the encapsulant effectively magnifies the size of the source by the square of the refractive index of the encapsulant, as discussed in chapter 9, specifically equation (9.1). Due to this magnification effect, the brightness of the source is also decreased by the same factor [88].

2.3.2 Chip shaping

To prevent TIR trapping light inside the LEDs until it is reabsorbed, the LED can be shaped so that a light ray reflected at one or several interfaces will eventually meet a sidewall at less than the critical angle and be extracted (see figure 2.10). This approach has been considered for as long as LEDs have been practical devices. The ideal solution of a hemispherical device with light emission at the centre so all the light emitted will meet the sidewalls at normal incidence, was considered by Carr and Pittman in 1963 for infra-red GaAs LEDs [89]. Later Carr and also Franklin and Newman considered other similar geometries as well as a truncated cone structure [90,91], but none of these have proved practical due to the associated device fabrication complexity. Krames et al. report
successful fabrication of truncated-inverted-pyramid AlGaInP/GaP LEDs which is shown in figure 2.10, cutting the sidewalls at $35^\circ$ using a beveled dicing blade [92]. This result led to a $1.4 \times$ improvement over a conventional structure. Research is ongoing into light extraction enhancement and fabrication techniques for angled-sidewall InGaN LEDs both for just the GaN [93, 94] and including the substrate [95] along with other geometries – triangular [96], circular [97] and parallelogram [98]. These approaches offer little control over the polar emission pattern from Lambertian [95, 96] and the experimental results range between 1.4 and $1.9 \times$ improvement over a control sample, speculatively giving an extraction efficiency of up to $\approx 45\%$ for unencapsulated devices.

![Figure 2.10: Truncated-inverted-pyramid LED. Reprinted from [92] with the permission of AIP Publishing.](image)

### 2.3.3 Surface roughening

Another option to reduce TIR is to roughen the reflecting interfaces to cause light rays to be scattered instead of reflected, as shown schematically in figure 2.11. Extraction enhancement by this method was first reported by Schnitzer et al. for GaAs LEDs using polystyrene nanospheres to form a random close packed array which is then used as an etch mask to create a rough surface [99]. The roughening of the surface results in an equal amount of optical intensity being scattered to all viewing angles if the roughness is greater than the wavelength of the light being scattered – i.e. all incoming photons are scattered rather than reflected, forming a Lambertian emission pattern which appears as a circle on a polar plot of the emitted intensity. In practice, this can be observed for LEDs with a less rough surface as photons will be incident on the surface at all angles, removing any distinct features in the emission pattern associated with specular reflection. Fabry-Pérot fringes are much weaker or not observed at all in LEDs with roughened surfaces due to the reduction of specular reflections.

An extraction enhancement of $1.62 \times$ was demonstrated in GaN LEDs by surface roughening p-GaN using hot phosphoric acid in conjunction with a self-assembled platinum etch mask by Huh et al. [101]. A mask-less wet etch method was developed for n-GaN by Gao et
al. using dilute potassium hydroxide (KOH) [102], which created roughness in the form of hexagonal pyramids as the etch rate of KOH is crystal-orientation dependent in GaN. As it will roughen n-GaN, this technique can be used for flip chip device designs (discussed below). Lin et al. had textured the LED sidewalls [86] to give $1.82 \times$ enhancement and Peng et al. performed a study which roughened both the top and bottom surfaces or just the top [100], achieving $2.77$ and $2.37 \times$ enhancement respectively over an unroughened device. Similar methods which rely on scattering light rather than reflecting involve patterning the substrate, usually referred to as PSS, from patterned sapphire substrate. For example, Tadatomo et al. report an approach on the micro-scale similar to chip shaping, where the light is scattered from regular patterning of the substrate surface out of the LED [103].

The roughening technique is used widely in commercial LEDs as it is a simple and versatile process which provides a good enhancement with little extra cost. However, it restricts the polar emission pattern of the LED to the Lambertian pattern, making it less suitable for étendue limited applications. Substrate patterning is also used widely in commercial LEDs and it has the additional advantage of acting to improve the quality of grown material.

### 2.3.4 Resonant cavity LEDs

With a thin film containing the QWs bounded by a reflector underneath, such as in the thin film flip chip device configuration discussed in §2.4.2, the emission from the active region is influenced by self-interference or resonances. Light emitted towards the reflective interface is directed back to the active region and interferes with light taking the opposite path; reflected back from the interface with air. The distance of the QWs from the reflector can be tuned to cause a substantial amount of the light to be emitted into the extraction cone [104] and the presence of the reflector creates a cavity which causes the emission from the QWs to be modified. Hunt et al. produced InGaAsP LEDs emitting at $1.3\mu m$ operating under this principle in 1992 [105].
The idea can be extended to any optical cavity which contains the QWs using a reflector underneath and the extracting interface above. The cavity can be tuned to create a resonance at the emission wavelength by setting its width to an integer number of half wavelengths. These devices, termed resonant-cavity LEDs (RCLEDs), have a very narrow emission band which depends primarily on the cavity resonance \[106\] and as a result, the performance of RCLEDs is highly dependent upon temperature \[107\]. It is challenging to fabricate structures in GaN LEDs thin enough to form cavities supporting only one resonance without having a significant negative impact on the IQE. The quality of epitaxial growth available to such thin films in GaN and the size required for an efficient active region are prohibitive. Distributed-Bragg reflectors (DBRs) are an option as they can be grown on top the GaN buffer layers below the active region, but the strain is hard to control, leading to large polarisation fields. Carlin et al. report achieving good results towards creating a cavity mode using AlInN/GaN DBRs by exploiting the lattice match of Al$_{0.83}$In$_{0.17}$N with GaN, preventing the build up of strain from mismatched layers. This study also reviews the problems surrounding fabrication of DBRs in III-nitride systems \[108\]. There has been some success in creating practical LEDs exploiting micro-cavity effects (MCLEDs), where the thickness is carefully tuned to a few wavelengths \[109,110\], but the results only focus on creating the cavity and its properties. The interaction of the cavity with the quantum well source changes the polar emission pattern, and so RCLEDs are a candidate for directional emitters, although they have proven challenging to fabricate and are limited to 35-45\% extraction efficiency \[111\]. The RCLED technique has largely been limited to creating vertical-cavity surface emitting lasers (VCSELs), where the cost of manufacture is less of a concern.

### 2.3.5 Photonic crystal LEDs

Photonic crystals (PhCs), which are formed by a periodic wavelength-scale variation in refractive index created using two materials with different refractive index, can also be used to extract light trapped inside a device. As the extraction process is coherent, photonic crystals offer control over the direction of light extraction and are therefore a good candidate for directional emitters — devices have been fabricated with 31\% of the extracted power within 30\° of surface normal \[112\], compared to 25\% for Lambertian. The remaining sections of this thesis focus on their use and design for light extraction, which is reviewed in chapter 4.

### 2.3.6 Summary

Several methods have been investigated to improve the extraction efficiency of III-Nitride LEDs, and are summarised in table 2.3.

The best results reporting extraction efficiency directly have used a combination of the
Table 2.3: Comparison of approaches for light extraction.

<table>
<thead>
<tr>
<th>Method</th>
<th>Fabrication complexity</th>
<th>Extraction enhancement</th>
<th>Directional emission</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>Low</td>
<td>Low</td>
<td>No control</td>
</tr>
<tr>
<td>Encapsulation</td>
<td>Low</td>
<td>Good</td>
<td>Detrimental</td>
</tr>
<tr>
<td>Chip shaping</td>
<td>Med-high</td>
<td>Moderate</td>
<td>No control</td>
</tr>
<tr>
<td>Surface roughening</td>
<td>Low</td>
<td>Good</td>
<td>No control</td>
</tr>
<tr>
<td>RCLED</td>
<td>High</td>
<td>Moderate</td>
<td>Some control</td>
</tr>
<tr>
<td>PhC LEDs</td>
<td>Med</td>
<td>Good</td>
<td>Most control</td>
</tr>
</tbody>
</table>

above approaches. For an encapsulated device, 89% extraction efficiency has been reported using a combination of chip shaping and surface roughening [113]. For an unencapsulated device, 73% extraction was achieved by combining a flip-chip RCLED with a photonic crystal [88]. The majority of commercial devices are encapsulated and use a combination of substrate patterning and surface roughening to enhance the extraction efficiency, but their extraction efficiency is unpublished.

2.4 Wall plug efficiency

The most significant factor contributing to the degradation of the wall plug efficiency (WPE) is the efficiency with which the electrical power from the initial supply can be converted to the correct voltage for the LED, but the design of efficient electronic power supplies is outside the scope of this thesis. Losses in efficiency from the methods of electrical injection into LEDs will also have an effect and are considered here as they depend upon device design.

2.4.1 Electrical losses and current spreading

The total electrical power consumed by an LED can be determined by multiplying the voltage (the energy of each electron) and current (the number of electrons) supplied to the device. As the energy level that the electron drops during recombination determines the energy of the photon emitted, there is a minimum voltage with which photon emission can occur; corresponding approximately to the band gap energy. This leads to a fundamental efficiency limitation in heterostructure LEDs as the p- and n-type bulk semiconductors will have a higher band gap energy than the active region – electrons will lose energy as they become trapped in the heterostructure. This limitation can be partly mitigated by carefully controlling the doping, but there is still energy loss through this process.

Other electrical loss mechanisms are caused by resistance in the electrical path through
the GaN and the contacts. The resistivity of GaN will depend upon the doping level – n-GaN is fairly conductive and so this is not a significant problem, but p-GaN is quite resistive, particularly parallel to the $c$-plane. The p-GaN is therefore typically kept thin and requires additional directly connected conductive current spreading layers to ensure all of the desired emission region in the LED receives adequate current. The n-GaN layer can normally be contacted more regionally as sufficient current spreading will occur in the n-GaN.

### 2.4.2 Device design

The design of the device can have a potent effect on the WPE through the series resistance as well as the light extraction. Designs often have to compromise between these in addition to other factors such as fabrication cost. GaN LEDs are typically grown with the p-side up as it is challenging to grow thick p-GaN films and the high electrical resistivity of Mg-doped p-GaN when compared to more conductive n-GaN. It is therefore usual to grow thick (a few $\mu$m) n-GaN buffer layers between the substrate and the active region for practical defect densities. The device configuration is influenced by contacting requirements, particularly for lateral current spreading under high current operation. For sapphire-grown devices, the n-layer has to be contacted from above after etching through the p-GaN as sapphire is electrically insulating. Four common device designs are shown in figure 2.12 and are discussed below.

In the conventional chip approach, an etch is performed to expose part of the n-type material for direct contacting. A thin semi-transparent current spreading layer such as Ni/Au or indium tin oxide (ITO) is deposited on the p-GaN to allow the light through whilst maintaining adequate electrical resistance. The primary advantages of this method are that it is cheap and simple to fabricate. However, the trade off between the resistance and optical absorption of the p-contact limits the performance to a maximum $\eta_{\text{ext}}$ of around 40\% when encapsulated, assuming some absorption in the p-contact and that all light emitted into the sapphire is extracted from the chip sidewalls [15]. As the intended injection current density is increased, the p-contact needs to be thicker to allow sufficient current spreading, which in turn will increase the optical absorption in this layer and lead to a reduced $\eta_{\text{ext}}$.

The flip chip approach for transparent substrates removes the problems of a partially absorptive current spreading layer by extracting the light through the substrate. In this case the n-GaN contacting remains the same as the conventional chip, but the p-GaN is coated with a highly reflective metal and then ‘flipped’ so light is emitted through the substrate. Light propagating from the active area away from the substrate is directed back towards the substrate by the reflector, where it can be extracted [114]. This p-contact will
Chapter 2. LED efficiency

Figure 2.12: Common device configurations for GaN LEDs on a sapphire substrate. Reproduced from [15], ©2007 IEEE.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conventional</td>
<td>Simple &amp; cheap to fabricate</td>
<td>Light emitted through p-contact</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Poor heatsinking</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Poor p-GaN current spreading</td>
</tr>
<tr>
<td>Flip chip</td>
<td>Mitigates disadvantages of conventional chip</td>
<td>Requires reflective p-contact</td>
</tr>
<tr>
<td></td>
<td>Good heatsinking</td>
<td></td>
</tr>
<tr>
<td></td>
<td>RCLED effects possible</td>
<td></td>
</tr>
<tr>
<td>Vertical thin film</td>
<td>Allows n-GaN to be roughened</td>
<td>Requires reflective p-contact</td>
</tr>
<tr>
<td></td>
<td>Good heatsinking</td>
<td>Requires top-side n-contact</td>
</tr>
<tr>
<td></td>
<td>MCLED effects possible</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Allows use of absorptive substrates</td>
<td></td>
</tr>
<tr>
<td>Thin film flip chip</td>
<td>Allows n-GaN to be roughened</td>
<td>Requires reflective p-contact</td>
</tr>
<tr>
<td></td>
<td>Improve light extraction</td>
<td>More complex to fabricate</td>
</tr>
<tr>
<td></td>
<td>Reduced material cost</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Good heatsinking</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MCLED effects possible</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Allows use of absorptive substrates</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.4: Comparison of device configurations.
not be 100% reflective and so will absorb a proportion of the light, but device performance is typically improved over the conventional chip approach. The reflective p-contact is very close to the active region of the LED and as a result also allows a channel for effective heat-sinking of the chip.

The vertical thin film approach can provide the advantages of the flip-chip method for absorptive substrates such as silicon and allows a more thermally conductive substrate to be used. After flipping, the p-contact is bonded to a host substrate and the original substrate removed from the n-GaN, for sapphire via laser lift-off, or for silicon destructively through polishing. Laser lift-off works by directing a high power UV laser through the substrate which is absorbed by the GaN but not the substrate to melt and/or denature the GaN at the interface [115], leaving the sapphire substrate intact and available for re-use to reduce manufacturing costs [116]. After substrate removal, the n-GaN can be thinned to take advantage of cavity effects, such as in an RCLED. The primary advantage of the vertical thin film over the flip chip option is that it allows access to the n-GaN to apply light extraction techniques such as surface roughening to improve extraction of light otherwise trapped in the GaN layers. For example, Haerle et al. report $\eta_{ext}$ of 75% using a vertical thin film design with a roughened n-GaN surface [117].

The thin-film flip chip gives the advantages of the vertical thin film design, but with reduced cost as there is no requirement for a host substrate and does not risk the quality of the reflective p-contact during the bonding process. It has been shown to give better light extraction than standard vertical and flip-chip LEDs [118], although heat extraction is more of a challenge. Absorption of trapped light in the contacting layers is restrictive to $\eta_{ext}$ in all the device configurations.

### 2.4.3 Contacting

Choice of an appropriate contact is complicated by the need to form an ohmic contact, where the current-voltage relationship remains linear. Non-ohmic contacts can form due to differences in the work functions of a contacting metal and the semiconductor – a pn junction will form as electrons flow in or out of the semiconductor to keep the Fermi level constant across the interface. This is known as a Schottky contact and results in a higher device voltage and electrical losses as the electrons must have extra energy to travel over the potential barrier created by the Schottky junction. Schottky contacts have also been shown to reduce reliability [119]. To avoid a Schottky contact, the work function of the contacting metal must be lower than the n-type semiconductor for the n-contact or higher than the p-type semiconductor for the p-contact. Depending upon the device configuration, the contact may need to be as reflective or transparent as possible.
Good contacts to n-GaN are easy to form by selecting a metal with an appropriate work function. Contacts based on Ti, Al, Ta and V, with combinations of other metals to mitigate the difficulties mentioned above have been investigated and shown to produce suitably low contact resistances down to $\approx 1 \times 10^{-8} \, \Omega \cdot \text{cm}^2$ [120]. Due to the lateral current spreading in n-GaN, the reflectance or absorption of the n-GaN contact is does not usually need consideration.

Good p-GaN contacts are harder to form as p-GaN is difficult to dope heavily and typically has a work function of $\approx 7.5 \text{eV}$, higher than most metals [121]. Thin Ni/Au (2nm/6nm) contacts were found to produce good semi-transparent contacts for conventional chip designs [122] after annealing in oxygen [123] and have been used widely in commercial devices. Improvements to contact resistance have also been using other techniques to increase the acceptor concentration at the p-GaN surface, for example treating the p-GaN to remove surface oxidation or to create Ga vacancies [120]. Indium tin oxide (ITO) is an electrical conductor with higher transparency than Ni/Au, so much thicker layers can be used. When combined with metal interlayers, very low contact resistance has been reported – Song et al. report transmittance of 96% at 460nm with Ag/ITO (1nm/200nm) contacts [124]. Most of these results rely at least partially on a tunnel contact, where the p-GaN should ideally be heavily doped to give a thin depletion region, allowing tunnelling through the potential barrier between the contacting metal with a lower work function and the p-GaN [120]. The value of the contact resistance characterises the resistance of this interface per unit area due to the tunnelling requirement.

Reflective p-GaN contacts are required for vertical and flip-chip LEDs. Ag, Al and Rh have been investigated due to their high reflectivity to blue light. For reflective contacts, there is a trade-off in the annealing step between the contact resistance which typically shows improvement with annealing conditions that degrade the reflectivity [125]. The use of interlayers has been investigated extensively [120] and has been shown to improve the thermal stability of the reflectivity, particularly with a thin nickel layer between the reflective contact and the p-GaN. Other reflective contact designs using DBRs and omnidirectional reflectors ODRs have been used successfully [126,127].

Other considerations of the material chosen to form the contact are the behaviour of the metal during further processing steps, notably diffusion of the metal into the GaN and reactions between GaN and the contact metal.
Contact | Type | Reflectance/transmittance | Contact resistance (Ω·cm²) | Ref.
--- | --- | --- | --- | ---
Ni/Au (2/6 nm) | Transparent | 85% | 1.7×10⁻² | [122]
Ag/ITO (1/200 nm) | Transparent | 96% | 1.2×10⁻⁴ | [124]
Ag | Reflective | 84% | 2.47×10⁻⁴ | [125]
Ni/Ag/Ru/Ni/Au (5/120/50/20/50 nm) | Reflective | 91% | 5.2×10⁻⁵ | [128]

Table 2.5: p-GaN contact resistance and optical performance.

### 2.4.4 Summary

The changes in device layout and contact technology have led to improvements in the efficiency. Some results for peak efficiency (pre-droop) are summarised in table 2.6.

<table>
<thead>
<tr>
<th>Efficiency</th>
<th>Method</th>
<th>Year</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.18%</td>
<td>First result, conventional chip</td>
<td>1991</td>
<td>[8]</td>
</tr>
<tr>
<td>5.4%</td>
<td>Conventional chip</td>
<td>1994</td>
<td>[129]</td>
</tr>
<tr>
<td>21%</td>
<td>Flip chip</td>
<td>2001</td>
<td>[114]</td>
</tr>
<tr>
<td>34.9%</td>
<td>PSS conventional chip</td>
<td>2002</td>
<td>[130]</td>
</tr>
<tr>
<td>34%</td>
<td>Vertical thin film</td>
<td>2004</td>
<td>[117]</td>
</tr>
<tr>
<td>56.3%</td>
<td>PSS conventional chip, ITO p-contact</td>
<td>2006</td>
<td>[131]</td>
</tr>
<tr>
<td>62%</td>
<td>Thin film flip chip</td>
<td>2007</td>
<td>[15]</td>
</tr>
<tr>
<td>57%</td>
<td>Semipolar roughened conventional chip</td>
<td>2010</td>
<td>[132]</td>
</tr>
<tr>
<td>63%</td>
<td>Vertical thin film</td>
<td>2015</td>
<td>[133]</td>
</tr>
</tbody>
</table>

Table 2.6: Efficiency of III-Nitride blue LEDs.

After the first results, the efficiency steadily improved up to the mid 2000s and published results flatten off around 60-65%, when the focus in academic research shifted to droop. Commercial development focussed on reproducing the high efficiency results with designs suitable for mass manufacture, which are now available [134]. Several groups began to pursue violet LEDs, as they suffer from less droop, and the best efficiency result to date known to the author is ≈80% from a 415nm violet LED [135].
2.5 Conclusion

Academic literature has provided results toward improving the internal and external quantum efficiencies through understanding of the limiting processes, and industrial product development has chiefly driven overall wall plug efficiency and performance of the whole device through optimisation. Research into the efficiency of LEDs is a mature topic and all of the factors which affect the overall efficiency of an LED have seen attention, but many avenues for further research remain. The best efficiency values for overall device performance are not clear as the approach from published work has largely been to conclude that a proposed method for improving a specific efficiency or limiting effect is or is not useful, and give a performance ratio over a control sample. This has left the complex multivariate optimisation problem of LED efficiency as an exercise for industrial efforts, which remain unpublished.

With double-heterostructure designs including an electron-blocking layer, the injection efficiency is considered to be very close to 100% by the majority of researchers, although some consider carrier overflow the cause or a contributor to efficiency droop. Results on the internal quantum efficiency show that 90% is achievable before the onset of droop through improvements to the crystallographic quality and reduction of the quantum-confined Stark effect. There appears to be little scope for improvement to these efforts due to their high values. Similarly, for issues relating to the overall wall-plug efficiency, understanding of the device configuration and electrical contacting is well described in the literature but its interplay with other device performance parameters is highly complex and therefore most suited to commercial optimisation.

Efficiency droop is a major limiting factor for high-brightness LEDs. Currently to produce high-brightness devices, manufacturers have to use a larger LED area or an array to avoid generating excessive heat at the high drive currents required. This increases the étendue of the source, making these devices unsuitable for étendue-limited applications such as projection or headlights. As droop is likely to be due to a material effect which is intrinsic to InGaN/GaN LEDs, two options remain to produce devices suitable for étendue-limited applications: the active area of the device must be increased without increasing the overall device area, using 3D geometries such as core-shell, and/or the directivity of the emission must be increased.

Whilst values of up to 90% for the light extraction efficiency have been reported, these rely on encapsulation of the light source, which is detrimental to its brightness and usefulness to étendue-limited applications. Light extraction of ≈75% has been achieved for an unencapsulated device, but the experimental parametric optimisation required did not consider control of the directivity of the light emission. The use of photonic crystals...
has allowed extraction of 31% of the extracted power within 30° of normal incidence, a 6% improvement over Lambertian emission from encapsulated surface-roughened devices with the same extraction efficiency, but there is a large scope for improvement as these devices only extracted 39% of the total light, giving only 12% extraction within 30°, compared to ≈22.5% for the best surface-roughened devices. Once the increase in étendue due to the encapsulant is taken into account, approximately a factor 2, the directional photonic crystal device can only just outperform the best surface roughened device in terms of flux throughput for matched étendue within 30° of normal incidence (see equation (9.1) and (9.2)).

In order to address the shortcomings of LEDs for high-brightness and étendue-limited applications, photonic crystals appear to provide excellent scope to improve unencapsulated extraction efficiency, whilst offering control of the direction of light extraction. Core-shell LED designs, which may be advantageous for mitigating droop, can also exhibit photonic crystal effects if they are fabricated in periodic arrays. The rest of this thesis focusses on the potential use of photonic crystals for addressing the shortcomings of current techniques.
Chapter 3

Physics outline

This chapter discusses the underlying physics behind the interaction of light with photonic crystals and typical LED structures. The information below is intended to provide background necessary for the concepts discussed in this thesis and there are many excellent textbooks which give much more detail\(^1\). The aim is to present a context for understanding the results obtained without the need for extensive reference to these complete texts.

3.1 LEDs as slab waveguides

Conventional LEDs can be modelled as slab waveguides as they are substantially larger in two dimensions (of the order of mm) than they are thick (a few \(\mu\)m). When solving Maxwell’s equations for light propagating in an infinite slab of high-index material with lower index materials above and below, there are a discrete number of permitted propagation constants if the light undergoes total internal reflection at both interfaces. These are the \textit{optical} or \textit{guided modes} of the slab within which the light can propagate. Two types of mode are found to exist corresponding to the two polarisations of light – TE, where the electric field is in the same plane as the slab layers and TM, where the magnetic field is in the same plane as the slab layers. To describe the situation using a photonic model, there are a discrete number of energy levels (equivalently frequencies from Planck’s theory) known as \textit{photonic states} which a photon in the waveguide can occupy, analogous to electrons trapped in a potential well. The mathematics are considered in more detail in chapter 5, and the rest of this section will provide a more qualitative description of this phenomenon.

A more intuitive consideration of modes in a slab waveguide is to consider the angles at which a light ray can propagate through the slab. When self-interference of the ray with its total internal reflections is taken into account, only a set of discrete light ray angles

\(^{1}\text{See, for example: Optical waveguide theory by Snyder \& Love [136], Photonic Crystals: Molding the flow of light by Joannopoulos et al. [137] and the work on Quasicrystals and geometry by Senechal et al. [138,139].}\)
are able to travel in the waveguide.

For a slab substantially thicker than the wavelength of light being considered, the number of modes is very large and can often be considered infinite, representing a continuum of modes – as if the slab were a homogeneous medium. When the slab is made thin enough, this number becomes smaller and there can no longer be considered a continuum of states. The distributions of electric field, magnetic field and optical power in the waveguide for each allowed mode are characteristic. The forms of these field distributions are called the mode profiles or envelope functions, examples of which are shown in figure 3.1a.

Each mode ‘feels’ a different effective refractive index $n_{eff}$ and has a characteristic in-plane or parallel component $k_\parallel$ of the wavevector $\hat{k}$ (often referred to as the propagation constant $\hat{\beta}$) where the wavevector has been resolved to the plane of the slab. $n_{eff}$ can be calculated for each mode using

$$n_{eff} = \frac{k_\parallel}{k_0} \tag{3.1}$$

where $k_0$ is the absolute value of the freespace wavevector (referred to as the freespace wavenumber) corresponding to the frequency $\omega$ of the light ($\omega \propto$ the photon energy).

To view the behaviour of a waveguide and the modes it supports, a dispersion diagram of the type shown in figure 3.1b can be used, where a waveguide comprising of a dielectric slab with $n = n_{slab}$ is surrounded by a material of lower index $n_{air}$ is considered. The blue lines and shaded area represent the allowed photon energies (y-axis) for a given $k_\parallel$. Each separate line corresponds to a single optical mode. The units have been normalised to the thickness of the slab $a$ under consideration as Maxwell’s wave equations are scalable with frequency and wavelength.

In the region above the light line $k_\parallel = k_0$, where $n_{eff} < n_{air}$, light emitted in the
high index slab is not confined and can propagate in a continuum of states in air known as radiation modes. In the case of an LED, any light emitted inside a semiconductor above the light line ($k_0 > k$) is in the extraction or air cone and does not undergo total internal reflection, but will still undergo Fresnel reflection. Between the light line and the dielectric line $k_0 = n_{slab}k_0$, light propagates in the discrete waveguide modes with $n_{slab} > n_{eff} > n_{air}$ and the fields are evanescent in air. Below the dielectric line, light cannot propagate. As the cavity becomes thinner or the frequency lower, higher order modes progressively move towards the light line and are ‘cut-off’ when they are no longer supported as discrete modes. Self-interference from Fresnel reflection at the interfaces for unguided light creates resonances, usually broad, similar to guided states called Fabry-Pérot modes, discussed in §2.3.

As there is no variation in the refractive index profile for all directions parallel to the 2D slab, this 1D model fully characterises the behaviour of the slab. As a consequence of the rotational symmetry perpendicular to the slab, there are an infinite number of degenerate modes with the same profile, covering all possible unique in-plane directions of travel.

To take into account absorption or loss in the waveguide, an imaginary part can be added to $k_{||}$ and $n_{eff}$ such that

$$k_{||} = \beta_{||} + \alpha_{||}i$$
$$n_{eff} = \tilde{n}_{eff} + \kappa_{eff}i$$

where $\alpha$ and $\kappa$ are referred to as the absorption and extinction coefficients respectively. This leads to a decay in intensity $I$ along the in-plane propagation direction $x$ of the form

$$I \propto e^{-2\alpha x}$$

From this, an in-plane absorption length can be defined as $\mu = 1/2\alpha$ or $\lambda_0/8\pi\kappa$, the distance over which the light has to travel within the waveguide to reach $1/e$ of its initial intensity.

Optical power which is lost to the air through diffraction from a slab waveguide containing a diffraction grating can be represented in the same way. This leads to an analogue to the absorption length known as the extraction length, which can be used as a measure of the efficiency of loss from the waveguide by diffraction. When combining this potentially useful loss mechanism with other non-extracting losses, the extraction efficiency from a slab can be found using (3.2), where $\mu_{PhC}$ represents the extraction length and $\mu_{loss}$ represents the absorption length of the loss mechanisms [140].

$$\eta_{ext} = \frac{\mu_{loss}}{\mu_{PhC} + \mu_{loss}}$$ (3.2)
3.2 Photonic crystals and photonic quasi-crystals

A photonic crystal (PhC) is an optical medium with a periodically varying dielectric constant. The variation can be in 1D, 2D or 3D and is referred to as a crystal lattice, originating from when the same phenomenon was investigated for electrons travelling in the periodically varying potential present in an atomic crystal structure. Typically the spatial variation in refractive index must be of about the same magnitude as the wavelength of the light it affects in order to exhibit interesting properties. A PhC can prohibit certain frequencies of light from travelling through it at some or all angles and polarisations, creating a band gap. PhCs can also act as diffraction gratings.

It should be mentioned that the behaviour of electrons is analogous to the behaviour of photons, where electric potential determines the energy of an electron and the dielectric constant the energy of a photon with a given freespace wavelength (although the relationship is opposite for photons; a photon in a material of lower dielectric constant has a higher energy than one in a higher dielectric constant). The wave-function and particle models for both cases produce the same results with the same consequences. As a result, many of the concepts in solid state physics have parallels in photonics.

1D, 2D and 3D PhCs have been experimentally shown to have photonic band gaps and are being investigated for use in a wide range of applications [137]. Distributed Bragg reflectors (DBRs) can be considered as 1D PhCs and are often used in lasers and sometimes LEDs as high-performance reflectors [108]. The application of PhCs to LEDs for light extraction usually uses 2D PhC lattices which have a non-infinite height known as photonic crystal slabs and are considered in the rest of this section.

A more mathematical consideration of the behaviour of PhCs is given in Photonic Crystals: Molding the flow of light by Joannopoulos et al. [137].

3.2.1 Diffraction by a periodic medium

It is widely known that the Bragg condition for diffraction by a periodic structure or grating is given by (3.3), which can be derived from analysing constructive and destructive interference of reflections from the grating elements. In (3.3), \( \lambda \) is the wavelength of the light, \( D \) is the period of the grating along the direction under consideration, \( m \) is the integer order of the diffraction and \( \theta \) is the angle at which constructive interference is observed.

\[
D \sin \theta = m \frac{\lambda}{2}
\]  

(3.3)

This specific formalism of Bragg’s condition is challenging to visualise in situations along more than one dimension and so it is useful to re-define it to allow it to be applied to \( n \)-dimensional PhCs.
Any \( n \)-dimensional regular periodic tiling or lattice can be represented by a series of points in space as in figure 3.2a, where a set of simple spatial vector transforms \( \{\hat{R}\} \), known as the lattice vectors, translate the lattice on to itself. There are obviously many values of \( \hat{R} \) which could be used, but the smallest are usually referred to, namely the values of \( \hat{R} \) that translate one point to its neighbouring point, which are represented in figure 3.2a as \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \). For 2D Euclidean tilings, combinations of integer multiples of two of these unit vectors give all \( \{\hat{R}\} \). Converting the spatial lattice into reciprocal space, sometimes called \( k \)-space\(^2\), yields the reciprocal lattice, which can be found by applying a Fourier transform to the spatial lattice and represents the periodicity of the crystal lattice.

A wavevector \( \hat{k} \) is the equivalent of wavelength in reciprocal space and so can be represented directly in reciprocal space by its value. In the case of a 2D slab waveguide, the unique omnidirectional \( k_\parallel \) for each guided mode is mapped as a circle of position vectors with radius \( k_\parallel \) in reciprocal space. This circle is made up of the individual wavevectors in every possible direction directed from the centre to the edge of the circle, where the position of the centre of the circle corresponds to an arbitrary point in space from which the phase of the wave in space and time is referenced.

\[ \{\hat{k}_d\} = \hat{k}_i + \{\hat{G}\} \]  \hspace{1cm} (3.4)

\(^2\)This is the same process as converting wavelength to wavenumber, i.e. \( k \propto 1/\lambda \).
As a consequence of (3.4), all the characteristics of the reciprocal (and spatial) lattice can be represented by the area closer to one reciprocal lattice point than any other as it can be translated to an equivalent place by adding or subtracting integer multiples of unit \( \hat{\mathbf{R}} \) or \( \hat{\mathbf{G}} \). This area is known as the first Brillouin zone, and it is shown in figure 3.2b for a regular hexagonal 2D lattice. Furthermore, the whole area of the first Brillouin zone can be uniquely represented by a subset of its area known as the irreducible Brillouin zone using rotational and translational transformations, which is shown in blue in figure 3.2c. Only the area inside the irreducible Brillouin zone needs analysing as it can be used to characterise the behaviour of any PhC completely. The vertices of the irreducible Brillouin zone are conventionally given the labels \( \Gamma \) at the centre of the reciprocal lattice and \( M \) and \( K \) at the edges for the 2D case\(^3\).

The order of the diffraction is rather harder to define in \( n \)-dimensions as an integer multiplier of the wavelength does not fully represent the tiling. The way that the order of diffraction is treated in the literature for 2D tiling varies, for example, the 2nd order may refer to the group of points which are twice one of the unit reciprocal lattice vectors, or the sum of both. The tiling is fully characterised only by the whole reciprocal lattice \( \{ \hat{\mathbf{G}} \} \), but subsets of the reciprocal lattice vectors \( \{ \hat{\mathbf{G}} \}_i \subset \{ \hat{\mathbf{G}} \} \) can be defined which are useful to represent the diffraction in some circumstances. These subsets are made up of groups of reciprocal lattice vectors with the same magnitude \( N \), and the order of each subset \( \{ \hat{\mathbf{G}} \}_i \) can be loosely defined by its magnitude normalised to the first order \( m_N \).

\[
m_N = \frac{N}{|\hat{\mathbf{G}}_1|} \tag{3.5}
\]

where \( \hat{\mathbf{G}}_1 \) refers to a first order point, chosen by the smallest non-zero value of \( N \in \{|\hat{\mathbf{G}}|\} \). Each different tiling will have a discrete set of \( m_N \) (e.g. \( \{0, 1, \sqrt{3}, 2, \sqrt{7}, \ldots\} \) for the hexagonal tiling). This convention will be used to refer to diffraction order throughout the rest of this thesis.

A technique known as Ewald construction, originally applied to X-ray diffraction [141], can be used to determine when the Bragg diffraction conditions are satisfied for an \( n \)-dimensional diffraction grating in a visual way. An example Ewald construction for a 1D line grating is shown in figure 3.3, where the grey points are the reciprocal lattice points of the grating and the black arrow represents the in-plane wavevector incident on the grating \( k_{i||} \). If the origin \( O \) for the wavevectors is positioned so the vector \( k_{i||} \) describes the transformation of the origin to a reciprocal lattice point, the diffracted in-plane wavevectors \( \{ k_{d||} \} \) are given by the vectors from the origin to every other reciprocal

\(^3\)Sometimes \( X \) and \( J \) are used instead of \( M \) and \( K \) respectively.
lattice point by applying (3.4).

(a) Real space schematic of a 1D waveguide grating. (Left) side view. (Right) plan view.

(b) Reciprocal space representation to create the Ewald construction where \( k_{\parallel} \) represents the wavevector incident on the grating. (Left) several possible diffracted wavevectors \( k_{d\parallel} \). (Right) only \( k_{d\parallel} \) inside the extraction cone, which is represented by the green circle.

**Figure 3.3**: Illustration of an Ewald construction for a 1D diffraction grating.

For the slab waveguide case, the diffracted light lies inside the extraction cone in only the locations where \( k_{d\parallel} < k_0 \). Some of the energy in the guided mode will be extracted or leaked to air. In the Ewald construction, this condition is satisfied only at reciprocal lattice points that lie inside the air cone (green line) in figure 3.3 with radius \( k_0 \), centred on \( O \).

To investigate more than one wavevector at a time, one can rearrange the Ewald construction process. The construct is centred about a reciprocal lattice point and the wavevectors translated by all \( \hat{G} \). This process is illustrated by rewriting (3.4) as

\[
\{\hat{k}_d\} = \hat{G} + \{\hat{k}_i\} - \Gamma
\]  

(3.6)

where \( \Gamma \) represents the reciprocal lattice point chosen to be the centre of the construct and \( \{\hat{k}_d\}, \{\hat{k}_i\} \) represent the set of all diffracted and incident wavevectors respectively.

Figure 3.4 shows an example for a 2D hexagonal lattice, where the green circle representing the extraction cone is now centred about the arbitrary reciprocal lattice point \( \Gamma \). The red circles with radius \( k_{\parallel} \) centred about each reciprocal lattice point show the loci of the incident wavevectors of a guided slab mode. Only part of the circles are shown in figure 3.4 for clarity. Where the red loci intersects the green air cone, the guided modes are diffracted to air.

The diffraction to the air cone from PhC slabs can be observed experimentally by viewing wavelength-resolved far-field intensity measurements. The intensity measurements are
collected over a hemispherical surface above a sample LED positioned at the origin of the hemisphere, so the axis of symmetry of the hemisphere is parallel to surface normal of the LED. Resolving the intensity measurements to in-plane reciprocal space can be achieved by projecting the positions on the hemispherical surface onto a 2D plane perpendicular to surface normal, discussed further in §6.2. Experiments of this nature comprise a significant part of this work and the experimental details are described in chapter 6.

Diffraction can be thought of as a process by which allowed states or photonic bands are transferred between Brillouin zones and is also known as band-folding; once a band has a large enough wavevector to be outside the irreducible Brillouin zone, it is folded back inside. This effect is illustrated in figure 3.5 where the thin grey straight lines represent the Brillouin zone boundaries, creating a hexagon around each reciprocal lattice point. An unfolded mode just outside the first Brillouin zone is shown in blue, and the band folding makes it appear geometrically ‘reflected’ by the zone boundary.

3.2.2 Photonic states in a periodic medium

To analyse the photonic states within a periodic medium, the refractive index contrast $\Delta n$ between two dielectric materials with lower $(n_l)$ and higher $(n_h)$ refractive index is considered. It is simplest to begin at the limit of $\Delta n \to 0$. Figure 3.6 shows the photonic states for a 1D PhC and a 2D PhC slab for $\mathbf{k}_\parallel$ at the edges of the irreducible Brillouin zone for $\Delta n = 0$. The wavevectors shown are only those that lie on the edges of the irreducible Brillouin zone as these will almost always give the maximum and minimum frequencies of the band\(^5\) [137]. The band folding can again be seen by the geometric ‘reflection’ of the lines at the edges of the Brillouin zone, where the band is folded back inside as its frequency increases.

Band folding can be applied to specific wavevectors to uncover the nature of the guided

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\(^4\)Band-folding is usually referred to as zone-folding in solid state physics textbooks referring to the similar quantum phenomenon for electrons in periodic media.

\(^5\)This is a useful property as it allows the limits of the bands and any gaps between to be investigated without needing to consider all possible states inside.
Chapter 3. Physics outline

C.J. Lewins

Figure 3.5: Illustration of band folding in reciprocal space for a hexagonal PhC slab. The red and blue circles represent two guided modes propagating within a PhC slab and the black circle represents the air cone. The edges of Brillouin zones are represented by thin grey lines. Reproduced from [140], ©2009 Wiley-VCH.

Figure 3.6: Dispersion diagram for a PhC at the limit of $\Delta n \to 0$.
states within a periodic medium. In a PhC, a wavevector $\mathbf{k}_1$ can be folded back into another Brillouin zone through the transformation $\mathbf{k}_1 + \mathbf{G}$, and will therefore have an equivalent wavevector to $\mathbf{k}_2 = \mathbf{k}_1 + \mathbf{G}$, from (3.4). There will be no discernible phase change between $\mathbf{k}_1$ and $\mathbf{k}_2$ as the phase between equivalent points in different Brillouin zones must be given by

$$\mathbf{R} \cdot \mathbf{G} = 2\pi N \quad (3.7)$$

where $N$ is an integer due to the translational symmetry. As a result, $\mathbf{k}_1$ and $\mathbf{k}_2$ are part of the same optical mode, so the mode profiles in the plane of the PhC must be periodic with the PhC lattice. The equivalence to (3.4) can be seen as the different values of $\mathbf{G}$ will produce harmonics of the lattice periodicity.

The same result can be found by solving Maxwell’s equations for modes in a periodic medium – the mode profiles are represented by a plane wave modulated by a function which is periodic with the PhC lattice, in general

$$\mathbf{H}_k(\mathbb{R}) = e^{i\mathbf{k} \cdot \mathbb{R}} \mathbf{u}_k(\mathbb{R}) \quad (3.8)$$

where $\mathbf{H}_k(\mathbb{R})$ represents the pattern of the mode profile as a function of real space $\mathbb{R}$, for each wavevector $\mathbf{k}$. $\mathbf{u}_k(\mathbb{R})$ is a function with the same periodicity as the lattice in space for each $\mathbf{k}$, i.e. $\mathbf{u}_k(\mathbb{R}) = \mathbf{u}_k(\mathbb{R} + \mathbf{R})$.

This result is known as Floquet’s or Bloch’s theorem, and the solutions to (3.8) representing guided light are called Bloch modes. Any frequency (corresponding to a unique value of $|\mathbf{k}|$ or $k_0$) may have any number of solutions to (3.8), or no solutions at all. As a result, the possible wavevector solutions for a given frequency may be highly directional, entirely omnidirectional or in a band gap. Bloch modes in a PhC which undergo diffraction or band folding to unguided radiation modes are known as leaky Bloch modes, as optical power propagating is lost to these unguided modes.

Considering the simple case of a 1D periodic dielectric shown in figure 3.7a, there are two possible arrangements of $\mathbf{H}_k(\mathbb{R})$ for any given solution, where the nodes could be in either material. These two arrangements represent the folded and unfolded states of a band. Using (3.1) and that $k_0$ is proportional to photon energy\(^6\), it can be seen that a higher $n_{eff}$ represents a lower energy state. Therefore, for a given $k_\parallel$, a state with a higher proportion of its optical energy localised in regions of high refractive index will have a lower frequency when compared to a state with its energy in regions with lower refractive index. At the limit of $\Delta n \to 0$, these states must converge to the same frequency as there can be no difference in their energy. However, for $\Delta n > 0$, the average index seen by the folded and unfolded bands becomes different and so the state splits, caus-

\(^6\)as $\omega$ is proportional to photon energy.
ing a band gap to appear. This is illustrated in figure 3.7b for small and large values of $\Delta n$.

![Diagram of band intensity profiles in 1D PhC and 1D PhC dispersion with $\Delta n = 0.14$ (left) and $\Delta n = 2.61$ (right).]

**Figure 3.7:** The origin of band gaps, adapted from [137].

The state below the band gap is commonly referred to as the dielectric band and the state above the gap as the air band$^7$ as the field is predominantly localised in the dielectric or air respectively. The band gap is referred to as a complete band gap if it prohibits all light in any polarisation of a certain frequency from travelling in any direction in the PhC. Non-complete gaps are seen when there is not a large enough difference in the average refractive index experienced by the intensity profiles of the two bands for some areas of the dispersion diagram and for where the two different light polarisations do not produce a gap at the same frequency. In PhC slabs, only incomplete band gaps can exist as light can exit the slab through the air cone at all frequencies, but complete gaps within the guided states can exist.

$^7$These are comparable to the valance and conduction bands respectively for electronic states in semiconductors.
3.2.3 Photonic quasi-crystals

There is a limit to the regular or Euclidean $n$-dimensional crystal lattices available. The upper bound to the available rotational symmetry is 6 for the 2D case, which corresponds to a hexagonal tiling of the plane. Quasi-periodic and non-periodic tilings of the plane can be formed using combinations of polygons or other algorithms and are often referred to as quasi-crystals. Quasi-crystal tilings can appear almost perfectly ordered through to amorphous, but they always have a degree of order and periodicity about them as can be seen in figure 3.8. Consequently, they exhibit a reciprocal lattice with points of varying intensity which may or may not be completely discrete. The intensity of each point is based on the frequency of occurrence of the spacings in the quasi-crystal pattern. Sharp diffraction points are observed in reciprocal space and so the tiling must show long-range order, but quasi-crystals always display some form of apparent short-range disorder with the length-scale over which this occurs dependent upon the pattern considered.

Quasi-crystals were first discovered in nature by Shechtman et al. in the molecular crystal structure of a Mn-Al alloy from X-ray diffraction through observation of icosahedral symmetry, not possible through the possible regular Bravais crystal lattices. 2D photonic quasi-crystals (PQCs) have been designed which show complete photonic band gaps initially theoretically and then experimentally. Much progress has been made in understanding their properties and designing useful PQC structures and it has even been shown that it is possible to design 2D PQCs which exhibit long range $n$-dimensional symmetry. For example, Lee et al. present a method which starts with the desired symmetry in reciprocal space and uses a digitisation of its inverse Fourier transform to produce a corresponding quasi-crystal pattern in real space.

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8Strictly the definition of a quasi-crystal is a tiling with no translational symmetry, but the literature on PhC technology typically refers to non-Euclidean tilings as quasi-crystals. As a result, this convention will be followed.
Figure 3.8: Quasi-crystal tilings and their reciprocal lattices, from [139]. (a-b): Binary tiling. (c-d) Penrose Rhomb tiling.
Chapter 4

Photonic crystal LEDs: literature review

Chapter 2 showed that there is substantial room for increase in performance of LEDs for high-brightness and étendue-limited applications, and that photonic crystals (PhCs) may provide a path to addressing the shortcomings of other approaches. The use of photonic crystals to extract light from LEDs has been investigated widely, with many different approaches and techniques considered both experimentally and theoretically in the literature. A summary is given by Noda and Fujita [148] and detailed review articles are presented by Wiesmann et al. [140] and David et al. [149]. The behaviour of PhCs in LEDs investigated to date has usually been classified under two operating regimes. This chapter is structured to discuss these two behaviours separately and then the fabrication methods which have been applied to create PhC LEDs.

Firstly, there is a diffractive or ‘weak’ regime where the PhC acts as a small perturbation to the slab waveguide formed by the epitaxial layers of the LED with little effect on the guided modes. These laterally guided modes undergo Bragg scattering to the extraction cone through the PhC acting as a diffraction grating, which is discussed in detail in §3.2.1. This operating regime has been widely investigated as an alternative to surface roughening to extract light trapped in guided modes. As diffraction is a coherent scattering process, information about the direction of light is conserved, allowing control over the far-field emission pattern. In contrast the random scattering from surface roughness produces a Lambertian emission pattern. Chapter 7 discusses experimental buried photonic crystal LEDs operating in this regime.

The second regime is the ‘strong’ or Bloch regime where the PhC significantly modifies the photonic states beyond diffraction or band folding of slab waveguide modes. In this regime, photonic band gaps can exist and their properties are available for exploitation. The behaviour has been widely investigated, particularly for the manipulation and localisation of light in the context of photonic circuits and high resonance microcavities [150–152]. In the III-nitrides and specifically applied to LEDs, this behaviour has not been reported
widely in theory or in experimental work. Chapter 8 reports experimental observation of strong photonic crystal effects in quantum disc and core-shell nanorod samples.

At this point, some conventional terminology will need to be defined when referring to PhC design criteria. The pitch \( a \) refers to the distance between adjacent points in a regular PhC lattice and usually a base unit distance between adjacent points for photonic quasi-crystals (PQCs). The filling fraction (usually air filling fraction, \( A_{FF} \) or dielectric filling fraction, \( D_{FF} \)) refers to the volumetric ratio between the two materials making up the PhC.

### 4.1 Strong photonic crystals

A PhC with a suitable band structure can be used to influence the behaviour of the spontaneous emission or to inhibit spontaneous emission into guided modes in an LED [140, 148, 149]. Yablonovitch first speculated that photonic band gaps could be used to influence spontaneous emission in 1987 [153] and in so doing coined the phrase ‘photonic crystal’. A decade later, Fan et al. showed that a source inside a suspended 2D hexagonal PhC slab of air holes in GaAs could be inhibited from emitting into guided slab modes by a PhC band gap and so only emit into the air cone [154] as in figure 4.1a. In this case, no in-plane waveguiding is allowed by the PhC band structure in a process sometimes referred to as Bloch-mode suppression, and so the extraction efficiency is very high. This concept was taken further by Lee et al. who report that 100% extraction efficiency may be achieved in this configuration [155]. However, they also point out the increase in surface recombination and other reductions to \( \eta_{IQE} \) caused by the presence of the PhC. These limitations were made clear in an experimental analysis, carried out in a 245nm thick slab of GaInAsP with an embedded QW, into which 2D PhCs with varying pitches were etched to investigate the effect of moving the band gap around the emission region [156]. A strong enhancement of the spontaneous emission in the direction perpendicular to the slab was observed when the band gap coincided with the photon emission, but the overall radiative recombination rate and therefore \( \eta_{IQE} \) is seen to reduce dramatically as there is a lower photonic density of states present to emit into in the gap. A similar influence on the radiative recombination rate has been reported for quantum dot (QD) emitters suspended in a 3D PhC [157] and this method for enhancing light extraction is therefore only effective at increasing the external quantum efficiency when the non-radiative recombination rate is very low.

Simple implementations using the band gap of a DBR or 1D PhC as a reflector underneath an emitting region creates a resonant-cavity or micro-cavity LED, which has already
been discussed in §2.3.4. It has been suggested that it is feasible to use a 2D PhC band gap in this manner as an alternative to a metallic mirror in a flip-chip configuration [158], reducing optical losses in the reflective layer. Figure 4.1b shows a similar approach with a PhC band gap to trap light emitted into guided modes near the active region, where it can undergo photon recycling until it is extracted [149]. This method places a heavy reliance on having a high $\eta_{IQE}$ of the device as several cycles are required to extract a photon, so is not particularly effective unless $\eta_{IQE} \approx 1$.

![Figure 4.1](image.png)

**Figure 4.1**: ‘Strong’ PhC configurations, from [149], ©2012 IOP Publishing.

Better performance may be possible by using the effect of a PhC on the level of spontaneous emission at frequencies away from a band gap [140]. The approach was first considered by Boroditsky *et al.* [159] and takes advantage of the spontaneous emission enhancement caused by an increased photonic density of states to improve the radiative recombination rate. This can occur at frequencies above a band gap, where the the magnitude of the in-plane wavevector depends less on the frequency in ‘flatter’ photonic bands. The light is then extracted by diffraction. Further studies on optimising the parameters for best emission enhancement and extraction from nano-patterned emitting regions have been carried out [160], but most research in this area is interested in exploiting the high density of states in these flat bands to create the conditions required for lasing [161, 162].

In addition to the tendency to reduce the radiative recombination rate caused by most strong PhC approaches, there are significant challenges associated with fabricating a practical device and only results using PL of suspended PhC slab LEDs have been reported to date [88, 140, 149]. A suspended slab is not suitable for high brightness operating currents as there is no heatsinking mechanism and requires good lateral current spreading for electrical injection, which is not available in GaN devices. Suspended slab structures are also fragile, cannot be used for large areas without supporting regions which will likely not exhibit the desirable properties and do not allow for structures without continuous connection across the slab, such as arrays of dielectric rods.
4.2 Weak photonic crystals as diffraction gratings

A PhC-based diffraction grating can be used to extract guided modes trapped in the waveguide created by a typical LED epitaxial structure through the process described in §3.2.1. Many different approaches to the design of devices using 2D PhC slabs have been investigated both experimentally and theoretically. The trapped light is guided in a plane and so 1D PhCs are not usually considered suitable for this mode of operation except in specialist applications as they can only extract light along one direction [163]. There are many reports in the literature which have experimentally shown an increase in light extraction using PhCs with a specific method or by varying one parameter over a wide range, but analytical studies of the characteristics and methods for optimisation are less common and will provide the focus of this review. Discussions of the overall factors affecting the optimal design of the PhC LED for light extraction can be found in e.g. references [88,140,149,164] and there are many other publications discussing specific design elements.

In the diffractive operating regime, it is considered that the PhC slab, placed somewhere in the structure and used for light extraction, acts only as a weak perturbation of the slab waveguide created by the rest of the LED structure. As a result, there are two design considerations which influence the extraction properties – the vertical structure design and the 2D in-plane PhC design, which can usually be considered separately. The former considers the location and depth of the PhC along with the other layers comprising the LED which largely determine the optical modes present in the device. The latter considers the pitch, lattice arrangement and filling fraction of the PhC which largely determine the diffraction and its efficiency. This separability of the 1D vertical structure and 2D PhC tiling is often used as a tool to simplify analysis of the behaviour of devices, and is referred to as the 1D-2D model throughout this thesis. These two parts are discussed separately below, firstly the placement of the PhC and then the choice of PhC tiling.

It should be noted that measurements of the light intensity which are only collected from part of the emitting hemisphere, such as use of a photodiode placed near the test sample, cannot be used to perform comparisons of light extraction performance without careful consideration. The emission direction of optical power from diffracted modes will depend upon the PhC geometry, so when the parameters are varied, a measurement of only part of the emission will not include the light outside the detector’s collection angle. Consequently, there is a level of uncertainty in some of the extraction efficiency enhancements claimed in the literature where these experimental details are not discussed.
4.2.1 Surface photonic crystals

The first reports attempting to improve the extraction efficiency using PhCs in GaN LEDs etched the PhC into the surface of a p-side up conventional chip device configuration (discussed in §2.4.2 and shown in figure 2.12). Oder et al. initially reported fabrication of PhCs by dry etching [165] and then reported enhancement of EL light output from blue and UV LEDs [166] using the structure shown in figure 4.2a without a pGaN current spreading layer. This study used PhC pitches of 700nm, but Jiang’s group at Kansas State University continued this work in UV AlN LEDs with smaller pitches and reported $2.5 \times$ enhancement [167]. At the same time, Orita et al. reported up to $1.5 \times$ enhancement of EL emission using a PhC on the surface of a device including a current spreading layer with a PhC pitch of $1.5 \mu \text{m}$ [168]. Wierer et al. also report $1.5 \times$ enhancement of EL emission but from four PhC LEDs with pitches from 270-340nm [169], with the configuration shown in figure 4.2b. This study considered the effect of the device configuration on the overall performance, employing an additional n-GaN layer with a tunnel junction above the p-GaN layer to address current spreading and challenges with etching p-GaN (discussed in §4.5 below). Figure 4.2 shows schematics which summarise this early work from the three research groups.

(a) Oder et al. Reprinted from [166] with the permission of AIP Publishing.

(b) Wierer et al. Reprinted from [169] with the permission of AIP Publishing.

(c) Orita et al. [168], ©2004 The Japan Society of Physics.

Figure 4.2: Early results using surface PhCs in GaN LEDs.
Many more studies which mostly focus on parameter sweeps and fabrication techniques have been presented which place PhCs on the p-GaN surface after this initial work in 2004. All these structures contain thick layers of semiconductor, which act as highly multi-moded slab waveguides and so the spatial overlap integral of the mode amplitudes with the adjacent surface PhC are not high. To a first-order approximation, the efficiency of the diffraction process for each guided mode present in the LED is dependent upon this overlap [164], and so the extraction of guided light is poor, especially for the well-confined low order modes which will carry a substantial proportion of the optical energy. David et al. performed an experimental study to investigate this behaviour and the photonic band structure of such an LED through observation of the diffraction of the guided modes [170]. They conclude that the 1D vertical waveguide structure must be designed for efficient operation and that guided modes can be present with negligible extraction. The detailed discussion of the design of the PhC depth in ref. [170] suggests that there is an optimal depth where the interaction of the modes with the PhC is best.

![Figure 4.3: Light emission restricted to cap layer and high order modes using a low index AlGaN layer to increase interaction with the surface PhC. Reprinted from [171] with the permission of AIP Publishing.](image)

To approach the problem of the limited interaction of the guided light with the PhC, David et al. presented a design using a lower refractive index AlGaN layer beneath the QWs to confine some of the trapped light above the AlGaN layer in modes that they term cap layer modes (CLMs) [171]. Their optical device design is shown in figure 4.3 and they argue that the formation of these CLMs increases the interaction of trapped light with the PhC which would otherwise propagate in low order modes and be poorly extracted in previous approaches. This is achieved without compromising the overlap of the higher order modes as they are not significantly affected by the addition of the AlGaN confining layer. The low order modes which exist in the GaN cavity below the AlGaN are not excited by the QWs as there is little or no spatial overlap of the QWs with their optical field profile and so the low overlap with the PhC is not of concern.

The designs discussed so far use a sapphire substrate, but do not consider the light lost to substrate modes. These modes have an even lower overlap with the PhC than the high order GaN modes and therefore poor extraction. The problem of substrate modes
was considered in GaAs LEDs before III-nitride LEDs. In the GaAs field, Delbeke et al. presented the analysis of a design where a DBR with high reflectivity at propagation angles corresponding to substrate modes was used to prevent the loss of light via this channel and increase the interaction of guided modes with a surface PhC [172], predicting a light extraction efficiency of 43%. Rattier et al. also reported a similar design in GaAs at about the same time [173], likewise avoiding losses by preventing light from entering the substrate with a DBR, achieving 28% extraction by using the leaky modes of the DBR, equivalent to diffraction by a 1D PhC. The logical extension is to make use of the thin film device configurations discussed in §2.4.2 which solve the same problem by removing the substrate entirely and additionally allows compatibility with established thin film LED processes. A report by David et al. etched a PhC into the nGaN surface after substrate removal and polishing to varying thicknesses in thin film LEDs [174]. They concluded that the efficiency in these geometries is limited by absorption in the metallic mirror. Varying the device thickness in the experiments combined PhC technology with thin film resonances previously exploited for extraction enhancement in MCLEDs. It was an optimisation of this PhC MCLED technology by Wierer et al. which has yielded the highest reported $\eta_{ext}$ to date of 73% for an unencapsulated LED [88]. Cho et al. presented a good experiment which should be mentioned as it directly compares their vertical LED with a conventional GaN on sapphire device with the same experimental parameters and includes comments on the overall device performance [175]. They found that the vertical LED produces a much higher light output ($2.05 \times$) without significant degradation of the electrical properties compared to the conventional LED, in line with other results [176].

### 4.2.2 Buried photonic crystals

To increase its interaction with the guided modes in the device, the PhC can alternatively be buried in the GaN below the active region, as shown in figure 4.4. The approach is similar to using an underlying AlGaN confining layer to increase the interaction of a surface PhC with the guided modes as the PhC layer can also confine light to the cap layer above. Embedding the PhC within the epitaxial layers provides the additional advantage of increased interaction with and therefore improved extraction of the high order GaN slab modes. Due to their unpatterned surface, the wafers with a buried PhC are compatible with standard planar device processing techniques. However, they do need a more complicated fabrication process to form the PhC, requiring the pattern to be etched into a GaN template and then overgrown before growth of the active region.

The effect of placing a 1D diffraction grating below the active region was investigated by David et al., who fabricated devices with two different cap layer depths (the layer above
the PhCs), as shown in figure 4.4. Kwon et al. found that the PL output from a 2D buried PhC LED and was increased by 17% over a control sample [177], but it is not clear if this enhancement was due to the increased extraction efficiency of the device or other experimental effects, such as increased in-coupling of the exciting laser light from diffraction by the PhC. A theoretical investigation into optimising structures containing buried 2D PhC was performed by Matioli et al., who argue that a single-moded cap layer can give best performance as a significant proportion of the power emitted from the QWs will be emitted into and then extracted from this first order CLM [178]. After optimising this process, they report an experimental $\eta_{ext}$ of 94% for an encapsulated device [179] using their own measurement technique [180] which relies on measuring the IQE of non-PhC devices on the same wafer. However, they did not comment on the variation of IQE over the wafer, which could be significant as the quality of the material may be substantially better or worse in the area where the GaN is coalesced over the PhC. Using a more conventional low temperature PL method with its own different set of assumptions, they reported $\eta_{ext}$ to be 59% for encapsulated and 46% for unencapsulated devices [181]. An experimental investigation of several thickness of multi-moded cap layers formed over buried photonic crystals was performed at the University of Bath, which concluded that many modes contribute significantly to the extraction [182]. This investigation partly confirmed Matioli et al.’s studies, but also commented on the significance of extraction of higher order modes. Chapter 7 of this thesis discusses the continuation of this work.

Some research has been undertaken into the effect of combining a buried PhC with a surface PhC, for example, a theoretical investigation by Charlton et al. compared the surface, buried and a combination of the two methods on a p-side up device [184]. The study found that combining the two approaches led to extraction of up to 73%, offering an improvement over devices with a similar epitaxial structure but just a surface PhC at $<$49% extraction. Jewell et al. reported very short extraction lengths using a double buried PhC structure which comprised a PhC either side of the QWs to confine the light.
into modes which is extracted by the PhCs well [185]. These designs may not be commercially feasible however due to the number of steps in the growth required during fabrication.

Buried PhCs have also been used to create LEDs with highly polarised emission using non-polar $m$-plane GaN epitaxial layers, which emit polarised light orientated along the $a$-axis. A 1D buried PhC was aligned with the $a$-axis to extract light in guided modes, and was observed to maintain the in-plane polarisation of the emitted light [163].

### 4.2.3 Photonic crystal lattice design

The tiling of the diffraction grating will determine the reciprocal lattice vectors, which in turn determine where in reciprocal space the guided modes are located after diffraction, (see §3.2.1). Due to the circular rotational symmetry of a slab waveguide around the axis perpendicular to the slab, the guided modes supported propagate with equal power in each in-plane direction, creating a circle in reciprocal space. The parts of this circle, corresponding to a range of in-plane propagation directions of the mode, which are inside the air cone (radius $k_0$ in reciprocal space) after diffraction can be extracted. Similarly, if inside the substrate cone (radius $n_{subs}k_0$ in reciprocal space), the light can be extracted to the substrate. If this diffracted light is inside the substrate cone but not the air cone, light will be lost to substrate modes which exhibit a poor spatial overlap with the PhC and, in the case of an absorptive substrate, lost completely. As a result, the pitch and the tiling pattern of the PhC determine which directions of in-plane propagation of the mode can be extracted, redirected to substrate modes or remain trapped in the GaN.

The air filling fraction ($A_{FF}$) of a PhC will affect the strength of diffraction to each order, and increasing (decreasing) the $A_{FF}$ will also push (pull) the optical mode energy profile away from (toward) the PhC, changing the spatial overlap. In light of these two factors, tuning of the $A_{FF}$ for a given crystal lattice is required for optimisation of the diffraction process to air. Both Long et al. and David et al. suggest that an $A_{FF}$ of $\approx 1/3$ gives optimum performance for a hexagonal tiling of air holes [164, 186].

There are many reports which compare the extraction enhancement for different pitches using hexagonal PhCs, predominantly via theoretical simulations. In the early results for surface PhCs, Orita et al. found larger pitches to be most effective [168], whilst others found structures with smaller pitches to be most effective [165, 169]. It is not clear why there is disagreement in the literature here, but it is most likely that differing device structures and assumptions were employed, and possibly affected by some groups choosing nanohole [165, 169] and others nanorod [168] PhC designs. Long et al. reported
a thorough investigation using simulations into varying several of the PhC parameters in both the surface and buried configurations for nanoholes [186]. They found the surface PhC to be best around 350-650nm, which would operate under the second Bragg order, and that the buried PhC is more sensitive to variation with its optimal pitch at 500-600nm for a 465nm source. Many other studies have experimentally swept through the parameters to determine the best value without analysing the cause, for example [167].

Diffraction of light to air, substrate or GaN modes leads to a trade off in the choice of diffraction order to operate at, which sets the pitch of the PhC. A larger pitch will allow diffraction from more Bragg orders to the air cone, and so a higher extracted power when in competition with absorptive processes, but will also increase the power diffracted to the substrate. By careful choice of the pitch and tailoring the guided modes through vertical structure design, the effect of diffraction to the substrate can be minimised at a chosen order, but as the order increases less design flexibility is available due to the larger area of reciprocal space diffracted to the substrate. The ratio of the optical power diffracted to the substrate and the optical power diffracted to air will ultimately increase with increasing diffraction order up to the ratio of the areas in reciprocal space extracted to each location\(^1\). The increased ratio of loss to the substrate acts against the improved performance compared to absorptive processes in the device and additionally, increasing the pitch of the crystal lattice will decrease the diffraction efficiency of each mode [164]. It has been suggested that selecting the pitch of the PhC to operate close to the second Bragg order provides a basic optimisation for a single waveguide mode and a hexagonal PhC tiling [149], in agreement with the simulations by Long et al. [186].

To minimise the power diffracted to the substrate at low orders, the optimal design of the lattice will need to consider the guided modes due to the vertical structure of the device. Under the simplifying assumption that light is not preferentially emitted into guided modes, David et al. considered these diffractive losses to the substrate. The optimal number of nearest neighbours to have in the reciprocal lattice to have in the reciprocal lattice is suggested to be 5 for GaN-based LEDs with a sapphire substrate, presenting the practical hexagonal Euclidean tiling with 6 nearest neighbours as a good solution [164]. A higher order of rotational symmetry, such as that present in a photonic quasi-crystal (PQC), will increase the diffraction to the substrate for the same reasons as described above for a higher diffraction order – again, with very high rotational symmetry, the ratio of the optical power

\(^1\)This can be understood using the reciprocal space model described in §3.2.1 – the ratio of light diffracted into the two extraction cones is given by the ratio of the arc lengths to the circumference inside each extraction cone. Taking a simplistic view at the limit with a very high order, all areas of reciprocal space have an equal power from the large number of diffraction paths for each mode and so, even assuming all light (including substrate-directed light) inside the air cone is extracted for the usual situation with a sapphire substrate (where \(n_{\text{subs}}^2 - n_{\text{air}}^2 > n_{\text{air}}^2\)), a larger proportion of the arcs cross through the substrate cone via the multiple diffraction paths than the air cone.
diffracted to the substrate and to air will increase up to the ratio of their area in reciprocal space. When substrate losses are not a concern, for example in devices where it has been removed or in the different situation where the substrate has a refractive index equal to or higher than the device, PQC lattices (see §3.2.3) have been found to be more effective in GaAs [187] and GaN [188] LEDs. The increased number of reciprocal lattice points and higher order of rotational symmetry available in PQC s compared to the Euclidean tilings can now increase the extraction efficiency without the concern of increasing the light trapped in the substrate. Indeed, the best reported extraction efficiency of 73% used an A13 Archimedean tiling on a thin film flip chip LED with the substrate removed [88].

The first use of PQC s in LEDs was as surface PhCs when Zhang et al. experimentally compared hexagonal PhCs with 8- and 12-fold PQC s and reported that the 12-fold PQC showed the best output enhancement of $1.7 \times$ [189, 190]. Buried PQC structures were investigated experimentally by Huang et al. who used SiO$_2$-filled holes [191, 192] and Charlton et al. who simulated air holes [184]. Both groups report enhancements to $\eta_{\text{ext}}$, again using 12-fold PQC s. Good results have also been obtained using Archimedean lattices [188]. It has been suggested by Bergenek et al. that using quasi-crystal lattices may not be required in multi-moded structures after observing that higher order diffraction contributes more to the overall light output than other studies seem to have assumed [193] and other groups have since presented results which reinforce this view [182, 184].

Another advantage regularly presented for the use of PQC s is that they diffract the light more omni-directionally, creating a better device through more even light output. For example, a comparison of the radial pattern from a square-lattice surface PhC with a PQC using simulations found the PQC output to be much more azimuthally omni-directional [194]. This behaviour was later characterised experimentally [195], in close agreement with the theoretical data.

### 4.2.4 Summary

In summary, the use of diffractive PhC s to improve the extraction efficiency and the effect of each parameter of the device and PhC are becoming well understood, with several groups releasing ‘design-guide’ style papers. Table 4.1 quantitatively summarises results, where available, from the work discussed above and shows the performance of different approaches.

There is such a wide parameter space to optimise that many groups seem to contradict each other and sometimes themselves in the literature, but this is likely due to the different configurations that have been investigated, along with differing interpretations of results. As can be seen from the table, there is no clear correlation between any one parameter and the extraction performance, suggesting that different studies have found different local
**Table 4.1:** Reported performance of blue PhC LEDs.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Lattice</th>
<th>$A_{FF}$</th>
<th>Etch depth</th>
<th>Enhancement</th>
<th>$\eta_{ext}$</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface PhC</td>
<td>700nm hex</td>
<td>0.17</td>
<td>225nm</td>
<td>1.63×</td>
<td></td>
<td>[166]</td>
</tr>
<tr>
<td>Surface PhC</td>
<td>1500nm hex</td>
<td>0.1</td>
<td>250nm</td>
<td>1.5×</td>
<td></td>
<td>[168]</td>
</tr>
<tr>
<td>Surface PhC</td>
<td>315nm hex</td>
<td>0.5</td>
<td>100nm</td>
<td>1.5×</td>
<td></td>
<td>[169]</td>
</tr>
<tr>
<td>Surface PhC</td>
<td>215nm hex</td>
<td>0.3</td>
<td>250nm</td>
<td>2×</td>
<td>24%</td>
<td>[171]</td>
</tr>
<tr>
<td>Surface PhC</td>
<td>1200nm square</td>
<td>0.33</td>
<td>900nm</td>
<td>2.05×</td>
<td></td>
<td>[175]</td>
</tr>
<tr>
<td>Surface PhC</td>
<td>450nm 12PQC</td>
<td></td>
<td>310nm</td>
<td>1.78×</td>
<td></td>
<td>[191]</td>
</tr>
<tr>
<td>Surface PhC</td>
<td>455nm A13 PQC</td>
<td>0.3</td>
<td>250nm</td>
<td></td>
<td>73%</td>
<td>[88]</td>
</tr>
<tr>
<td>Buried PhC</td>
<td>230nm hex</td>
<td>0.12</td>
<td>100nm</td>
<td></td>
<td>46%</td>
<td>[181]</td>
</tr>
</tbody>
</table>

minima. Nevertheless, photonic crystals have produced the best unencapsulated extraction efficiency known to the author, which used a surface photonic quasicrystal in a thin film flip chip configuration [88]. This result was 73%, still leaving scope for improvement. Buried photonic crystals have produced promising results of 46% extraction, but have not been nearly so widely investigated.

### 4.3 Nanorod and core-shell LEDs

Nanorod LEDs have been investigated in both core-shell and quantum disc configurations [196], and the work presented in chapter 8 investigates PhC effects in such structures. The devices typically consist of arrays of nanorods of the order of 50-1000nm in diameter and can be fabricated using a ‘top-down’ method, which etches down into a planar template to define the nanorods, or a ‘bottom-up’ method, which grows the nanostructures upwards. Interest was initially sparked as using the ‘bottom-up’ method could be used to produce high quality planar material through the ELOG process discussed previously.

The quantum disc configuration incorporates a planar active region into each nanorod, typically fabricated by etching through the active region in a planar device. In a $c$-plane template the quantum wells will be strained, leading to a large quantum-confined Stark effect (QCSE) and therefore a reduction of the radiative recombination rate, as discussed in §2.2.2. If nanorods are etched into a $c$-plane template, a reduction of the QCSE has been observed through a blue-shift in the emission compared to a planar template in a
number of studies [61,197,198], due to the strain relaxation of the quantum wells. Varying the nanorod diameter between 50-300nm [61,198] or the penetration depth of the electron beam in CL studies [198] have shown that the blue shift, and therefore the strain relaxation, is much more significant at the edges of the nanorods than the centre.

Due to etching through the active region in the ‘top-down’ approach, these structures suffer damage to the crystal surfaces during the etching process, leading to an increase in surface recombination [199], observed as yellow-band emission. Most research groups employ techniques to recover the surface, for example through annealing [60] or using KOH etching under UV illumination [62]. Remarkably, even with the vastly increased surface area when compared to planar LEDs, the surface leakage increase in nanorod devices has been found by several studies to only be approximately one order of magnitude worse than planar equivalents after recovery [61,199,200].

![Figure 4.5: Core-shell LED structure. Reprinted from [196] with the permission of AIP Publishing.](image)

An alternative approach is to use the core-shell configuration, shown in figure 4.5 and compared with quantum disc nanorods in table 4.2. These structures can be grown onto etched nanorods, which provide an excellent method for recovering the surface after etching [201,202], or grown directly on the substrate through a mask [203] or self-assembled under carefully controlled conditions [204,205], producing material with very low defect densities. The core-shell structure presents several advantages over the quantum-disc nanorod structure. As the active regions are located around and often on top of the nanorods, the emitting surface area for the chip area is greatly increased over a planar device, up to $10 \times$ for currently achievable aspect ratios [196]. The increased emitting area offers a higher brightness or the potential to mitigate droop through requiring a lower current density for the same light output as a planar device [67]. For $c$-plane substrates, the emitting sidewalls are formed of non-polar facets, which reduces the QCSE in the quantum wells, and allows well developed and simpler growth on $c$-plane templates to produce non-polar heterostructures with a good material quality. Due to the encapsulation of the nanorod by the active region, surface recombination is no longer a significant concern in these structures as the area of the surfaces adjacent to the active region is comparable or lower than for planar devices with a similar active area. During the growth of the
quantum wells, different In mole fractions of InGaN can be deposited over the rods [206], or the diameter of the nanorods varied [207] which offers the possibility of phosphor-less white light emitters.

One of the primary challenges of nanorod structures is making electrical contact to them. Most approaches fill in the spaces between adjacent nanorods with a transparent dielectric material [199, 208], allowing 2D processing techniques to be used [196]. Working quantum disc nanorod LEDs have been demonstrated through EL. Early examples showed unfavourable IV characteristics due to high series resistance [199], but more recent examples have been demonstrated with only a small 20mA turn-on voltage increase from a comparable planar device, for example [200] (3.26V nanorod, 3.07V planar) and [208] (3.29V nanorod, 3.14V planar) with operation reported up to 300mA device current. There have also been some initial results with turn on-voltages of 5V presented using graphene sheets laid over the nanorod array as transparent contacts, thus avoiding the need for planarisation [209, 210].

Core-shell designs can be contacted in a similar way [211], or by overgrowing a planar layer at the top of the nanorods [212], but have the additional challenge of current spreading over the shell and core layers to give a homogeneous current density over the active region. The specific design using an overgrown layer considered in ref. [213] showed a 10% increase in wall plug efficiency over a planar device when taking into account increased absorption from their transparent contact.

<table>
<thead>
<tr>
<th>Design</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nanorod</td>
<td>Photonic crystal effects</td>
<td>Etch damage</td>
</tr>
<tr>
<td></td>
<td>Simple to fabricate</td>
<td>Lower active area than planar</td>
</tr>
<tr>
<td></td>
<td>Increased IQE: strain reduction</td>
<td>Large surface recombination area</td>
</tr>
<tr>
<td>Core-shell</td>
<td>Photonic crystal effects</td>
<td>Current spreading in core and shell layers a challenge</td>
</tr>
<tr>
<td></td>
<td>Increased IQE: non-polar QWs</td>
<td>Increased fabrication complexity</td>
</tr>
<tr>
<td></td>
<td>Increased IQE: strain reduction</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Higher active area than planar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Low surface recombination area</td>
<td></td>
</tr>
</tbody>
</table>

**Table 4.2:** Comparison of nanorod and core-shell designs.

Table 4.2 summarises the advantages and disadvantages of nanorod and core-shell geometries, which offer a promising approach to improving the performance of III-Nitride LEDs. When fabricated in periodic arrays, these designs could potentially exploit PhC effects, in addition to the other advantages they offer. Little research into photonic crystal effects in periodic arrays of III-nitride nanorod and core-shell arrays has been carried out, and is the subject of investigation in chapter 8, as there is some indication they may operate in the ‘strong’ or Bloch regime [214].
4.4 Directional emission

As discussed previously in §2.3 and explained in detail in chapter 9, the proportion of the power emitted from a source which can be coupled through a complete optical system with étendue-limited components depends critically on the étendue of the source. For these applications, such as projection or car headlamps, a more directional source will provide improvements to the performance and the efficiency compared to a less directional source.

PhCs offer the potential to control the directivity of the emission from LEDs, and various studies have come to different conclusions about which geometric parameters of a device affect the polar pattern of the light emitted from PhC LEDs most profoundly. Even in initial studies of surface PhCs, the polar emission pattern of the light output was commented on, for example, Wierer et al. found that small changes in the pitch changed the emission pattern markedly [169]. Charlton et al. report little change in directivity with PhC depth for buried and double-patterned LEDs [184], whereas Rangel showed that the depth can be used to tune the directivity in flip chip surface patterned LEDs [215]. This contrast is representative of the literature as there are few studies of how the device behaviour affects the overall directivity, but many which consider how it varies with a single parameter.

The most successful attempts at creating more directional PhC devices operate in the weak behavioural regime, where the optical slab modes are controlled carefully and the PhC lattice designed to preferentially diffract these optical slab modes to normal incidence [112, 216, 217]. This approach is described in detail in §9.2. Both Rangel et al. [216] and Lai et al. [217] produced very similar designs using a thin film flip chip LED with a metal reflector, with similar polar emission patterns. A PhC was etched into the surface after flipping the LED, creating a thin optical waveguide between the bottom of the photonic crystal and the reflector, with the active region positioned to preferentially excite a second-order slab waveguide mode. However, this design is limited by competition between PhC diffraction to extract light and absorption by the reflector. Wiesmann et al. used a multi-moded approach to avoid this effect and reduce the fabrication complexity by designing the PhC lattice to extract the range of modes carrying the highest proportion of the guided power to normal incidence [112]. This approach is in principle less effective, but due to the practical constraints of the single-moded design, was able to produce approximately the same performance in a practical device, as shown in table 4.3. 12% extraction inside 30° for an unencapsulated device is comparable to a high performance Lambertian emitter, once the effect of encapsulation is taken into account. For single-moded operation, the maximum possible performance has been considered for a single
emission frequency to be 50\% within 30^\circ from normal incidence [112]. The operating principle and practical factors affecting the performance of these devices is investigated for practical device linewidths in §9.2 of this thesis.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Proportion of power emitted inside 30^\circ</th>
<th>Total power extracted inside 30^\circ</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-moded</td>
<td>≈30%</td>
<td>Not stated</td>
<td>[216]</td>
</tr>
<tr>
<td>Single-moded</td>
<td>Not stated (similar polar emission to [216])</td>
<td>Not stated</td>
<td>[217]</td>
</tr>
<tr>
<td>Multi-moded</td>
<td>31%</td>
<td>12%</td>
<td>[112]</td>
</tr>
</tbody>
</table>

Table 4.3: Comparison of directional emission using the weak PhC behavioural regime.

A theoretical study by Fehrembach et al. considered operation in the strong or Bloch regime for producing directional emission [218], which is described in §9.3.1. For single wavelength operation, this design was predicted to emit up to 80\% of the optical energy into a cone of half angle 0.2^\circ from normal incidence. The same operating principle is considered in §9.3 for a realistic III-nitride LED design with practical emission linewidths.

### 4.5 Fabrication of photonic crystals

The fabrication process for a PhC can typically be split into two steps; the first is lithography, which defines the 2D tiling pattern of the PhC and the second is the process of creating the PhC in the vertical direction. The considerations for process choice in commercial manufacture are the cost, yield, the speed and if any damage is caused to other parts of the device, whereas a process for the purposes of research and development is more concerned with the cost of fabricating a small number of devices needs to be more customisable.

#### 4.5.1 Lithography

In nanofabrication, lithography is the process of defining where a process should and should not be applied at later fabrication steps. A resist is applied as a film to the surface to be patterned, usually as drops of solvent containing the resist. The substrate is spun to form a film, and then baked to remove the carrying solvent. In microelectronics the most widely used lithography process is photolithography, where a UV light-sensitive resist is illuminated through a mask, which selectively shadows the sample. Other methods for exposing the resist are discussed below. The chemistry of the exposed regions of the resist is changed, usually by cross-linking, and then a developer solvent is used to dissolve either the exposed (positive) or unexposed (negative) areas, depending upon the polarity of the
resist. It might be necessary to perform an inversion process to swap the areas which are
and are not processed, depending upon the technique and the availability of resists with
the correct polarity. If a metal is required to form a pattern to mask another process, such
as etching, then the metal must be deposited by thin film deposition techniques, and then
the exposed resist dissolved to ‘lift-off’ the metal in the areas not to be etched.

Conventional photolithography is not suitable for PhC lithography except at the largest
pitches as it is limited to a minimum pitch size of about 1\(\mu\)m [140] by the diffraction of
light around features on the mask. Deep-UV techniques to mitigate diffraction challenges
do exist which allow fabrication down to tens of nanometres, but have not been applied to
PhCs, likely as they prove too expensive to be considered for manufacture or in research.
Much work had been done in fabricating nano-structures in GaAs, but due to the smaller
pitches required to operate at shorter wavelengths and the different chemistry of GaN,
these technologies must be adapted.

An alternative technique to expose the desired parts of a resist is electron-beam lithog-
raphy (EBL), in this method, an electron beam is directed to specified locations on the
surface to ‘write’ the desired pattern. The number of electrons or dose deposited into
the resist at each location can be controlled directly through the beam current and the
energy of the beam can affect the feature size and shape due to electron scattering. This
technique is commonly used in research due to its flexibility as it does not require a costly
pre-fabricated mask, can be programmed to produce any feature shape and be carried out
in a modified scanning electron microscope (SEM), available at most research institutions.
The smallest features which can be produced with EBL are usually limited by the quality
of the electron optics used to focus the beam and the quantity and energy of secondary
electrons scattered from the main beam travelling in the resist and substrate. Feature sizes
down to \(\approx 20\text{nm}\) or smaller [140] are possible, but the use of EBL in industry is limited
to specialised applications by the time required to write all the features over a large area
and secondarily the cost of the equipment. The first results in InGaN LEDs used this
method [165,219] and EBL continues to be used in research extensively, particularly when
varying PhC parameters are investigated.

Nano-imprint lithography (NIL) uses a stamp or master, patterned with the features
to be transferred to the GaN, and may take the form of a patterned laminar sheet or
roller. The master or roller is pressed against a soft resist which is then heated to high
temperature and/or exposed to UV to harden, leaving the resist thinner in the imprinted
areas. In most methods, the resist is then etched for the correct time to remove only
the imprinted areas and expose the material below, which could be either the GaN or an
intermediate layer for further pattern transfer before an etch step. NIL allows a whole
wafer to be patterned at the nano-scale very quickly with an easily scalable process for
feature sizes down to 10-20nm [140]. It initially requires an expensive imprint master to be fabricated which can be reproduced, making the process inflexible and so not feasible for low-volume or one-off patterning. The uniformity of the process can be limited by the lifetime of the imprint masters and the uniformity of pressure across the sample as a result of wafer bow or other fluctuations on surface of the wafer to be patterned. NIL cannot typically be aligned accurately, and so is not suitable for designs which require alignment with features already present in the devices. Many groups have successfully used NIL to produce PhCs in GaN [220–223] and this technique combined with an inversion process is employed extensively to create metal etch masks at the University of Bath [224]. The NIL process used to fabricate the samples investigated in chapter 8 of this thesis is summarised in figure 4.6.

![NIL process diagram](image)

**Figure 4.6:** University of Bath nano-imprint lithography process.

In laser interference lithography (LIL), the interference pattern from two coherent laser beams is used to pattern a photo-sensitive resist, allowing fabrication of any regular pattern which can be produced from the interference. For example, the pitch of the resulting pattern can be varied by changing the angle between the laser beams. This technique is limited in its application to PhC fabrication as it cannot be used to for features below $\lambda/4$ where $\lambda$ is the wavelength of the lasers [225] due to diffraction of the beams, without applying any specialist methods to decrease the diffraction limit. LIL is suitable for one-off production or research as there is no requirement for a prefabricated mask and it can be set up reasonably cheaply. Some publications report using LIL to produce GaN PhC LEDs [226].

**Nanosphere lithography** uses nanospheres which will self-arrange into close packed hexagonal arrays in two dimensions, applied typically by spinning on a suspension of the spheres in a solvent. The packed spheres can be used to create an etch mask through further processing or directly, as shown in figure 4.7a. The method is quick and cheap, but the quality of the results are limited by the variation in diameter of the spheres, the absence of long-range ordering and difficulty in achieving uniform coverage over large ar-
4.5.2 Creating the photonic crystal

In the literature, the fabrication of the PhC from the lithography has almost exclusively been by etching. The fabrication of PhC structures requires a directional or anisotropic etch to create the vertical topology, the exact nature of which prevents wet processes (chemical etching by a fluid) being suitable for PhCs etched into c-plane GaN as it will etch underneath the mask.

Some solvents with a high etch rate in the direction of the non-polar axes compared to the c-axis are available for GaN, but no studies known the author have reported attempting to fabricate a PhC in non-polar GaN by this method. Some studies have used these facet-dependent wet etches, such as hot potassium hydroxide (KOH), after a dry process in c-plane structures to improve the smoothness of the resulting PhC. For example, it can be used to widen nano-holes and will transform circular holes from a dry etch process into hexagonal holes, conforming to the GaN facets [182].

Dry etching techniques are widely employed for PhC fabrication in GaN, reactive ion etching (RIE) and inductively coupled plasma (ICP) etching have been used extensively. The exact process by which these techniques work is not well understood, but it is through a mixture of chemical and kinetic etch processes. For GaN, a Cl₂/Ar plasma is most
often employed, with the chlorine acting chemically on the GaN and the argon thought to predominantly provide a kinetic sputtering effect. The gases are ionised using radio frequency energy to form the plasma and then accelerated towards the sample using a DC voltage bias between the sample and the plasma source. Highly directional anisotropic etching can be achieved under the correct optimisation of temperatures, plasma power, pressure and gas flow rates. The primary limitations of this method for creating high aspect ratio features are the rate at which the plasma also etches the mask and mask undercutting which acts to widen features under the mask. The sidewall profile of the features in the mask will be transferred during a long etch as the mask is gradually removed.

Unfortunately, the dry etch process has been shown to significantly degrade the characteristics of p-GaN due to damage to the GaN structure from ion penetration, especially at the sidewall surfaces, which reduces the performance of the device [229] (described in §2.1.2 and §2.2.1). Results using wet processes designed to recover the sidewall surfaces after etching have been used successfully [62], as has annealing [60]. Core-shell devices fabricated by the ‘top-down’ method undergo regrowth after etching, which recovers the sidewall crystal structure. More detail of this complication for nanorod structures is discussed in §4.3. For PhC LEDs, a method to eliminate the effect on the p-GaN entirely has been to employ flip-chip device designs to allow the PhC to be etched into the n-GaN surface, which is much less sensitive to the dry etch. The alternative method to the subtractive etch process is to use selective area growth (SAG) to add material to form the PhC, which avoids the problems of etch damage entirely, but introduces significant fabrication challenges. Efficiency enhancements under EL have been demonstrated after the growth of hexagonal arrays of nano-pyramids on the surface of the p-GaN using a nanohole SiO$_2$ growth mask [230]. The inverse pattern of a layer of p-GaN nano-holes using a SiO$_2$ nano-pillar mask has also proved successful [231]. When using a buried PhC configuration, novel growth methods also need to be applied as high quality material needs to be grown over the PhC in a thin layer to produce high quality QWs as close as possible to the PhC. Coalescence of smooth, high quality films have been demonstrated grown over 1D and 2D SiO$_2$-filled nanostructures [183, 232] and air-filled structures [33, 232, 233]. Some results of this work are shown in figure 4.8. The buried PhC configuration has the advantage of avoiding etch damage to the active region as the PhC is etched before growth of the QWs.
4.6 Conclusion

Photonic crystals offer scope for improving the performance of LEDs for high-brightness and étendue-limited applications. They have been used successfully to produce high unencapsulated extraction efficiency and directional emission. Devices are considered to operate in one of two regimes, the ‘weak’ or diffractive regime, where the PhC acts as a diffraction grating and the ‘strong’ or Bloch regime, where the periodicity of the PhC significantly affects the dispersion of supported guided modes. The Bloch regime has only been observed in suspended slabs structures, unsuitable for high-brightness devices.

The diffractive regime has been investigated widely as a means of improving the extraction efficiency of III-nitride LEDs, using several device configurations with different advantages and disadvantages. The operation of these LEDs can be considered to be split into two parts; a 1D part describing the vertical structure of the device and its guided modes, and a 2D part describing the PhC lattice. A substantial amount of published work focusses on the performance of surface PhC LEDs, and the best unencapsulated extraction efficiency known to the author of 73% was produced by a surface photonic quasicrystal etched into a thin film flip chip device. However, low-order modes in this configuration do not interact well with the PhC. Buried PhC LEDs place the PhC inside the device structure to increase the interaction with the guided modes, and have been demonstrated with 46% extraction efficiency, but have not been so widely investigated. No studies have considered whether the 1D-2D model is suitable for buried quasicrystal LEDs. Chapter 7 investigates this model for LEDs containing a buried photonic quasicrystal and studies the feasibility of buried PhC LEDs for improving unencapsulated extraction efficiency.
Nanorod and core-shell device structures have been shown to offer increased performance compared to planar LEDs, for example, increased IQE due to strain relaxation and increased active area for the device area to mitigate efficiency droop. These structures can be fabricated in regular arrays, but little research has been carried out into the photonic crystal effects exhibited by these devices. Chapter 8 experimentally investigates the nature of photonic crystal effects in regular arrays of core-shell and quantum-disc nanorod LEDs, and shows that they can operate in the Bloch regime.

PhC LEDs have been reported which emit \( \approx 30\% \) of the extracted power within \( 30^\circ \) of normal incidence by confining light to specific guided modes and choosing a 2D PhC lattice to diffract these modes close to normal incidence. As discussed in the conclusion of chapter 2, the best result for total extraction efficiency within \( 30^\circ \) of normal incidence of \( \approx 12\% \) only just provides better performance than the best encapsulated surface-roughened devices, giving substantial scope for improvement. Using PhCs, in theory the best performance requires a single-moded design, but the best experimental results are comparable between a less complex multi-moded design and the single-moded design, due partially to absorption in the reflector in the single-moded devices. The buried PhC configuration may be able to overcome some of the limitations of the single-moded design by avoiding reflector absorption whilst maintaining operation of a thin slab waveguide, and is discussed in chapter 7. With operation in the Bloch regime, which is demonstrated experimentally in chapter 8, ultra-directional emission may be possible. The limits to the performance of diffractive PhCs for directional emission and the performance of a design operating in the Bloch regime are investigated in chapter 9.

The fabrication of PhC LEDs requires two principal steps; using lithography to define the 2D pattern of the PhC and removing or adding material to form the PhC. Several techniques suitable for commercial production exist for each step, but fabrication is more costly than for surface-roughened devices. As encapsulated surface-roughened devices can produce very high extraction efficiency with low fabrication complexity, PhCs are not likely to replace this technique for low-cost applications such as space lighting where encapsulation and Lambertian emission do not impact performance. However, the market for directional and high-brightness LEDs is well suited to the increased complexity of fabrication of PhC LEDs where surface-roughening is performance limiting in more specialist étendue-limited applications such as car headlamps or projection.
Chapter 5

Slab waveguide modelling

Typical planar LEDs can be modelled accurately as slab waveguides, an attribute that has been heavily exploited throughout this work. This chapter describes the implementation of the model used when calculations of slab waveguide properties have been presented.

5.1 A transfer and scattering matrix model for slab waveguides

In order to investigate the behaviour of planar epitaxial layers in practical LED structures, a model for waveguiding in arbitrary slab structures was implemented. Due to the flexibility required, a completely generalised analytical approach is not feasible and a numerical method is required. Several suitable techniques exist, the simplest of which is the plane wave expansion method, where any electromagnetic field distribution can be broken down into the sum of plane waves of different wavevector and frequency. A transfer and scattering matrix implementation of this method was chosen as it is accurate, computationally reasonable and straightforward for arbitrary structures. This technique offers the flexibility required to model arbitrary layer stacks and emission from sources therein, with little restriction on their composition. Many other people have discussed and implemented similar models in the past and their work has provided excellent guidance on the development of the model used in this thesis [109,234–236]. A model has been implemented as part of this work as existing freely-available software does not allow for the power flows between the waveguide layers due to a source to be calculated.

5.1.1 A note on notation and coordinates

This method requires the use of field vectors and their components travelling in different directions. Conventional symbol notation has been used where possible, but in some places this would lead to unclear statements. Figures are used to illustrate the meaning of symbols throughout and for reference, this chapter uses the following symbol conventions:
A – an italic letter represents a scalar quantity or vector component in the direction given in subscript.

\( \mathbf{D} = \begin{bmatrix} D_x \\ D_y \end{bmatrix} \) – a bold letter with a hat above denotes a vector quantity, for example the displacement field vector.

\( \mathbf{E} \) – a bold letter represents a magnitude in the direction of the corresponding field vector (the value can be positive or negative), for example the magnitude of the electric field vector.

\( \mathbf{H} \) – arrows above a quantity represent the direction of travel perpendicular to the plane of the waveguide, for example the magnitude of the left travelling magnetic field. Two arrows, \( \mathbf{H} \), are used as a shorthand for both quantities.

\( k_{x1} \) – a subscript represents a direction and/or the layer(s) of the stack the quantity refers to, for example the \( x \)-component of the wavevector in layer 1.

\( M_{ij} \) – for matrices representing the properties of one or several layers. The order of the layers in the subscript states the direction of the matrix, for example the transfer matrix from layer \( i \) to layer \( j \).

\( S_{(a,b)} \) – subscript coordinates represent a specific element of a matrix, i.e. \( S = \begin{bmatrix} S_{(1,1)} & S_{(1,2)} \\ S_{(2,1)} & S_{(2,2)} \end{bmatrix} \)

The geometry used is shown in figure 5.1. The \( z \)-direction is perpendicular to the waveguide and increases from the superstrate (left) towards the substrate (right). The propagation vector of light is always considered to be in the \((x, z)\) plane and the waveguide media are invariant over the \((x, y)\) plane. Geometrically, the system can be rotated about the \( z \)-axis to consider all possible propagation directions. Where spherical coordinates are needed for investigating source emission, \( \theta \) refers to the angle from the \( z \)-axis and \( \phi \) the angle within the \((x, y)\) plane.
5.1.2 Light propagation in layered media

Maxwell’s equations describing the behaviour of electromagnetic fields are [237–239]

\[
\nabla \cdot \mathbf{D} = \rho \tag{5.1}
\]
\[
\nabla \cdot \mathbf{B} = 0 \tag{5.2}
\]
\[
\nabla \times \mathbf{E} = -\partial_t \mathbf{B} \tag{5.3}
\]
\[
\nabla \times \mathbf{H} = \mathbf{J} + \partial_t \mathbf{D} \tag{5.4}
\]

Solving Maxwell’s equations for a vector field \( \mathbf{F} \) in a homogeneous sourceless medium \( \mathbb{R} \) for a specific wavevector \( \mathbf{k} \) gives

\[
\mathbf{F}(\mathbb{R}) = Ae^{i(\omega t - \mathbf{k} \cdot \mathbf{R})} \tag{5.5}
\]

where \( \omega \) is the angular frequency of the wave and \( A \) its amplitude. More details of this process are well described in most introductory electromagnetics textbooks. Equation (5.5) describes a plane wave, where parallel planes of constant field magnitude form perpendicular to the direction of propagation represented by \( \mathbf{k} \) at a constant frequency. As this investigation is interested in the spatial behaviour of electromagnetic waves in an arbitrary planar geometry rather than their evolution over time, the time dependence \( \omega t \) can be set to zero.

Due to the principle of superposition, any spatial field distribution due to a propagating wave with a single frequency can be described as the sum of the field components of a set of plane waves \( \{\mathbf{k}\} \) propagating with different \( \mathbf{k}_i \) weighted by expansion coefficients \( A_i \) [240]:

\[
\mathbf{F}(\mathbb{R}) = \sum \{k\} A_i e^{-i\mathbf{k}_i \cdot \mathbf{R}} \tag{5.6}
\]

When a waveguide is considered, \( \{\mathbf{k}\} \) will be a discrete set for guided light and a continuum for unguided light, as discussed in §3.1 previously.

In the case of plane waves travelling in the \((x, z)\)-plane in a 3-dimensional Cartesian space, as will be considered in the rest of this chapter and shown in figure 5.1, \( \mathbf{k} = (k_x, k_y, k_z) \) where \( k_y = 0 \) and \( k_x \) represents the parallel component of the wavevector referred to as \( k_{||} \) previously. For a plane wave with amplitude \( A \) in medium 1 (where \( z < 0 \)) incident upon an interface (at \( z = 0 \)) with medium 2 (where \( z > 0 \)) as shown in figure 5.2, the wave will be reflected and transmitted with amplitudes \( B \) and \( C \) respectively.

It can be seen in figure 5.2 that the total field due to this plane wave is given by the
sum of the two fields from the counter-propagating plane waves:

$$
\begin{align*}
F_{z<0} &= Ae^{-i(k_{x1}x-k_{z1}z)} + Be^{-i(k_{x1}x+k_{z1}z)} \\
F_{z>0} &= Ce^{-i(k_{x2}x-k_{z2}z)} + De^{-i(k_{x2}x+k_{z2}z)}
\end{align*}
$$

(5.7)

where for the specific situation shown in figure 5.2, $D=0$, but will be non-zero due to reflections if there are further interfaces for $z>0$. Equations (5.7) can instead be represented by position dependent field magnitudes e.g. for $z<0$,

$$
\begin{align*}
\vec{F}_{z<0}(x,z) &= Ae^{-i(k_{x1}x-k_{z1}z)} \\
\vec{F}_{z<0}(x,z) &= Be^{-i(k_{x1}x+k_{z1}z)}
\end{align*}
$$

(5.8)

where the arrow above the field quantity represents the direction of propagation along $z$. When several parallel interfaces are combined in a stack, the total field magnitude for this plane wave in any layer for fixed $x$ can be described in terms of the two field magnitudes corresponding to counter-propagating waves due to reflections off the interfaces:

$$
F(z) = \vec{F}(z) + \vec{F}(z)
$$

(5.9)

A multilayer slab system consists of layers of homogeneous optical media and the interfaces between them. To summarise the method presented below, the interface conditions found from Maxwell’s equations show that the two fields on one side of an interface depend directly upon the two fields on the other side of the interface. It is obvious from (5.5) that this relation also applies to the fields inside a layer. Therefore, the fields for both directions of travel $\vec{F}$, can be found anywhere in a multilayer slab system from a known or incident initial field $\vec{F}_0$ somewhere in the system – the reverse-travelling partner of this initial field $\vec{F}_0$ can be found from the reflectance of the system, and then the pair propagated through each layer and interface in the slab to find the fields elsewhere. The initial fields can be set arbitrarily or from an incoming field or source condition.
5.1.3 Transfer and scattering matrices

A transfer or scattering-matrix model is very general and can be applied to any physical system with observables which can be related together by a series of interactions applied in the sequence determined by the system. In the case of a multilayer stack, these observables are the pairs of fields and the interactions describe their propagation through the layers and interfaces in the stack. Consider the system shown in figure 5.3, where the input and output fields at any interface between two layers $i$ and $j$ can be related together by reflection $r_{ij}$ and transmission $t_{ij}$ coefficients, for example layer 1 to layer 2:

\[ \begin{align*}
\vec{F}_2 &= t_{12} \vec{F}_1 + r_{21} \vec{F}_2 \\
\vec{F}_1 &= r_{12} \vec{F}_1 + t_{21} \vec{F}_2
\end{align*} \tag{5.10} \]

This can be put into matrix form

\[ \begin{bmatrix} \vec{F}_2 \\ \vec{F}_1 \end{bmatrix} = S_{12} \begin{bmatrix} \vec{F}_1 \\ \vec{F}_2 \end{bmatrix} \tag{5.11} \]

where

\[ S_{ij} = \begin{bmatrix} t_{ij} & r_{ji} \\ r_{ij} & t_{ji} \end{bmatrix} \] (≡ \begin{bmatrix} S_{ij(1,1)} & S_{ij(1,2)} \\ S_{ij(2,1)} & S_{ij(2,2)} \end{bmatrix})

is the scattering matrix of the system.

These relations can also be rearranged to give the two fields on the right of the system from the fields on the left:

\[ \begin{bmatrix} \vec{F}_2 \\ \vec{F}_1 \end{bmatrix} = M_{12} \begin{bmatrix} \vec{F}_2 \\ \vec{F}_1 \end{bmatrix} \tag{5.12} \]

where

\[ M_{ij} = \begin{bmatrix} t_{ij} - r_{ij}t_{ji}^{-1} & r_{ji}t_{ji}^{-1} \\ -r_{ij}t_{ji}^{-1} & t_{ji}^{-1} \end{bmatrix} \]

is the transfer matrix of the system. The two formalisms are equivalent mathematically, but using both to describe these systems becomes important in a numerical implementation of the method, as will be discussed later. Transfer matrices have the useful property that they can simply be multiplied to find the transfer matrix for several cascaded sub-systems, e.g. for a system $ac$ which consists of the two subsystems $ab$ and $bc$:

\[ M_{ac} = M_{ab} \times M_{bc} \quad \text{or more generally,} \quad M_{1N} = \prod_{i=1}^{N-1} M_{i,i+1} \tag{5.13} \]

for a system with $N$ cascaded sub-systems.
Scattering matrices require some rearranging to cascade,

\[
S_{ac} = \begin{bmatrix}
XS_{ab(1,1)}S_{bc(1,1)} & S_{bc(1,2)} + XS_{ab(1,2)}S_{bc(1,1)}S_{bc(2,2)} \\
S_{ab(2,1)} + XS_{bc(2,1)}S_{ab(1,1)}S_{ab(2,2)} & XS_{ab(2,2)}S_{bc(2,2)}
\end{bmatrix}
\]

(5.14)

where \( X = \frac{1}{1 - S_{ab(1,2)}S_{bc(2,1)}} \)

which can be iterated to cascade more than two sub-systems.

\[\text{Figure 5.3: Fields in an optical system.}\]

For modelling light in a multilayer stack, two types of matrix exist; propagation matrices, which characterise the propagation of the fields through a layer in the stack and boundary matrices, which describe the interaction of the fields with a change in refractive index between two layers in the stack. These matrices can be found for each part of the stack and combined to give the transfer or scattering matrix for the whole system.

5.1.4 Propagation and boundary matrices in multilayer slabs

Propagation of the fields through a layer is the application of (5.5) to each field:

\[
\begin{align*}
\mathbf{F}_2 &= e^{ikzd} \cdot \mathbf{F}_1 + 0 \cdot \mathbf{F}_2 \\
\mathbf{F}_1 &= 0 \cdot \mathbf{F}_1 + e^{ikzd} \cdot \mathbf{F}_2
\end{align*}
\]

(5.15)

where \( d \) is the thickness of the layer. The non-physical increasing exponential fields in unguided media where the fields are evanescent are discarded by taking \( k_z \) to have a positive imaginary part, hence the sign change of the exponent from (5.5). This gives the propagation matrices

\[
S_p = \begin{bmatrix}
e^{ikzd} & 0 \\
0 & e^{ikzd}
\end{bmatrix}
\]

(5.16)

\[
M_p = \begin{bmatrix}
e^{ikzd} & 0 \\
0 & e^{-ikzd}
\end{bmatrix}
\]

(5.17)
and for cascading the scattering matrix $S$ through a homogeneous layer, (5.14) simplifies to

$$S_{\text{new}} = \begin{bmatrix} S_{(1,1)}e^{ik_1d} & S_{(1,2)}e^{2ik_1d} \\ S_{(2,1)} & S_{(2,2)}e^{ik_2d} \end{bmatrix}$$  \hspace{1cm} (5.18)$$

To find the boundary matrices, the interface conditions for the fields at a dielectric-dielectric boundary can be derived from the integral form of Maxwell’s equations. Assuming unity relative permeability ($\mu = 1$) and no source currents at the interface, the tangential electric ($E_x, E_y$) and magnetic fields ($H_x, H_y$) are constant across the boundary. Applying the conditions to the situation in figure 5.2 allows the field reflection ($r_{12} = B/A$) and transmission ($t_{12} = C/A$) coefficients to be found. For the case of TE polarisation, where

$$\hat{E} = \begin{bmatrix} 0 \\ E_y \\ \hat{z} \end{bmatrix} \quad \text{and} \quad \hat{H} = \begin{bmatrix} H_x \\ 0 \\ \hat{y} \end{bmatrix}$$  \hspace{1cm} (5.19)$$

imposing the interface continuity conditions to the $E_y$ field requires

$$Ae^{-ik_1x} + Be^{-ik_2x} = Ce^{-ik_2x}$$  \hspace{1cm} (5.20)$$
at the interface $z = 0$. Applying continuity of the tangential $\hat{H}$-field, $H_x$ yields

$$k_1Ae^{-ik_1x} - k_1Be^{-ik_1x} = k_2Ce^{-ik_2x}$$  \hspace{1cm} (5.21)$$
which is found by applying Faraday’s law (5.3) and the relation $\hat{B} = \mu_0\mu\hat{H}$ to equation (5.20):

$$\frac{\partial E_y}{\partial z} = -i\omega\mu_0\mu H_x$$  \hspace{1cm} (5.22)$$

As a result, both (5.20) and (5.21) lead to $k_{z1} = k_{z2}$, confirming the continuity of $k||$ through all layers of the stack. For all $x$, the following two electric field amplitude relations therefore apply:

$$A + B = C$$  \hspace{1cm} (5.23)$$
$$k_{z1}A - k_{z1}B = k_{z2}C$$  \hspace{1cm} (5.24)$$

The reflection and transmission coefficients are found by solving (5.23) and (5.24)

$$r_{12(TE)} = \frac{k_{z1} - k_{z2}}{k_{z1} + k_{z2}} \quad \text{and} \quad t_{12(TE)} = \frac{2k_{z1}}{k_{z1} + k_{z2}}$$  \hspace{1cm} (5.25)$$

A similar process gives the coefficients for the electric field amplitude for TM polarisation ($\hat{H} = H_y\hat{y}$):

$$r_{12(TM)} = \frac{n_2^2k_{z1} - n_2^2k_{z2}}{n_2^2k_{z1} + n_1^2k_{z2}} \quad \text{and} \quad t_{12(TM)} = \frac{2n_1n_2k_{z1}}{n_2^2k_{z1} + n_1^2k_{z2}}$$  \hspace{1cm} (5.26)$$
Equations (5.25) and (5.26) are known as the Fresnel equations and can be used directly to give the scattering matrices at a boundary for each polarisation state in the multilayer slab. As the intensity of the light is proportional to the square of the electric field strength, the square of these field coefficients will give the reflection and transmission of power by the boundary. To get the transfer matrices, some rearranging is required:

\[
M_I(TE) = \frac{1}{2kz_2} \begin{bmatrix}
k_{z1} + k_{z2} & k_{z2} - k_{z1} \\
k_{z2} - k_{z1} & k_{z1} + k_{z2}
\end{bmatrix}
\]

\[
M_I(TM) = \frac{1}{2kz_2n_1n_2} \begin{bmatrix}
n_2^2k_{z1} + n_1^2k_{z2} & n_1^2k_{z2} - n_2^2k_{z1} \\
n_2^2k_{z2} - n_1^2k_{z1} & n_2^2k_{z1} + n_1^2k_{z2}
\end{bmatrix}
\]

(5.27)

With this information, the transfer and scattering matrices for an arbitrary layered stack can be found using (5.13) and (5.14) at a frequency of interest from the refractive index and the thickness of each layer.
5.2 Implementation of the model

A function library was written in MatLab to implement the transfer matrix model. A simple structure has been used to test the model, consisting of a suspended 500nm thick slab with refractive index 2.5 surrounded by a semi-infinite air superstrate and substrate.

5.2.1 Guided slab modes

![Diagram showing fields on the left and right sides of the interfaces in a multilayer stack with semi-infinite superstrate and substrate layers L and R.]

Figure 5.4: Fields on the left \( l \) and right \( r \) sides of the interfaces in a multilayer stack with semi-infinite superstrate and substrate layers \( L \) and \( R \).

The conditions giving rise to guided modes can now be imposed to the matrices describing the slab waveguide. When optical power is guided inside the stack, the incoming fields will be zero\(^1\), but there will be non-zero outgoing fields. For the layered stack shown in figure 5.4, the incoming fields \( \vec{F}_{r,L} \) and \( \vec{F}_{l,R} \) are set to 0 and equation (5.12) becomes

\[
M_{LR} \begin{bmatrix} 0 \\ \vec{F}_{r,L} \end{bmatrix} = \begin{bmatrix} \vec{F}_{l,R} \\ 0 \end{bmatrix}
\]

(5.28)

i.e.  \( M_{LR(2,2)} = 0 \)  (5.29)

As \( k_x \) is constant for all layers, the values of \( k_x \) which satisfy (5.29)\(^2\) can be used to give the effective refractive indices \( n_{eff} \) of the allowed guided modes for a frequency of interest. Alternatively, \( k_x \) could be fixed and the system parameters determined as a function of \( k_0 \) if desired to find the dispersion relation. A root finder can be used to solve (5.29). For lossless waveguides comprised of layers with real refractive index \( n \) values, \( k_x \) will be real, whereas for lossy (or amplifying) layers with complex \( n \), \( k_x \) will be complex. The built-in MatLab function \texttt{fzero} was used to solve the guiding condition (5.29) in this work for lossless waveguides.

The 500nm test slab of refractive index 2.5 suspended in air supports 6 TE and 6 TM guided modes for light with a wavelength of 450nm in air. The \( n_{eff} \) values are shown in

---

\(^1\)Imposing this restriction is equivalent to using perfectly-matched layer (PML) boundary conditions at the edges of the waveguide.

\(^2\)for \( k_z = \sqrt{k_0^2 n^2 - k_x^2} \), choosing the root with a positive imaginary part
In addition, a freely available slab waveguide solver called CAMFR [236] was used to validate the results produced by the MatLab model. CAMFR makes use of perfect electrical conductors (PEC) at the edges of the simulation region to allow more advanced functionality, so the air superstrate and substrate for the test slab were represented by layers 500µm thick to prevent parasitic reflections affecting the results. The results produced by CAMFR are also shown in Table 5.1. As long as the optical thicknesses of the substrate and superstrate are made large enough in the CAMFR model, the results agree for arbitrary stacks.

<table>
<thead>
<tr>
<th>Mode index</th>
<th>This work</th>
<th>CAMFR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.46783127539409</td>
<td>2.46783127534</td>
</tr>
<tr>
<td>2</td>
<td>2.36919152363911</td>
<td>2.36919152326</td>
</tr>
<tr>
<td>3</td>
<td>2.196932475681524</td>
<td>2.19693247568</td>
</tr>
<tr>
<td>4</td>
<td>1.936014851369893</td>
<td>1.93601485137</td>
</tr>
<tr>
<td>5</td>
<td>1.555992629113419</td>
<td>1.55599262911</td>
</tr>
<tr>
<td>6</td>
<td>1.027012902046905</td>
<td>1.02701290205</td>
</tr>
</tbody>
</table>

(a) TE.

<table>
<thead>
<tr>
<th>Mode index</th>
<th>This work</th>
<th>CAMFR</th>
</tr>
</thead>
<tbody>
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<td>2.460794174554515</td>
<td>2.46079417455</td>
</tr>
<tr>
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<tr>
<td>3</td>
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</tr>
<tr>
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<td>1.78864433312</td>
</tr>
<tr>
<td>5</td>
<td>1.296625856110832</td>
<td>1.29662585611</td>
</tr>
<tr>
<td>6</td>
<td>1.001372361158670</td>
<td>1.00137236116</td>
</tr>
</tbody>
</table>

(b) TM.

Table 5.1: \( n_{eff} \) values produced by CAMFR and the MatLab model developed for a 500nm thick slab suspended in air with refractive index 2.5 for light with a wavelength of 450nm.

### 5.2.2 Field profiles

Once the in-plane wavevector \( k_x \) for each mode is known, the field profile in the slab can be found for each mode. The reverse and forward travelling field magnitudes can be found by setting the total field at a point in the stack to a value and propagating it out from this point through the slab layers.

The initial field values can be chosen arbitrarily, in which case only the shape of the field conveys any useful meaning and the numerical relationship between the field magnitudes for different modes only has meaning after some sort of normalisation is applied, for example to represent emission from a source as discussed below in §5.2.3.

In a numerical implementation where the field values are represented by floating point
numbers, care must be taken when propagating the fields through the structure. Using only the transfer matrix method to propagate through the layers requires the addition of very small numbers to very large numbers due to the opposite signs of the exponential terms in (5.17). For floating point number representations, these small terms can be beyond the precision of the large terms, so addition may not change the value of the large term thus introducing numerical instabilities. These can be avoided by using only one sign of exponential.

The numerically stable method used in this work uses a combination of both the transfer and scattering matrix approaches. The fields are propagated through each layer from an adjacent layer using an iterative process which avoids using both the decreasing and increasing exponential terms when propagating the fields through each layer. Referring to the notation used in figure 5.4, the fields at any position in layer \( N \) (\( \vec{F}_N(z) \)) can be found from the fields on the left side of layer \( N+1 \) (\( \vec{F}_{l,N+1} \)).

Firstly, the counter propagating fields \( \vec{F}_{l,N+1} \) and the interface transfer matrix \( M_{I(N+1,N)} \) for the boundary \((N+1, N)\), are used to find the reverse travelling field on the right side of layer \( N \) (\( \vec{F}_{r,N} \)) using (5.12),

\[
\vec{F}_{r,N} = M_{I(1,1)} \vec{F}_{l,N+1} + M_{I(1,2)} \vec{F}_{l,N+1}
\]

This field is propagated through \( N \) to give the reverse travelling field at the far left side of layer \( N \) (\( \vec{F}_{l,N} \)) with (5.5), i.e.

\[
\vec{F}_{l,N} = \vec{F}_{r,N} e^{ik_N z_N}
\]

where \( d \) is the thickness of the layer. By changing the value of \( d \), the field at any point in layer \( N \) can be found as a function of position. The scattering parameters of the left side of the structure (\( S_{LN} \)) are used to reflect \( \vec{F}_{l,N} \) to find the corresponding forward travelling field \( \vec{F}_{l,N} \), with (5.11)

\[
\vec{F}_{l,N} = S_{LN(1,1)} \vec{F}_{r,L} + S_{LN(1,2)} \vec{F}_{l,N}
\]

where the incoming field from the superstrate, \( \vec{F}_{r,L} \) is known to be zero. Finally, using (5.5) the forward travelling field magnitude can be found at any point in layer \( N \)

\[
\vec{F}_N(z) = \vec{F}_{l,N} e^{ik_N z}
\]

Both the coefficients used to propagate the fields through the layer have positive exponents, and the method is equivalent to using the scattering parameters for propagation in layer \( N \) given in (5.16). The fields \( \vec{F}_{l,N} \) can be used to repeat the process for layer \( N-1 \).
The obvious implementation of this method is to set the outgoing field at one side of the multilayer stack to an arbitrary value and propagate this field through as above (with the incoming field set to 0). However, as the $n_{\text{eff}}$ for each mode cannot be represented perfectly in a numerical system, errors in the values of $k_x$ and $k_z$ become apparent as minute field discontinuities at the interfaces. These discontinuities become significant as the evanescent fields become very small in thicker regions for which the light is not guided and can cause unstable non-physical results. The mitigation is to set the initial field conditions for an interface inside the stack where the fields are evanescent and the incoming field can be approximated to zero, rather than at the true edge of the stack. This ensures the method remains stable and physical at the cost of an insignificant field discontinuity at the interface chosen. Errors can be prevented when investigating weakly coupled guides by avoiding approximating fields to zero between guiding regions.

To find the fields in the superstrate and substrate, the field at the boundary is propagated outwards using (5.5) for the desired distance. For the evanescent fields of guided modes in the superstrate and substrate, $k_z$ will take a purely imaginary value, leaving (5.5) as an exponential decay.

Now that the reverse and forward travelling field magnitudes are known through the structure, the components of the electric and magnetic field vectors as a function of $z$-position can be determined. The total field is then given by the sum of the reverse and forward travelling fields. In this work, the convention is chosen that the field magnitudes represent the electric field. The relationship between the fields can be determined from (5.3) and (5.4).

For the TE fields

$$\vec{E}_y = \vec{E}$$

$$\vec{H}_z = -\frac{k_x}{k_0 c \mu_0} \vec{E}$$

$$\vec{H}_x = \frac{k_{zi}}{k_0 c \mu_0} \vec{E}$$

and similarly for the TM fields

$$\vec{H}_y = \vec{H} = c \epsilon_0 n_i \vec{E}$$

$$\vec{E}_z = \frac{k_x}{k_0 n_i} \vec{E}$$

$$\vec{E}_x = \frac{k_{zi}}{k_0 n_i} \vec{E}$$

$$\vec{E}_x = -\frac{k_{zi}}{k_0 n_i} \vec{E}$$

where $\vec{E}$ is the electric field magnitude as a function of $z$ position and subscript $i$ represents the layer for the $z$ position under consideration.
The time-averaged intensity or Poynting vector [241] as a function of position can be found using the fields

\[ \hat{S} = \frac{1}{2} \text{Re} \left( \hat{E} \times \hat{H}^* \right) \]  

(5.36)

where \( \hat{H}^* \) is the complex conjugate of the magnetic field.

![Electric field amplitude](image)

(a) This work.

![Electric field amplitude](image)

(b) CAMFR.

**Figure 5.5:** Electric field variation with position for the first 4 TE modes in a 500nm thick slab with refractive index 2.5 for a freespace wavelength of 450nm.

Figure 5.5a shows how the \( E_y \) field for the first four TE modes varies with position in the test slab. The initial value for the field is set at the interface between the guide and the substrate (\( x = 500 \text{nm} \)), giving all the fields here the same sign. The same output from CAMFR is displayed in figure 5.5b, which is identical except for the signs of modes 3 and 4. Close inspection of all the field profiles produced by the MatLab library shows them to be highly accurate.

### 5.2.3 Modelling emission from source layers

In the presence of a source, the outgoing field magnitudes will be set by the interaction of the source with its surroundings. Considering a plane source with fixed position in \( z \) and invariance in the \( x \) and \( y \)-directions, the multilayer stack can be split by the source into left (\( z < z_s \)) and right (\( z > z_s \)) stacks with scattering parameters \( S_{ls} \) and \( S_{sr} \) respectively, shown in figure 5.6. Inside the source itself, there will be a field in each direction due to the excitation, referred to here as \( \vec{A} \) and \( \vec{A}^\prime \) as a function of \( \theta_s \), the angle of propagation from the \( z \)-axis in the source layer. In order to include the effect of evanescent coupling from the source to all of the layers in the structure, we must embed the source in an infinitesimal layer \( n_s \) with the real part of its refractive index equal to or greater than all the other layers in the system.

To find the two sets of counter-propagating field magnitudes \( \vec{F}_l \) and \( \vec{F}_r \) in \( n_s \) either side
of the source, the approach considers what happens to the field $\vec{A}$ attempting to leave the source. This field is repeatedly bounced off the left and right stacks, with the reflectance on each round-trip given by the product of the reflectance of each stack $S_{ls(1,2)}S_{sr(2,1)}$. After an infinite number of trips, this converges to

$$\frac{\vec{A}}{1 - S_{ls(1,2)}S_{sr(2,1)}}$$

(5.37)

exiting the source. To find the total outgoing field, we must also include the contribution of $\vec{A}$ reflected off the opposite side of the structure

$$\vec{F}_l = \frac{\vec{A} + S_{sr(2,1)}\vec{A}}{1 - S_{ls(1,2)}S_{sr(2,1)}}, \quad \text{and similarly,} \quad \vec{F}_r = \frac{\vec{A} + S_{ls(1,2)}\vec{A}}{1 - S_{ls(1,2)}S_{sr(2,1)}}$$

(5.38)

The fields travelling towards the source are found by reflecting these outgoing fields off the surrounding stacks

$$\vec{F}_l = \vec{F}_l S_{ls(1,2)} \quad \text{and} \quad \vec{F}_r = \vec{F}_r S_{sr(2,1)}$$

(5.39)

$\vec{F}_l$ and $\vec{F}_r$ can now be propagated through the various layers of the system as desired.

The procedure for determining $\vec{A}$ is now described. The coupling strength of a dipole $\hat{J}$ with a field scales with the dot product of the dipole and the field vector

$$\vec{A} \propto \hat{J} \cdot \vec{F}$$

(5.40)

Isotropic sources can be modelled as the sum of three dipoles orientated perpendicularly, aligned along each of the $x$, $y$ and $z$-axes for simplicity. This gives three sets of source fields; those due to two horizontal dipoles $- \vec{A}_x$ and $\vec{A}_y$ — in the plane of the waveguide and a vertical dipole, $\vec{A}_z$. Only fields with components of the field vector along the direction of the dipole orientation will be excited. Specifically for electric dipoles, only TE modes will be excited by $\vec{A}_y$ and only TM modes for $\vec{A}_x$ and $\vec{A}_z$ where (5.40) gives the following
source terms

\[ \vec{A}_x = \sqrt{\frac{3\mu_0 c}{8\pi n_s}} \cos(\theta_s) \quad \text{and} \quad \vec{A}_x = -\vec{A}_x \tag{5.41} \]

\[ \vec{A}_y = \sqrt{\frac{3\mu_0 c}{8\pi n_s}} \tag{5.42} \]

\[ \vec{A}_z = \sqrt{\frac{3\mu_0 c}{8\pi n_s}} \sin(\theta_s) \tag{5.43} \]

as a function of propagation angle \( \theta_s \) to the z-axis in the source layer. In the x case, the source terms must be given opposite signs as the x-component of the propagation vector does not change sign between the forward and backward travelling waves. Normalisation constants have been added to scale the emission so that the surface integral of the Poynting vector over a sphere is equal to 1 for the combined horizontal dipoles and for the vertical dipole in a homogeneous medium.

This method can be implemented simply by calculating the fields inside the source layer as a function of a discrete grid of the propagation angle in the source layer, \( \theta_s \). (5.36) is used to calculate the power flow due to each of the fields for the desired parts of the structure, which represents an energy flux per solid angle. The total power emitted from the source as a function of \( \theta_s \) can be found by calculating the difference between the power leaving the source layer and the power returning after reflection off the structure. When performing this subtraction, the z-components must be given opposite signs due to their opposing directions of travel

\[ \hat{\mathbf{S}} = \begin{bmatrix} \hat{s}_x \\ \hat{s}_y \\ \hat{s}_z \end{bmatrix} - \begin{bmatrix} \hat{s}_x \\ \hat{s}_y \\ -\hat{s}_z \end{bmatrix} \tag{5.44} \]

for the left side of the source. \( \hat{\mathbf{S}} \) can be integrated over all or a range of \( \theta_s \) and through the sphere surface subtended to find the total power emitted, simply

\[ \Phi = \int_{0}^{2\pi} \int_{0}^{\theta_s} |\hat{\mathbf{S}}| \, d\theta_s \, d\phi \tag{5.45} \]

as \( \hat{\mathbf{S}} \) is orientated along the propagation direction, \( \theta_s \). To account for both directions of emission and polarisation for horizontal dipole emission, \( \Phi \) can be found for each of these and summed to give the total emission as all the powers are time averaged and incoherent. If all \( \theta_s \) are considered, the normalisation constants will give \( \Phi \) to be unity for homogeneous media for each dipole type (horizontal, vertical) or otherwise the emission enhancement factor for the multilayer stack.

Performing this integration (5.45) for guided modes produces a problem. For guided light in a lossless waveguide, both the numerator and denominator of (5.38) become zero.
which (in this case, from limit theory) produces a delta function at each mode and zero elsewhere. Physically this makes sense\(^3\) as no energy loss is encountered under these conditions so all the guided energy emitted travels along the \(x\)-direction for an infinite distance. Whilst analytically the integral of this delta function may produce the value for the energy emitted, it is obviously not possible to evaluate it numerically. The solution is to add a small imaginary term to the refractive index of the layers surrounding the source, representing an absorptive loss of energy in those layers. This causes the guided delta functions to broaden and the peak to become finite without significant error when determining the area underneath.

To compute the energy emitted into low-loss guides accurately and efficiently, an adaptive grid for theta can be used with more points near guided modes and fewer away from them for low-loss guides. This allows investigation of how much power is emitted as a function of cavity properties, for example its thickness for a source in the centre, as shown in figure 5.7. To find the power in each mode, the integration is performed only over the range of \(\theta_s\) corresponding to emission into the specific mode. As the cavity increases in thickness, the power in each mode initially climbs as the mode moves away from cut-off to become more confined and then falls away. As the source is placed in the centre of the cavity, only odd modes are excited.

![Power emitted into TE modes as a function of cavity thickness for a 500nm thick slab with refractive index 2.5 at freespace wavelength 450nm. An extinction coefficient of 0.001 has been added to the refractive index.](image)

**Figure 5.7:** Power emitted into TE modes as a function of cavity thickness for a 500nm thick slab with refractive index 2.5 at freespace wavelength 450nm. An extinction coefficient of 0.001 has been added to the refractive index.

The power leaving the waveguide into the substrate or superstrate can be found using the same process as before in (5.44) for the power flows at the inside edges of the guide.

\(^3\)As far as perfectly lossless media do, along with infinite slabs and frictionless vacuums.
Finding the power here, rather than over the critical angle in the source layer ensures that the effects of Fresnel reflection at the interface and absorption in the guide on the power flow are included. To find the extraction efficiency for source emission in a multilayer stack, the ratio of the power leaving the waveguide to the total power emitted from the source can be found from (5.45).

However, to calculate the emission pattern of intensity observed in the substrate or superstrate medium, the energy flux per solid angle will change due to refraction across the boundary. The solid angle must be converted to the new propagation medium with (5.46). \( \hat{S}(\theta_{\text{out}}) \) and then provides a quantity proportional to observed intensity.

\[
\hat{S}(\theta_{\text{out}}) = \hat{S}(\theta_{\text{s}}) \frac{n_{\text{s}}^2 \cos \theta_{\text{s}}}{n_{\text{out}}^2 \cos \theta_{\text{out}}}
\]

(5.46)

where \( n_{\text{out}} \) and \( \theta_{\text{out}} \) represent the refractive index and propagation angle in the outside medium. Figure 5.8a shows the TE and TM emission pattern into air for the test slab, with the source positioned in the centre for horizontal dipoles. Moving the source to 100nm from the substrate as in figure 5.8b, shows that the emission into the superstrate is greatly increased.

(a) Source positioned in the centre of the cavity.  
(b) Source positioned 100nm from the substrate.

Figure 5.8: Simulated TE (blue) and TM (red) emission to the surrounding medium for a 500nm thick slab with refractive index 2.5 for horizontal dipoles emitting at freespace wavelength 450nm. Both plots have the same radial scale.
5.2.4 Application to InGaN LEDs

In wurtzite semiconductors, the valence band states split into three bands formed of crystal, light and heavy holes in typical order of increasing energy [242,243]. The dominant radiative recombination will be the lowest energy transition, which for the In$_{1-x}$Ga$_x$N system is always between the conduction band and the heavy hole valence band. This transition leads to emission polarisation parallel to the $c$-plane [244, 245] and so when modelling $c$-plane InGaN quantum wells, the optical emission can be considered to come from only horizontal dipoles.

The consequence of this is not only to simplify the computation but also, where the value of (5.41) (which gives the TM-polarised source field due to an $x$-directed dipole) is small, there is little TM excitation. The energy emitted into low order modes, where $\theta_s$ is near to 90°, is almost entirely TE polarised in $c$-plane InGaN QWs as a result. This result is consistent with the experimental observations discussed in §7.3.2 and results from other groups [109].

In order to confirm these assumptions, the emission pattern was measured from an InGaN/GaN MQW LED commercially grown on a sapphire substrate with a roughened back side. The sample comprised of six $\approx2.5$nm wide QWs with 10nm barrier layers, situated 122nm below the epitaxially smooth top surface. Reflectometry measured the total GaN thickness to be 5275nm thick. The measured TE and TM polarised emission patterns are shown in red and blue on the left ($-90^\circ \leq \theta \leq 0^\circ$) and right ($0^\circ \leq \theta \leq 90^\circ$) sides respectively of figure 5.9. As the emission from each QW is incoherent, the emission for each one was modelled separately and the results combined to give the emission pattern, shown in black in figure 5.9. The model assumes only GaN layers with perfectly smooth interfaces, surrounded by an air superstrate and a sapphire substrate, with equal weighting given to the emission from each QW.

![Figure 5.9](image_url): Experimental (coloured) and simulated (black) emission patterns for a planar LED. TE emission is on the left ($-90^\circ \leq \theta \leq 0^\circ$) and TM on the right ($0^\circ \leq \theta \leq 90^\circ$).

The simulation fit is good, with an apparent broadening in the experimental data between 30 and 90° which could be due to measurement inaccuracies in the thicknesses in the layers, or scattering effects caused by non-ideal surfaces as the experimental sample
contained a substrate with a roughened back-side.

5.3 Conclusion

A model for simulating the behaviour of guided light in a slab waveguide consisting of arbitrary layers has been developed and validated against an alternative model. The model has been extended to include the effect of adding a source layer into the waveguide, and it has shown an excellent fit with experimental data from a planar LED sample.

This model is used throughout this thesis when LEDs are considered as slab waveguides. In chapter 7 it has been used to interpret experimentally observed diffraction of guided modes in buried photonic crystal LEDs, and to investigate the effect of vertical device parameters on the possible performance of such devices. In chapter 8, the confinement of light to the periodic regions of devices with shaped nanorods is considered, providing understanding of the behaviour of such devices. The model is used to provide insight into feasible device designs for highly directional emission in chapter 9, exploiting the results from chapter 8. In conclusion, this model provides a valuable tool for quick and accurate simulation of the interaction of light with layered slab structures.
Chapter 6

Angular luminescence

Band folding or diffraction of light to the air cone from a sample LED can be observed directly using wavelength and angle-resolved far field intensity measurements. These observations can be viewed and analysed to understand the behaviour of confined light in a PhCLED through mapping the data to reciprocal space and dispersion relations, as discussed in §3.2.1.

6.1 Experimental system

A system was set up to allow an optical spectrum to be taken from an LED at any point around a hemisphere above it. A flexible optical fibre bundle is used to collect the light and deliver it to a spectrometer with a CCD detector (Andor Shamrock 303i). The fibre is attached to an arm built from aluminium profile and manipulated in a spherical coordinate system using two high precision stepper motors (ThorLabs NanoRotator NR360) – one to control the azimuthal angle and one to control the angle from normal incidence or the inclinal angle. The system is shown in figure 6.1, situated on an optical bench with pneumatic legs for vibration isolation.

A pair of small lasers are used to align the system; one for each motor. Firstly, the lasers are aligned to point perpendicular to the plane of rotation of each motor and then centred on the axis of rotation. The structure is adjusted using spring washers to align the axis of rotation of the two motors so they become perpendicular, using the aligned beams. The fibre holder is aligned to the azimuthal laser beam with the inclinal motor positioned at zero degrees to calibrate the normal incidence position. The sample is positioned where the alignment lasers cross at the origin of the motors’ coordinate system and the top surface of the sample is levelled using its reflection of the azimuthal laser.

Taking into account the tolerance of the optical equipment used and flexing of the structure, a pessimistic estimate of the uncertainty in position over the whole coordinate system is less than $0.16^\circ$, illustrated in figure 6.2. As the position of the fibre bundle is
aligned at normal incidence, the uncertainty at normal incidence is more accurate at $0.11^\circ$.

**Figure 6.2:** Illustration of the uncertainty of the system for any points $a$: the actual position of fibre, and $m$: the position of the fibre read out from the motors, where $\psi_{\text{err}} < 0.16^\circ$. 
For a point source, the angular resolution is limited by the solid angle subtended by the fibre bundle, which has a collecting diameter of just under 1mm. Depending upon the sensitivity required, the position of the bundle can be varied up to 300mm away from the sample, giving a maximum angular resolution in each direction of $\approx 0.19^\circ$. As a result, scans taken at a resolution of $0.19/2\approx 0.1^\circ$ allows the data collected to be limited by the angular resolution of the system.

A 100mW 405nm diode laser with a highly stable output (Vortran Stradus) is used as a photoluminescence (PL) source. The laser is focussed by a fused silica lens into a small spot to approximate as close to a point source as possible. The wavelength was chosen as it allows direct excitation of typical InGaN QWs with low absorption in the surrounding GaN layers to increase the signal-to-noise ratio at the detector. Contacted devices can be probed for electroluminescence (EL) measurements, but are limited by the size and shape of the devices.

When using the diode laser as a PL source, an optical long-pass filter (Semrock Bright-Line) is used to prevent laser light diffracted, reflected or scattered by the sample affecting the measurements. A polarising cube can be placed between the sample and fibre bundle to investigate the polarisation of emitted light in the plane of the sample. The polariser in the angular luminescence measurements is always perpendicular to the direction of propagation and is aligned in one of two ways; to measure the intensity of light polarised with the E-field parallel to the plane of the device and perpendicular to the propagation direction (TE) or to measure the E-field perpendicular to the TE field and the propagation direction (TM). In this case, the fibre bundle acts as a depolariser, so any polarisation dependence of the spectrometer grating will not affect the measurement.

The spectral resolution of the experiment is determined by the slit width and choice of grating in the spectrometer. The data collected for this thesis used a 600 lines/mm grating, which gives a resolution of approximately 0.13nm per CCD pixel for 400-700nm wavelengths. The slit width can be varied upwards from 10µm, and is limited to a maximum of 125µm by the diameter of the fibre bundle cores. As the slit is imaged onto the CCD, its width also limits the full-width at half-maximum (FWHM) of the spectral resolution ($\approx 0.25$nm for small slit widths) and so a trade-off between signal level (directly affecting experiment time) and spectral resolution is encountered. The slit width it typically kept at 20µm or below to maximise resolution and the exposure time varied to control the measured light fluence, but for some of the samples investigated with lower brightness the slit was opened up as far as 100µm so the experiments could be performed over practical time-scales.


## 6.2 Data visualisation and processing

As the data are collected, they are saved into a binary file by the LabView virtual instrument controlling the hardware. Two other files are created; a dark background spectrum of the CCD for the exposure settings used and a header file which contains the experiment parameters and a spectrometer calibration, performed using mercury or sodium emission lines. To allow visualisation and manipulation of the data, a library of MatLab functions was written. The binary file is read into a data structure based on the experiment parameters in the header and the background spectrum is subtracted from each spectrum in the file. The data contains intensity information as a function of wavelength, azimuth and angle from normal incidence, \( I(\lambda, \phi, \theta) \). The data can be viewed on 2D intensity plots, showing a subset of up to two of the three variables in the data or as time-varying animations. Figures 6.3 and 6.4 show example far field patterns from a planar control LED with a smooth top surface, where white and black represent higher and lower intensity respectively.

Figure 6.3a shows the intensity variation with the angle from normal incidence (\( x \)-axis) and the freespace wavelength (\( y \)-axis) for observation at a fixed angle of azimuth. This can be projected into \( k \)-space to produce a dispersion diagram by converting the freespace wavelength to freespace wavenumber (\( k_0 = \frac{2\pi}{\lambda_0} \)) and resolving with the angle of observation from normal incidence to give the parallel wavevector (\( k_\parallel = k_0 \sin \theta \)). The dispersion diagram for the planar LED is shown in figure 6.3b with \( k_0 \) on the \( y \)-axis and \( k_\parallel \) on the \( x \)-axis.

![Far field intensity plots of a planar control LED at fixed azimuth.](image)

**Figure 6.3**: Far field intensity plots of a planar control LED at fixed azimuth.
Alternatively, the variation of intensity with azimuth and inclinal angle can be viewed for a single wavelength, represented by the detection on a single CCD line. Figure 6.4a shows this variation for the planar LED projected onto the surface of a sphere for a fixed wavelength of 460nm. When this sphere is viewed from surface normal, the plot is resolved to a plane representing the variation of the parallel wavevector with azimuth, as shown in figure 6.4b.

![Figure 6.4: Intensity plot for single wavelength (460nm) from a planar LED – from surface normal to 60° inclinal angle, 10° azimuthal data taken and rotated around normal incidence – plan view.](image)

The planar LED sample with no light extraction enhancement techniques applied shows concentric rings on the single wavelength plot and broad, sweeping curves on the fixed azimuth plots. These rings and curves are the Fabry-Pérot fringes arising from vertical cavity resonances of the parallel-sided dielectric slab forming the LED. The features are not visible at oblique angles (close to 90° from normal incidence) and away from the quantum well wavelength range due to the lower intensity of the light emitted. As the contrast range in the data is high, simply changing the brightness and contrast will not allow the features in all these regions to be visible at once. To overcome this problem, a normalisation algorithm was devised to enhance the visible contrast of the features when displayed by removing the intensity dependence of the quantum well emission and observation angle.

The algorithm removes the gross intensity variations from the wavelength and angle-dependence in two separate steps, shown in figures 6.5a and 6.5b. In the formalism that follows, the dataset $D$ is defined as intensity values $I(\lambda, \mathbf{R})$ which vary with wavelength and angular position $\mathbf{R} = (\theta, \phi)$, collected for a discrete list of coordinate pairs $\{\mathbf{R}\}$ and wavelengths $\{\lambda\}$. To remove the wavelength independent variation of intensity with angle,
the mean intensity value at each angle is found

$$\bar{I}(R) = \frac{1}{|\{\lambda\}|} \sum_{\lambda} I(\lambda, R) \quad (6.1)$$

and then each spectrum is divided by its mean value

$$\tilde{I}_R(\lambda, R) = \frac{I(\lambda, R)}{\bar{I}(R)} \quad \forall \ R \in D \quad (6.2)$$

Similarly, to remove the angle independent variation with wavelength, the mean intensity value at each wavelength is found and then the intensity data at each wavelength is divided by its mean value

$$\tilde{I}_\lambda(\lambda, R) = \frac{I(\lambda, R)}{1/|\{R\}| \sum_{R} I(\lambda, R)} \quad \forall \ \lambda \in D \quad (6.3)$$

The two steps are combined to remove both variations by substituting $\tilde{I}_{\lambda}(\lambda, R)$ for $I(\lambda, R)$ in (6.3). The combined effect is shown for the planar LED in figure 6.6. It can be seen that there is some noise introduced, particularly in the areas which were not visible to start with. This is due to the much lower signal-to-noise ratio present in these very dim areas\(^1\).

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\(^1\)Image/data processing techniques could be used to reduce or remove the noise if desired, but this has not been done because all the techniques known to the author, for example, morphological techniques or median filters, will reduce the resolution of the data, and the features are visible enough for analysis.
sion intensity of two features is required, it must be extracted from unprocessed data.

The system can also be used to examine the polar intensity of the light source by integrating over a range of wavelengths and azimuth to get a plot of intensity against angle from normal incidence, $\bar{I}(\theta)$. As the fibre bundle collects from a fixed surface angle, its measurement is directly related to the intensity (i.e. power per surface area) of the light detected. This is shown in figure 6.7a for the planar control sample (blue line) and a perfect Lambertian emitter (black line).

Knowledge of the relative radiant flux ($\Phi(\theta)$) for each inclinal angle of emission, i.e. the integration of the emission pattern over azimuth, would be more useful when investigating the performance of directional sources. This can be calculated in this case by multiplying the intensity measured by the surface area of the measurement sphere for each inclinal angle interval in the dataset. When applied to the discrete data set and using the trapezium
rule for the intensity, this becomes

\[ \Phi(\theta) \propto (\cos \theta_i - \cos \theta_{i+1})(\bar{I}(\theta_i) + \bar{I}(\theta_{i+1})) \]  \hspace{1cm} (6.4)

where \( \theta \) is the inclinal angle from normal incidence, halfway between the two adjacent data points \( (\theta_i & \theta_{i+1}) \), \( i \) represents the index of the angle and constants have been dropped. This is shown in figure 6.7b as the dashed line for the Lambertian emitter, where it can be seen that little emission occurs near normal incidence (due to small surface area) or at oblique angles (due to low emission intensity). In order to calculate the proportion of radiant flux \( \eta \) emitted from a sample within a given angle range \( (\alpha, \beta) \), \( \Phi(\theta) \) can simply be integrated over the range and its ratio with the total emitted flux taken:

\[ \eta = \frac{\sum_{\{\theta\} = \alpha}^{\beta} \Phi(\theta)}{\sum \Phi(\theta)} \hspace{1cm} \text{for} \hspace{0.5cm} 0^\circ \leq \theta < 90^\circ \]  \hspace{1cm} (6.5)

For the case of a Lambertian emitter where \( \Phi(\theta) = \cos^2 \theta \), the proportion of the power emitted within half angle \( \theta \) from normal incidence simplifies to \( \sin^2 \theta \), shown as the solid line in figure 6.7b. For small values of theta, this proportion is very low, with 0.76% of the power within 5° and 3.02% within 10° of normal incidence.
Chapter 7

Buried photonic quasi-crystal LEDs

7.1 Introduction

Most effort directed towards exploiting the effects of a photonic crystal (PhC) in LED devices have focussed on increasing the light extraction. Typically, the PhC is placed at the surface of the device where it has little interaction with the low order guided modes due to their low overlap with the edges of the LED. An alternative is to bury the PhC in the epitaxial structure of the device below the QWs where it can interact much more due to the larger overlap with these modes, which carry a significant proportion of trapped light in the LED. Additionally, buried PhCs can be fabricated without etching towards the active region, which causes degradation of the performance of the QWs [229].

The application of buried PhC layers has not been widely investigated, but thin buried PhC layers have shown promising results for light extraction enhancement, with good effect on both low and high order modes evanescent outside the GaN layers [179]. A more detailed review is given in §4.2.2. The best result reported for a buried PhC is an unencapsulated extraction efficiency of 46% [181], compared to 73% for a surface PhC [88], leaving scope for improvement and understanding what the limit of unencapsulated light extraction performance may be for buried PhC devices.

For directional emission using PhCs operating in the diffractive regime, the ideal device configuration requires a thin slab containing the active region to confine light in these specific guided modes, discussed in detail in §9.2. The slab could be formed either with a reflector on one side in a thin film flip chip configuration, which suffers from metal absorption of light trapped in the guided modes [176] or by embedding low index waveguiding layers, which offer limited confinement and create epitaxial strain-management challenges [171]. Thicker buried PhCs with higher air filling fractions ($A_{FF}$) tend to confine light to the layer above in a thin cap layer, supporting a small number of cap layer
modes (CLMs, shown in figure 7.16a) and do not rely on a lossy metal layer or the use of other materials with different crystallographic lattice constants. In this case, the cap layer above the PhC can be considered to be decoupled from the GaN buffer layer below the PhC. These confining PhCs have not been looked upon favourably due to their tendency to increase the extraction length of the guided light, which is detrimental to overall extraction efficiency, and as a result have not been studied in detail. However, they have potential for use in directional emitters to confine optical power to specific guided modes, which can then be extracted near to normal incidence by the PhC. The effect of the PhC and device parameters on the properties of cap layer modes has not been investigated in depth, but is required for their exploitation in directional devices.

In order to facilitate the design of buried PhC LEDs with a specific goal in mind, design tools will prove invaluable to avoid many costly and time-consuming trial and error steps requiring the fabrication of devices. Previously, the behaviour of LEDs comprising a PhC acting to diffract guided modes has been successfully predicted using two independent models (1D-2D); a 1D slab waveguide for the vertical confinement of light and a 2D consideration of the diffracting properties of the PhC tiling, which was discussed in §4.2. This method has been shown to produce good results when compared with measurements for surface and thin buried PhCs, but has not been investigated for devices containing thick buried PhC layers or for photonic quasi-crystals. Once the behaviour is understood, a wide range of design parameters can then be investigated to produce design rules for controlling the optical behaviour of buried PhC LEDs for both directional emission or light extraction enhancement.

Quasi-crystal tilings were chosen as they have a greater degree of rotational symmetry than Euclidean tilings and photonic quasi-crystals give more azimuthally invariant extraction of guided modes [194, 195] and so seemed well suited to applications requiring good control of emission. Devices with quasi-crystal tilings were fabricated previously and are available for investigation, although they can lead to increased diffraction to the substrate, as discussed in §4.2.3. Previous work has almost exclusively focussed on Euclidean tilings, and no work on buried photonic crystals outside the University of Bath has considered quasi-crystal tilings.

This chapter experimentally characterises and investigates the behaviour of buried photonic quasi-crystal LEDs with different etch depths and fill fractions, and considers the application of the 1D-2D model to these devices. The use of buried photonic crystals for the different goals of unencapsulated light extraction enhancement for high-brightness devices and for confining optical power to specific guided modes for directional emitters is then discussed.
7.2 Fabrication overview and sample characterisation

LEDs with a buried photonic quasi-crystal (PQC) slab were fabricated previously by Dr P. Shields at the University of Bath. The structure and fabrication method is summarised in figure 7.1 and is now described. \( c \)-plane \( n \)-GaN on sapphire wafers patterned with a PQC tiling using nano-imprint lithography were sourced (Luxtaltek, Taiwan) with a pitch of 400nm (a in figure 7.3a). In vertex notation, the tiling is classified as \((3^6; \ 3^2.4.3.4; \ 3^2.4.3.4)\) with \( p6m \) symmetry\(^1\) [246] and is shown in figure 7.3. The lithography was used to create a nickel nanohole mask and the pattern transferred into the GaN using \( \text{Cl}_2/\text{Ar} \) ICP etching. The holes were smoothed in a 1M 80\(^\circ\)C potassium hydroxide (KOH) solution for 30 minutes, which recovered the facets inside the holes at the surface, shown in figure 7.3c. A pulsed MOVPE technique was used to produce a coalesced GaN layer over the holes [233], after passivating the inner surfaces of the holes to prevent epitaxial growth in the air gaps. Finally, a commercial MQW LED structure was grown on top by IQE Plc, emitting at approximately 450-460nm. The structure comprised six QWs and an electron blocking layer and is shown in figure 7.2.

Two samples were not rotated during the growth of the coalescence layer, which gave a smooth variation in the thickness of the cap layer above the PQC surface, the measurement method used to find these depths is described later and the results shown in figure 7.6. Samples with different PQC layer depths were fabricated by varying the ICP etch time, and it was later found that the passivation process used to prevent growth on the nanohole sidewalls was not entirely successful in all the samples, leading to much smaller air holes, shown in the SEM images in figure 7.4.

After angular PL measurements, some of the wafers were processed into 1\( \text{mm}^2 \) devices for EL measurements. The transparent p-contact was made using a 5/5nm Ni/Au film in order to minimise their effect on the optical modes in the devices. Attempts were made to characterise the electrical properties of the LEDs and their dependency on the cap and PQC layer thicknesses and the \( A_{FF} \) but the passivation used on the hole sidewalls acted as a mask during the mesa etch. The contacts formed were poor and inconsistent from sample to sample, so comparative measurements were not possible.

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\(^1\)This particular tiling is sometimes referred to as the Archimedean A13 tiling in the context of photonic crystals; although strictly it is not Archimedean as it is 3-isogonal (requiring 3 vertices to fully describe), but a modification of the truly Archimedean \((3.12^4)\) tiling \((1\text{-isogonal})\).
Chapter 7. Buried photonic quasi-crystal LEDs

C.J. Lewins

Figure 7.1: Buried PQC LED structure and fabrication process.

Figure 7.2: MQW structure grown over photonic quasi-crystal, modified from [247].

Figure 7.3: The photonic quasi crystal (plan view).
7.2.1 Measuring cap and photonic crystal layer thicknesses

Initial values for the device parameters were obtained during fabrication from process times. The PQC layer depths of the 1300nm and 300nm were measured directly from SEM images of wafer cross sections (figure 7.4). A magnification reference standard grating along with image analysis software (ImageJ) were used to calibrate the measurements from the SEM by obtaining a width measurement for each pixel at each magnification. The 650nm depth has not been measured, but inferred from the ICP etch rate of the 1300nm deep PQC sample.

A method was devised to map the thickness of the cap layer over the wafers not rotated during the coalescence growth step. It is not practical to cleave these samples into enough pieces to characterise the thickness variation by SEM; this would make angular luminescence difficult and prohibit future device processing. Instead, a thin film reflectometry system (Filmetrics F20) was used to measure the variation in depth of the different layers over the wafers by analysing the variation in Fabry-Perot fringes with wavelength (see §2.3). The system software (FILmeasure) fits the depth values for each layer, based upon the refractive index values for the materials. The system cannot take into account the effect of absorption in the quantum well layers on the reflectance and refractive index, so the reflectance data where these effects are significant was excluded from the fitting process by discarding data for wavelengths below 500nm. Figure 7.5a shows the reflectance of a planar control LED with its periodicity corresponding to a GaN depth of 5275nm. Figure 7.5b shows the reflectance of the sample with the 1300nm deep PQC. Two periodic variations can be seen; the slow variation is from the capping layer and the faster variation due to the whole structure from the GaN surface to the sapphire. Without further consideration, this method is only able to analyse planar thin films as the reflectivity function and refractive index of the PQC layer are not well known.

SEM cross section images as in figure 7.4b were used to measure the layer depths from two cleaved wafers with the same PQC layer and a consistent cap layer depth over the wafer. The reflectometry system was then configured to create a model for this thin PQC layer to be used for analysing other samples. The known depths of the cap layer and underlying n-GaN were entered as constants and the software set to fit for a refractive index at each wavelength and corresponding depth for the PQC layer. The models obtained from the two cleaved wafers were very similar, and were each validated by confirming the accuracy of the layer thickness measurement against the thickness acquired from the SEM cross sections for both samples. Development of this method allowed non-destructive testing of the samples with variation in the cap layer depth over the wafer and its result is shown in figure 7.6. The parameters of the samples are listed in table 7.1.
Chapter 7. Buried photonic quasi-crystal LEDs

Figure 7.4: SEM cross sections of the samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Cap layer depth (nm)</th>
<th>PQC depth (nm)</th>
<th>GaN depth (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>243v6</td>
<td>450-675</td>
<td>300</td>
<td>4440</td>
</tr>
<tr>
<td>240v3</td>
<td>630-1000</td>
<td>300</td>
<td>4285</td>
</tr>
<tr>
<td>242v2</td>
<td>500</td>
<td>300</td>
<td>4620</td>
</tr>
<tr>
<td>240v2</td>
<td>790</td>
<td>300</td>
<td>4900</td>
</tr>
<tr>
<td>242v4</td>
<td>600</td>
<td>(\approx 650)</td>
<td>(\approx 3830)</td>
</tr>
<tr>
<td>243v4</td>
<td>600</td>
<td>1300</td>
<td>3180</td>
</tr>
<tr>
<td>Control</td>
<td>0</td>
<td>0</td>
<td>5275</td>
</tr>
</tbody>
</table>

Table 7.1: Sample parameters measured from test samples.
Chapter 7. Buried photonic quasi-crystal LEDs

Figure 7.5: Reflectance measurements.

(a) Planar control sample with GaN depth 5275nm.

(b) 1300nm deep PQC sample.

Figure 7.6: Interpolated depth maps (nm) for wafers with non-uniform cap layer thickness due to failed rotation during overgrowth.

(a) Wafer 243v6 with 450-675nm cap layer depth variation.

(b) Wafer 240v3 with 630-1000nm cap layer depth variation.
Figure 7.7: PL intensity variation shown for 460nm wavelength. 30° of data have been collected and tiled.

Figure 7.8: EL intensity variation shown for 460nm wavelength. 30° of data have been collected and tiled.

Figure 7.9: EL Intensity variation with wavelength.
7.3 Observation of guided modes: 2D model

Angular luminescence measurements are initially presented for the sample with the 1300nm deep PQC layer and 600nm deep cap layer. The data was acquired and normalised using the procedures described in chapter 6. Figures 7.7 and 7.8 display single wavelength intensity measurements of the emitted PL and EL respectively. The PL was exciting using a 405nm laser diode source. The plot is characterised by twelve pairs of concentric arcs, which are caused by diffraction of guided slab modes to the air cone, showing that the buried PQC with 12-fold rotational symmetry is acting in the diffractive regime. As discussed in §3.2.1 and shown in figure 3.5, a hexagonal tiling would only show six pairs of these arcs due to the 6-fold rotational symmetry. In addition, the Fabry-Pérot fringes expected from a planar LED (figure 6.6) are only faintly visible.

The PL and EL show very similar modal features, but the PL in figure 7.7 appears darker at large angles of incidence with lower contrast between the background and the modal arcs and Fabry-Pérot fringes when compared to the EL in figure 7.8. This is due to the reduced signal (mode)-to-noise (background) ratio as the emission intensity of the PL is much lower than that of the EL, resulting in the much lower detector signal-to-noise ratio as a much longer integration time was used. When the normalisation procedure is applied, it enhances the contrast of the features relative to the mean intensity, which is predominantly the background emission level, which, in the case of the PL, is increased substantially by noise. This increased noise can be seen at the larger angles of incidence from surface normal for the PL in figure 7.7a compared to the EL in figure 7.8a. The slight difference in the location of the modal features is discussed later at the end of §7.4.

The variation in intensity for a single azimuth shown in figure 7.9a allows visualisation of how the diffraction varies with wavelength. Sharp, diagonal lines which are most distinguishable by their reflective symmetry about normal incidence can be seen in addition to the residual Fabry-Pérot fringes. The expected 12-fold rotational symmetry from the PQC was confirmed using the variation in intensity for a single inclinal angle shown in figure 7.9b.

7.3.1 Diffraction of guided modes by a photonic quasi-crystal

When the single wavelength plots are viewed from above, they represent a projection of the data to the in-plane k-space or reciprocal space within the air cone. In this projection, guided slab modes diffracted to air manifest as arcs centred on the reciprocal lattice points for the PhC, dependent on the 2D properties of the PhC tiling used. With knowledge of the reciprocal lattice of the PQC pattern, the in-plane components of the wavevectors \( k_{||} \) of the guided slab modes can be determined, as described in detail in §3.2.1. The twelve
Chapter 7. Buried photonic quasi-crystal LEDs

(a) Simulation.

(b) Vectorised positions. The concentric rings show the order \( m_N \) of the points they pass through.

**Figure 7.10:** Reciprocal lattice of the PQC tiling.

(a) One reciprocal lattice point from each order, \( m_N \approx 1.42, 1.93, 2.40, 2.73, 2.91 \), shown in red in figure 7.10.

(b) All reciprocal lattice points.

**Figure 7.11:** Simulated single wavelength far-field intensity plots at 460nm for \( n_{\text{eff}} \) in bulk GaN \((n=2.459)\).
duplets of parallel arcs visible in these projections of the data (figures 7.7b and 7.8b) must each be centred around a reciprocal lattice point. The different radii of the two sets of arcs corresponds to a different $k_||$ value and so are caused by the diffraction of two separate guided modes.

A model was established to allow further analysis of the far-field diffraction patterns from the reciprocal lattice of a given photonic crystal pattern, which calculates the diffraction to the air cone from guided modes with specified effective index values. The variation in refractive index for GaN with $k_0$ is taken into account using the method presented by Shokhovets et al. [248] to account for material dispersion. The far-field pattern is calculated for a discrete range of freespace wavelengths and observation angles so that the results of these simulations can be analysed with the same methods as the experimental data. The ‘diffraction arcs’ produced are widened using a Guassian blur\(^2\) to improve the clarity of the image and their intensity is determined from the brightness of each reciprocal lattice point.

As the PQC tiling is non-Euclidean, a simple pair of characteristic reciprocal lattice vectors do not exist for the tiling. For further analysis, the reciprocal lattice of the PQC was determined numerically from a 10x10 tiling of the PQC unit cell using an algorithm for the transform based on that presented in §8.4.1 of Quasicrystals and geometry [139]. The vector positions of the reciprocal lattice points were then determined from the centre of mass of each connected region using image processing techniques to allow sub-pixel resolution, and an intensity value stored for each point. Weak reciprocal lattice points were discounted. Figure 7.10 is the result of this process applied to the PQC tiling used in the experimental samples, where the reciprocal lattice shows characteristics of fractals and archimedean tilings. Results from the simulation are shown in figure 7.11.

At this point, it is useful to clarify what is meant by diffraction order in these tilings as multiple conventions exist and do not apply well to PQC lattices. The formalism described in §3.2.1, specifically equation (3.5), will be used. Referring to figure 7.10b, the magnitude of each reciprocal lattice point ($N$) from $\Gamma$ normalised to the first order ($m_N$) is used to represent its order. The first order ($m_N=1$) will be taken to be the circle of the twelve nearest neighbours to the centre point, $\Gamma$, the magnitude of which is $2\pi/a$. Concentric circles are labelled in figure 7.10b to display the value of $m_N$ for some of the points.

To measure $k_||$ for each mode in the data, Ewald constructions can be used to analyse the diffraction of the PQC in the far-field patterns, where the radii of the arcs give $k_||$. However, determining the radii of each family of arcs directly from the far-field data

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\(^2\)This is a spatial convolution with a discrete Gaussian function, frequently used in digital image processing.
projected into k-space requires lengthy measurement runs to collect 3D data for every sample and is not able to produce particularly accurate results. Alternatively, a much faster single azimuth measurement, such as that shown in figure 7.12 can be used. In the single azimuth projection, the modes are observed as families of sharp diagonal lines. At the freespace wavelength that these are all seen to cross ($\lambda_x$), labelled 1-4 in figure 7.12, the arcs that would be observed in the in-plane reciprocal space plots meet at normal incidence. Here, $k_{||}$ can be directly obtained from the distance of the reciprocal lattice point to the centre of the reciprocal lattice. It now it makes rather more sense to characterise each mode by its effective refractive index $n_{eff}$ as $k_{||}$ scales with wavelength;

$$n_{eff} = \frac{k_{||}}{k_{0x}} = |\hat{G}_{m_N}| \lambda_x$$

where $|\hat{G}_{m_N}|$ gives the reciprocal distance of order $m_N$ from $\Gamma$ at normal incidence.

To confirm the value of $m_N$ for the four $\lambda_x$ seen in figure 7.12, a simulation of the far-field diffraction due to a single point from each order (the red points in figure 7.10b) was performed. A guided mode with a effective index corresponding to GaN was simulated, chosen as it will be close to the effective index of low order guided modes. A single wavelength intensity plot at 460nm viewed from above is displayed in figure 7.11 and reveals that the strongest features observed in the experimental data primarily come from the order $m_N=1.93$. Substituting into (7.1) gives

$$n_{eff} = \frac{1.93\lambda_x}{a}$$

which is mapped onto the $y$-axis on the right side of figure 7.12.

The effective refractive indices of the two modes ($\approx 2.409$ & $2.326$) giving rise to the strongest PL were extracted by this method and entered into the simulation. A comparison of the simulated and experimental data is shown in figure 7.13 and shows an excellent fit of the modal features. The skirt of features around the outer circumference of the data is shown to be caused by $m_N=1.42$ and $m_N=2.73$ diffraction. This fit of the guided modes shows that the 2D part of the 1D-2D model depending upon the PhC tiling is valid for the PQC lattice.

7.3.2 Polarisation of light output

Figure 7.14 shows polarisation-resolved fixed azimuth intensity plots from the sample with the 1300nm deep PQC. The sharp straight features are revealed to be TE polarised, whereas the more curving features further from normal incidence are predominantly TM polarised with respect to the plane of the LED.
Figure 7.12: Finding effective indices of the modes from single azimuth plots.

Figure 7.13: Single wavelength far-field intensity plots at 460nm for PL excitation of sample with 1300nm PQC and 600nm cap layer.
To understand the cause of these results intuitively, one needs to consider the fields of the incident and diffracted waves. The fields of the incident wave couple to the fields of the outgoing diffracted wave. Equivalently, the magnetic and electric fields of the incident wave can be viewed to act as two dipoles (one electric and one magnetic) orientated along each of its field directions which couple according to (5.40). To predict the amplitude $A$ of the two observed polarisation components of the wave, each field should be coupled to the two measurement directions ($\hat{E}_{dTE}$ & $\hat{E}_{dTM}$) separately. For the electric field

$$A_{eTE} \propto (\hat{E}_i \cdot \hat{E}_{dTE})$$

$$A_{eTM} \propto (\hat{E}_i \cdot \hat{E}_{dTM})$$

and for the magnetic field

$$A_{hTE} \propto (\hat{H}_i \cdot \hat{H}_{dTE}) \equiv (\hat{k}_i \times \hat{E}_i) \cdot (\hat{k}_d \times \hat{E}_{dTE})$$

$$A_{hTM} \propto (\hat{H}_i \cdot \hat{H}_{dTM}) \equiv (\hat{k}_i \times \hat{E}_i) \cdot (\hat{k}_d \times \hat{E}_{dTM})$$

where the subscripts $i$ and $d$ refer to the incident and diffracted waves, the subscripts $e$ and $h$ refer to the amplitude due to the electric and magnetic fields, and arbitrary constants representing the diffraction efficiency have been dropped. The fields due to each dipole can then be summed and finally squared to scale to intensity $I$

$$I_{TE} = A^2_{TE} = (A_{eTE} + A_{hTE})^2$$

$$I_{TM} = A^2_{TM} = (A_{eTM} + A_{hTM})^2$$

As discussed in §5.2.4, one can assume that the guided modes emitted from these InGaN/GaN QWs are TE polarised and so only the case where the E-field of the incident wave is parallel to the plane need be considered. For the measured data, the E-field is parallel to the plane of the device for TE and perpendicular to the TE E-field and wavevector for TM. This is most easily derived by resolving the E- and H-fields into components perpendicular and parallel to the plane and treating separately

$$A_{TE} \propto \cos \theta + \cos \phi_d \cos \phi_i \cos \theta + \sin \phi_i \sin \phi_d$$

$$A_{TM} \propto \sin \theta \cos \phi_d + \cos \phi_i \sin \theta + 0$$

where $\theta$ is the angle between the in-plane components of $\hat{k}_i$ and $\hat{k}_d$ and $\phi$ is the angle between $\hat{k}$ and normal incidence. The three terms in each expression come from the in-plane E-field, the in-plane H-field and the H-field perpendicular to the plane respectively.

Figure 7.15 shows a simulation of the TE and TM emission using this method and shows a good fit with the experimental data in figure 7.14. This fit provides further evidence that the assumption that only TE polarised low order modes are significantly
excited is valid. If both TM and TE modes were present, the variation in the polarisation of the diffracted features would not be seen.\(^3\)

\[\text{Figure 7.14: Normalised single azimuthal intensity plots for the sample with the 1300nm deep PQC layer for polarised light.}\]

\[\text{Figure 7.15: Simulated polarised single azimuthal intensity plots for the dominant two modes.}\]

\(^3\)The far field polarisation for TM modes is found simply by swapping the terms in 7.6 for the TE and TM cases to reflect the swap in field direction, which yields the opposite polarisation in the far field pattern, for which there is no evidence.
7.4 Slab modelling of buried photonic crystal LEDs: 1D model

A significant challenge with modelling the PQC layer is the non-regularity of the pattern on short scales and the size of the unit parent cell, with the result that typical PhC modelling techniques such as FDTD cannot be implemented without excessive computational effort. Instead, 1D slab waveguide modelling was used to match the observed guided modes with the optical behaviour of the device.

For this technique to be applied, the PQC layer must be represented as a homogeneous slab layer with a characteristic refractive index. Aspnes provides a method for determining the effective refractive index of a layer composed of nanostructures of two materials from the relative volumes of each material and their dielectric constants \[249\], which lies between

\[ n_{\text{eff}} = \sqrt{A_{\text{FF}} + (1 - A_{\text{FF}})n_{\text{GaN}}^2} \]  \hspace{1cm} (7.7)

for no screening of the E-field and

\[ n_{\text{eff}} = \left( \sqrt{A_{\text{FF}} + \frac{(1 - A_{\text{FF}})}{n_{\text{GaN}}^2}} \right)^{-1} \]  \hspace{1cm} (7.8)

for maximum screening of the E-field, where \( A_{\text{FF}} \) is the air filling fraction of the PhC. For the PQC devices, it is unclear which to choose as for TE modes, since the E-field runs both parallel (7.7) and perpendicular to sides of the air holes (7.8), as well as parallel to the interface with the PhC. The version given in (7.7) has been used by other studies e.g. [181, 215], but without further justification. Both the choice of expression and the validity are worthy of investigation as expressions (7.7) and (7.8) rely on the pitch of the patterning being small compared to the wavelength of light considered, which is certainly not the case here.

Three families of optical modes guided in the GaN with evanescent field profiles elsewhere were predicted to be present in these devices and are shown in figure 7.16a, in line with previous work, reviewed in §4.2.2. These are cap layer modes, (CLMs) where the majority of the optical power is confined to the structure above the PQC, low order modes in which the power is confined mainly to the GaN buffer layer and high order modes where the optical power is distributed through both the cap and buffer layers. As the MQW is situated in the cap layer in the device, modes confined to the GaN buffer layer with a negligible field amplitude in the cap layer will not be emitted into significantly.

The sample with the 1300nm PQC and 600nm cap layer was modelled for \( A_{\text{FF}}=33\% \), estimated using plan view SEMs as in figure 7.3c. Four separate CLMs were found and
Chapter 7. Buried photonic quasi-crystal LEDs

(a) Modes in the device:
CLM – Cap layer mode
LOM – Low order mode
HOM – High order mode

Figure 7.16: Mode profiles in the devices.

Table 7.2

<table>
<thead>
<tr>
<th>Method</th>
<th>Mode 1</th>
<th>Mode 2</th>
<th>Mode 3</th>
<th>Mode 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel (eq. 7.7)</td>
<td>2.396</td>
<td>2.335</td>
<td>2.252</td>
<td>2.167</td>
</tr>
<tr>
<td>Perpendicular (eq. 7.8)</td>
<td>2.394</td>
<td>2.328</td>
<td>2.236</td>
<td>2.114</td>
</tr>
<tr>
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<td>2.326</td>
<td>2.219</td>
<td>2.095</td>
</tr>
<tr>
<td>Experimental EL</td>
<td>2.413</td>
<td>2.347</td>
<td>2.246</td>
<td>2.132</td>
</tr>
</tbody>
</table>

Table 7.2: $n_{eff}$ values for 1300nm PQC, 600nm cap layer.

Figure 7.17: Comparison of simulated and measured $n_{eff}$ values.

(b) 1300nm PQC layer – 1-4th orders.
their profiles are shown in figure 7.16b, confirming that the diffraction arcs observed in the experimental data are due to cap layer modes. None of the CLMs have any significant energy in the GaN buffer layer, showing that the cap and buffer layers are decoupled for low order modes by the deep (1300nm) PQC. Both models (equations (7.7) and (7.8)) for the PQC layer were tested and the effective refractive indices produced by the simulations are shown in table 7.2. The simulation was performed at the same wavelength as the experimental effective index was measured for each mode to take into account material dispersion. Figure 7.17 shows a comparison of the simulated and experimentally measured $n_{eff}$ values with quantitative estimates of the uncertainties. The uncertainty in the simulated values is due to the 5% uncertainty in the measurements of the cap layer depth with the SEM – the maximum and minimum layer depths were simulated to produce the error bars. The uncertainty in the experimentally derived values is due to the accuracy to which the freespace wavelength values where the diffracted arcs of the mode meet at normal incidence ($\lambda_\times$) can be determined from the data and measured by the spectrometer. Also included is the uncertainty in the measurement of the pitch of the PQC pattern.

For low order TE modes, these data suggest that the perpendicular model is probably more accurate but it is likely that, as the index of the mode increases, the effective medium model becomes less valid due to increased overlap of the mode and therefore interaction with the nanostructure itself. Additionally, the model does not take into account the change in refractive index of the QWs with wavelength and relies heavily on the accuracy of the refractive index used for GaN, which is doped in the experimental samples. As a result, this method cannot be relied on to give precise numerical values when compared with experimental devices, but will allow valuable insight from an engineering perspective into the overall behaviour of a device, particularly for low order modes.

Table 7.2 also compares the effective indices measured from the PL sample with a planar top surface with the EL sample with a 5/5nm Ni/Au contact layer above. The indices for the EL sample are higher, which is not explained by including the metal contacts in the slab simulation. For the EL experiments, a current of 150mA is injected into a 1mm$^2$ device on-wafer with no heatsinking, and so the change may be due to an increase in the refractive index of GaN with temperature [250].

The fit between the effective indices of the measured and modelled modes shows that the 1D part of the 1D-2D model describing the vertical confinement of the light provides a good guide, but is unlikely to be able to produce precise values. Other studies have selected equation (7.7) to describe a homogenised refractive index for the PhC layer without considering equation (7.8). In this work, it was not clear which equation should be used due to the uncertainties in the measurement of the parameters of the experimental samples and that future work should be cautious before selecting a volume-averaging method.
7.5 Effect of varying vertical device parameters on guided modes

7.5.1 Photonic crystal layer thickness

The depth of the PQC was varied between 650 and 1300nm intentionally in the experimental samples, and the failure of the passivation layer during the growth step created a shallower PQC with a triangular shape and much lower $A_{FF}$. By comparison of the cross section SEM images of the samples, the $A_{FF}$ of the shallow PQC was estimated to be $\approx 10\%$ and its thickness 300nm. Figure 7.18 compares single azimuth and single wavelength intensity plots acquired from PL of samples with a fixed cap layer thickness of 600nm and the three different PQC layers.

The two devices with thicker PQC layers display very similar far-field behaviour (figures 7.18a-7.18d). This similarity is also visible in the simulated cap layer mode profiles for the 650nm thick PQC layer shown in figure 7.19a when compared to 7.16b, although a tiny portion of the fourth order mode interacts with the GaN buffer below the PQC. In contrast, the far-field data for the shallow PQC layer (figures 7.18e and 7.18f) displays a change in the behaviour of the cap layer modes. As before, four groups of features are present. The first and second order cap layer modes are distinct, but as the mode order increases the modes become less well defined and instead groups of closely spaced modes are seen. Figure 7.19b summarises the typical calculated profiles of modes which have significant interaction with the cap layer for the thin PQC sample. In this case, a small proportion of the energy in the first and second CLMs propagates in the GaN buffer layer but above the second order, the effect of the thin PQC become much more significant. There are no longer distinct cap layer modes but instead groups of higher order modes resonant with the cap layer. The existence of many more modes on the single azimuth intensity plot (figure 7.18e) can now be explained for this structure. They belong to four distinct groups – the lowest and most distinct corresponding to a single cap layer mode, and the higher groups corresponding to higher order modes with third and fourth order resonances in the cap layer.

For modes guided in the GaN, the device structure acts as two waveguides – one in the cap layer and the other in the GaN buffer – with the interaction between them dependent on the properties of the PQC layer. The devices with the deepest (1300nm) PQC layer act in a decoupled regime, where the waveguides have little or no interaction with each other. The 650nm deep PQC devices essentially operate in this regime, whereas in the devices with a 300nm deep PQC and lower $A_{FF}$, the observed diffraction features show that the light is trapped in coupled waveguide modes.
Figure 7.18: Normalised single azimuth (left) and single wavelength at 470nm (right) intensity plots for samples with a 600nm deep cap layer. 30° of data have been collected and tiled for the single wavelength plots.
7.5.2 Cap layer thickness

Two of the wafers with the shallowest (300nm) PQC were not rotated during the growth of the coalesced layer above the PQC, leading to a variation of the cap layer thickness which is mapped in figure 7.6. Angular PL data were taken at fixed azimuth for several points on the wafer with the cap layer varying from 450 to 675nm. Figure 7.20 shows a subset of this data for 445, 507, 561 and 623nm thick cap layers. The other samples with the 300nm PQC layer (figure 7.20) all show similar behaviour.

The effective indices of the cap layer modes move to higher values as the cap layer depth is increased. The 445 and 507nm samples support three cap layer resonances and the thicker 561 and 623nm samples support four. It is also clear that the intensity of each mode is different for each cavity thickness; there is a similar intensity for both the first and second order modes for the thinnest cap layer and the intensity of the second order mode increases relative the the first order as the cap layer becomes thicker. This is likely due to the change in relative position of the MQW with respect to the cavity and a change in the density of states for the modes as the thickness varies, thereby affecting the power emitted into each mode. In order to investigate, simulations were performed. The thickness of the coalescence layer is varied for a modelled device with a 1300nm thick PQC, which gives the strongest confinement of light to the cap layer. In line with the measured samples, the QW is fixed at 150nm from the top surface. Figure 7.21 shows the integrated emission into the two well-confined cap layer modes and is qualitatively similar to the measured trend, which suggests that the placement of the QW is more significant than the cap layer thickness. Additionally, a change in the overlap with the PQC layer which will affect the diffraction efficiency and so stronger diffraction is expected of higher order modes.

![Figure 7.19: Cap layer mode profiles in the devices with fixed 600nm thick cap layers.](image-url)

(a) 650nm PQC layer – 1-4th orders.
(b) 300nm PQC layer – 1st, 2nd, and quasi-3rd orders.
Figure 7.20: Normalised single azimuthal intensity plots for samples with a varying depth cap layer and 300nm PQC depth.

Figure 7.21: Simulation of power emitted into the first two cap layer modes as a function of cap layer thickness. The QW is positioned 150nm from the top surface.
7.5.3 Summary

For modes guided in the GaN, the device structure acts as two waveguides – one comprising the cap layer and the other in the GaN buffer – with the interaction between them dependent on the properties of the PQC layer. The devices with deeper PQC layers have been shown to act in a decoupled regime, where the two waveguides have little or no interaction with each other, and the shallower PQC layer with lower $A_{FF}$ acts in a more coupled regime. The cap layer thickness can be chosen to trap light in guided modes with desired effective indices and the 2D tiling of the PhC optimised to extract the modes efficiently and control where the diffracted power is directed.

It is clear from these results that if the depth and/or the $A_{FF}$ of the PQC is high enough, there is a decoupling effect for modes confined in just the GaN layers (i.e. $n_{eff} > 1.8$). It is likely that the depth required for a 33%$A_{FF}$ to perform the decoupling effect is somewhere close to 650nm due to the small intensity in the GaN buffer for the fourth CLM in the simulation of the 650nm PQC depth. However, this only considers a 600nm thick cap layer and the decoupling effect will vary with its thickness. There is also no data to determine the range of $A_{FF}$ required to decouple the guides.

7.6 Design rules for buried photonic crystal LEDs

Buried photonic crystal devices are good candidates for both directional emitters and high-brightness devices. A directional emitter using a photonic crystal as a diffraction grating requires as much light as possible to be confined to a small number of guided modes, such as cap layer modes, as shown in figure 7.19a. The previous section showed it was possible to decouple the cap layer from the GaN buffer layer below for guided light with a photonic crystal which has a large enough thickness or air filling fraction. This decoupling of the cap layer has been shown to provide the small number of guided modes required for directional emission. When the GaN buffer and cap layers are coupled, this situation does not arise, and so is not considered suitable for directional emission.

For enhancing the light extraction efficiency, as much light as possible must be extracted, but the direction is not important. Previously, the coupled regime has been investigated experimentally and proposed to be a good candidate for extraction efficiency due to increased interaction of guided light with the PQC, as can be seen in figure 7.19b. In addition, the decoupled regime may be suitable for high extraction efficiency if it can decouple substrate modes and prevent light loss to the substrate.

The parameters required to decouple the cap layer will now be investigated, and then the suitability of both the coupled and decoupled regimes investigated for high light extraction efficiency.
7.6.1 Decoupling the cap layer for directional emitters

The range of the decoupling conditions for the guided modes can be more precisely investigated through slab modelling of the emission from a source into devices with varying PQC thickness and air filling fraction. As discussed in §5.2.3, a small loss term has been added to the guiding layers in the model to allow integration of the power emitted into guided modes. By considering the guided power flows into and out of the interface between the GaN buffer layer from the PQC layer, a ratio between the power lost to the buffer layer and the useful power confined the cap layer and PQC can be used to define the coupling between the two regions. The experimental results show clearly that the air filling fraction and or the PQC depth have a significant effect on the coupling – lowering the filling fraction and PQC layer thickness will increase the coupling. Additionally the cap layer thickness and the position of the QWs can be varied.

Considering the PQC layer as an effective medium, there are two ways that guided power can be lost to the buffer layer. Firstly, if the air filling fraction is too low, some of the guided light is not evanescent in the PQC layer due to its higher refractive index and can propagate in the cap, PQC and buffer layers as high order modes. If the PQC layer is too thin, the light can ‘tunnel’ through the PQC layer, when the evanescent tails from the cap layer and buffer layer modes couple. Thinner cap layers will increase the tunnelling effect as the penetration depth of the evanescent tails in the PQC layer will be increased for modes with smaller effective indices. These effects are illustrated by modelling a coupled case with $A_{FF}=33\%$ and PQC thickness of 100nm ($0.50 \frac{\lambda}{n}$) and a decoupled case with $A_{FF}=33\%$ and PQC thickness 1300nm ($6.45 \frac{\lambda}{n}$). As the focus is on producing rules for the parameters required for decoupling, the following simulations use equation (7.7) to provide an upper limit to the index of the PQC layer.

Figure 7.22 shows the ratio of the TE guided power lost to the buffer layer as a function of cap layer thickness ($y$-axis) and relative QW position ($x$-axis) and illustrates the two loss mechanisms of direct coupling and tunnelling. In the decoupled case, power is only lost to the buffer layer for QW positions that overlap with a high order mode, at the distinct peaks in figure 7.22a, and does not depend significantly on the cap layer depth. For the coupled device in figure 7.22b, power is lost to the buffer layer for all modes through the tunnelling process and the overlap of the QW with the high order modes becomes a secondary effect. There is more dependence on the cap layer depth; a thicker cap layer increases the effective index of the cap layer modes and so the evanescent tail in the PQC layer becomes smaller.

Figure 7.23 shows the total TE power confined to the cap and PQC layers to include the cavity enhancement effects due to the QW placement. Varying the position of the QW has a more profound effect on the total confined power than the cap layer thickness.
(a) Decoupled case, PQC thickness $6.45\, \lambda/n$ and 33% $A_{FP}$.
(b) Coupled case, PQC thickness $0.50\, \lambda/n$ with 33% $A_{FP}$.

**Figure 7.22**: Ratio of guided TE power in GaN buffer layer to total guided TE power.

(a) Decoupled case, PQC thickness $6.45\, \lambda/n$ and 33% $A_{FP}$.
(b) Coupled case, PQC thickness $0.50\, \lambda/n$ with 33% $A_{FP}$.

**Figure 7.23**: Total TE power confined to cap and PQC layers.
Figure 7.24: Effect of varying the PQC parameters on the ratio of guided TE power in the GaN buffer layer to total guided TE power for $2.40 \frac{\lambda}{n}$ cap layer thickness and QW 25% from the top of the device. The blue regions represent decoupled operation, and the red coupled operation.
for the decoupled case in figure 7.23a, as it determines which of the cap layer modes are preferentially excited. As long as the cap layer is sufficiently thick, the precise thickness and QW placement present options for ‘fine-tuning’ the confined power, rather than determining the device behaviour.

To determine the decoupling parameters for the PQC layer, a cap layer thickness of 485nm (2.40 $\lambda/n$) was chosen and the QW positioned 25% from the top of the cap layer, to give near-optimal decoupling from the buffer layer, based on the model shown in figure 7.22a. Figure 7.24 shows the effect of varying the $A_{FF}$ ($x$-axis) and thickness of the PQC layer ($y$-axis) on the guided power distribution in the device and presents contours for clarity. The graph illustrates the two mechanisms causing loss to the buffer layer and corresponding values for the $A_{FF}$ and PQC thickness. Once the $A_{FF}$ is sufficiently high, fixing the $A_{FF}$ and increasing the PQC thickness from zero gives an exponential relationship, confirming that the evanescent tails of the modes are responsible for the tunnelling mechanism of the coupling in this case. An approximately parabolic relationship is seen for varying the $A_{FF}$ for fixed PQC thickness as the effective refractive index (which depends on $\approx \sqrt{A_{FF}}$) of the PQC layer is roughly proportional to the ratio between the available states in the buffer layer and the cap layer. The locus of the 10% contour in figure 7.24b gives a safe estimate of the parameters required to be in a decoupled regime for optimised cap layer thickness and QW placement with a high level of certainty due to the choice of (7.7) for calculating the refractive index of the PQC layer and longer wavelength (490nm) used for the simulation. To provide a general rule, the PQC is able to decouple at least 90% of the guided power for PQC thicknesses over 300nm ($\approx 1.5\lambda/n$) with an air filling fraction over 30%.

7.6.2 Light extraction efficiency

So far, decoupling of the cap layer for the power trapped in guided modes has been considered in detail, but this does not cover all the available states in the device. To optimise the total extraction efficiency, the power emitted into substrate and radiation modes must be considered. Previous work has considered the coupled regime due to increased interaction between guided modes and the photonic crystal providing a higher diffraction efficiency.

Referring again to the experimental results for the varying PQC thicknesses shown in figure 7.18, the fast-period Fabry-Pérot fringes due to the GaN-air and GaN-sapphire interfaces observed on the single azimuth emission plots appear more intense for the 650nm PQC layer than the 1300nm PQC layer. The slow fringes ($\approx 20$nm wide with a 40nm period) due to the GaN-air and GaN-PQC interfaces are more intense for the deeper PQCs
than the 300nm thick PQC. As discussed in detail in the previous section, the coupling between the cap and buffer layers through the PQC layer increases as light becomes less well confined in the cap layer, i.e. as the size of the in-plane wavevector $k_{||}$ of the mode decreases. The comparison of the Fabry-Pérot fringes for the 650nm and 1300nm deep PQC samples indicates that this decoupling relationship may continue past the guided modes confined in the GaN layers to smaller values of $k_{||}$ representing the substrate and radiation modes. Further investigation will determine what limits there are to the extracted power from buried PQC devices and if there are similar threshold PhC parameters for the decoupling of substrate modes from the cap layer as there are for high order GaN modes – devices with significant decoupling may show improved light output over coupled devices by limiting the optical energy directly emitted or diffracted into substrate modes, reducing the light lost to absorption through these channels.

**Coupled case**

As discussed previously, one of the reasons for choosing the buried PhC device configuration is specifically to increase interaction of the PQC with the guided modes to reduce the extraction length. For best extraction of guided modes, the air filling fraction needs to be low enough for some overlap of the modes with the photonic crystal. However, it may be possible to improve the overall extraction efficiency by decoupling the substrate modes, which will be considered below. A device with a 100nm (0.50 $\lambda$/$n$) PhC layer and $A_{FF}$=33%, which is known not to decouple the guided modes significantly is initially chosen to consider a good overlap case. As power emitted into substrate and superstrate modes includes states which are not just propagating near to parallel with the plane of the slab, the TM emission due to horizontal dipoles can no longer be approximated to zero and must now be included. To represent a best-case scenario for the maximum effect on the substrate modes, eq. (7.8) has been chosen to calculate the homogeneous equivalent refractive index of the PQC. Figure 7.25a and 7.25b show that the power entering the substrate and superstrate respectively varies considerably with the choice of QW position ($x$-axis) and cap layer thickness ($y$-axis). Intuitively, best performance should be achieved by minimising the substrate losses while maximising the superstrate emission, but the figure-of-merit representing the performance must be considered carefully to avoid misleading conclusions.

Typically, extraction efficiency ($\eta_{ext}$) is used experimentally as a figure-of-merit for the performance of such structures. A best-case for the extraction efficiency is estimated from the distribution of power across the states in the device by considering the substrate, superstrate and guided powers separately as follows:
Figure 7.25: Effect of QW position and cap layer thickness on power emitted from a device with PQC thickness 0.50 \( \lambda/n \) and 33% \( A_{FF} \).
The powers calculated for the substrate and superstrate represent optical energy leaving the device, so the useful extracted power must include all the superstrate power ($P_{\text{superstrate}}$). $P_{\text{superstrate}}$ is small compared to the guided and substrate power, as can be seen in figure 7.25.

The PQC diffracts guided power in the device and so a proportion ($\eta_{\text{diff}}$) of this power ($P_{\text{guided}}$) will be ultimately directed towards the superstrate in states that can exit the device as useful power.

A final term ($P_{\text{loss}}$) is included to represent light diffracted from states other than the guided modes$^4$. To summarise, a lower limit can be set to the extraction if all the power emitted to the substrate is assumed lost

$$P_{\text{ext}} \geq P_{\text{superstrate}} + \eta_{\text{diff}}(P_{\text{guided}} + P_{\text{loss}}) \quad (7.9)$$

The value taken by $\eta_{\text{diff}}$ representing the proportion of diffracted power which actually leaves the device through the GaN-superstrate interface requires consideration. In the coupled case, there is little waveguiding effect of the PQC on the superstrate and substrate modes to redirect the light after diffraction and so it seems reasonable to assume that half of the diffracted power is directed towards the superstrate and half towards the substrate. This diffracted power will all be below the critical angle of the substrate and possibly the superstrate, as GaN states would be evanescent$^5$. Considering the unrealistic best case, where all the diffracted light directed towards the superstrate leaves the device (even if it cannot escape as it is in the substrate cone but evanescent in the superstrate) without undergoing any further diffraction, Fresnel reflection or material absorption, the upper limit of $\eta_{\text{diff}}$ is 0.5. If all the power diffracted or emitted directly into substrate modes is assumed completely lost, the best case is therefore that $\eta_{\text{ext}} (= P_{\text{ext}}/P_{\text{Total}})$ cannot be much greater than 50% (as $P_{\text{superstrate}} \ll P_{\text{Total}}$) in the best case where no power at all is emitted by the source directly to substrate modes:

$$P_{\text{ext}} < P_{\text{superstrate}} + \eta_{\text{diff}}(P_{\text{Total}} - P_{\text{superstrate}}) \quad (7.10)$$

This is shown in figure 7.25c.

With the assumption that all power in substrate modes cannot be extracted, the

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$^4$This term considers unguided light which was emitted by the source into the superstrate (or substrate) extraction cone but is instead modelled to be absorbed by the material loss (due to the loss terms in the model) before it can leave the device. For example, light travelling at angles which do not undergo total internal reflection, but are close enough to the critical angle to have high Fresnel reflection coefficients at the interface between GaN and air may undergo significant absorption. This absorbed power is not included in the calculation of $P_{\text{superstrate}}$ (or $P_{\text{substrate}}$) by the model. This light could well be diffracted to angles which can escape with much lower Fresnel reflection coefficients, and so the mechanism should be included by assuming that this power is diffracted in the same way as the guided power, and is therefore included in the useful extracted power.

$^5$Except for the unusual case where diffraction from one guided state to another is possible – considering e.g. figure 7.7 presented earlier, this occurs where two of the arcs meet.
parameter optimisation should be directed predominantly towards minimising substrate losses to maximise $\eta_{\text{ext}}$, seen by comparing figure 7.25c estimating the extraction efficiency with figure 7.25a emission to the substrate. The values of CL thickness and QW position which give low substrate loss correlate with the values that give the best extraction efficiency. However, when the total extracted power is considered (shown in figure 7.25d) rather than the extraction efficiency, it becomes clear that where the substrate loss is minimal the power is not predominantly made up for in other states contributing to the extracted power, but is instead mostly missing. The cause of this peculiarity is found by considering the meaning of the value taken on by power in this model – the source terms include the cavity effects on the spontaneous emission rate or Purcell factor. Emission of the missing power is inhibited by the effect of the cavity on the source and so does not contribute to the extracted power. This leaves the choice of $\eta_{\text{ext}}$ as a sole indicator of optical performance rather open to misleading inflation which does not necessarily represent best overall device performance\textsuperscript{6}.

By assuming that all the light travelling in substrate modes is lost, it is clear that considering the light directed towards the substrate before or after diffraction is rather important. To realise a buried PhC device with $\eta_{\text{ext}} \gg 50\%$, the substrate modes must be given at least equal consideration to optimising the efficiency of diffraction of light guided in the cap and buffer layers. Typically, substrate modes are not well extracted by PhCs due to their low overlap, so other techniques may be required.

**Decoupled case**

To investigate if it is possible to improve extraction efficiency performance by decoupling the substrate and superstrate states with the PQC, the effect of varying the PQC thickness and $A_{\text{FF}}$ on the power emitted to the substrate is considered in figure 7.26. Figures 7.26a and 7.26b show the upper and lower limits for the homogeneous refractive index of the PQC layer, given by (7.7) and (7.8) respectively. A cap layer thickness of 600nm (2.96 $\lambda/n$) and QW placement 0.25 from the top is chosen to be representative of the experimental samples to see if the observation of apparent change in intensity of Fabry-Pérot fringes with changing PQC thickness can be explained. In both cases in figure 7.26, increasing the PQC thickness has little effect once thicker than about 300nm (1.5 $\lambda/n$) and the behaviour is determined by which side of a ‘threshold’ $A_{\text{FF}}$ the parameters lie. As TM

\textsuperscript{6}To clarify what this means for the device performance, the radiative recombination rate will be reduced by the optical cavity, impacting the IQE of the device. As this work concerns only factors affecting the extraction efficiency, one could perhaps choose to consider $\eta_{\text{IQE}} = 100\%$ as the eventual goal of other researchers and continue without due consideration – many practical and theoretical studies choose to present results as ratios of ‘before’ and ‘after’ light intensity measurements without discussing if this effect is taken into account. It is not assumed in this investigation that a reduction of the radiative recombination rate is not detrimental to device performance.
polarised power contributes significantly to the unguided light, the best and worse case threshold $A_{FF}$ values will be pulled toward the same $A_{FF}$ as the electric field vector is no longer entirely in one orientation and so a mix of (7.7) and (7.8) is likely to be most representative – a real device should lie somewhere between figures 7.26a and 7.26b. For the experimental results, these simulations suggest the change observed in the intensity of the fringes is brought about by the change in filling fraction from $A_{FF} \approx 10\%$ to $\approx 33\%$, rather than the depth of the PQC etch, assuming decoupling of the substrate provides a suitable analogue for the effect on the superstrate light. This implies that perhaps the threshold $A_{FF}$ is closer to the best-case than the worst-case but it is not possible to quantify, particularly once scattering from rough surfaces is considered – the different etches may well produce different surface roughness. To answer the question posed about whether similar threshold parameters exist for decoupling substrate modes as for cap layer modes, the PQC layer thickness required is similar, but the requirements on $A_{FF}$ are rather more stringent.

For the buried PhC device design, it turns out that the reduction in the substrate power brought about by increasing $A_{FF}$ does bring a corresponding increase to the guided power. This can then contribute to useful extracted power and hopefully increase $\eta_{diff}$, unlike in the coupled case where the emission was inhibited. However, increasing $A_{FF}$ will increase the extraction length and lead to the best-case assumption that the extraction length is short enough that all the guided power is extracted before it can be absorbed (i.e. $\mu_{ext} \ll \mu_{loss}$) becoming unrealistic. Therefore, choosing to reduce substrate emission in favour of guided power by increasing the $A_{FF}$ is counteracted to at least some degree by a decrease in the ability of the PhC to extract the guided states well. By extension, it is clear that the aim of increasing the decoupling properties of the PQC in order to prevent light being lost to the substrate directly conflicts with the principle of using a buried PQC for its increased overlap with and therefore good extraction of guided modes; any decoupling effect will be more potent for the guided modes than the unguided states, thus pushing the mode tails away from the diffracting PQC and increasing the extraction length. This observation is illustrated by comparing the regions of figure 7.24a below and to the left of the 0.1 contour line where some power is coupled between the cap and GaN buffer layers for guided modes (i.e. there is a chance of good overlap with the PQC for some of the higher order modes) with the regions which provide significant reduction of substrate losses for the best-case scenario shown in blue in figure 7.26b – there is no overlap (note the different $y$-axis scales). Further investigation for several values of cap layer thickness and QW position with different substrate losses also displayed this behaviour, although an exhaustive search is not possible with the computational resources available.

What does remain open to question, is what effect a fully decoupled device might have
on where guided light that has been diffracted is directed. If the substrate is decoupled, the following questions arise: can any power diffracted in this direction be redirected back towards the superstrate and potentially extracted? Or can diffraction to these states be inhibited (although this will likely lead to an increase in the extraction length)? Optimisation then becomes a case of balancing this possible gain to the useful extracted power against the likely reduced diffraction efficiency and so increased material absorption, which will be highly dependent upon where the threshold $A_{FF}$ for decoupling lies in reality. The balance becomes rather precarious when one considers the available figures; the best extraction lengths for low $A_{FF}$ in practical structures has been measured to be no better than 75µm [179] (more realistically, 100µm [251]) and the absorption length of MOVPE GaN-on-sapphire measured in the region of a few hundred microns, becoming lower once the dopants required for the active layer are introduced [252,253], before even considering the detrimental effect of re-absorption by the QWs for $\eta_{IQE} < 100\%$.

![Figure 7.26: Effect of PQC parameters on power exiting to substrate.](image)

7.6.3 Summary

In buried photonic crystal LED configurations, one has the freedom to decide which states are confined in the capping layer through choice of the thickness and air filling fraction of the PhC layer. For the case where the PhC is made thick enough with a high enough air filling fraction to optically decouple the cap layer and GaN buffer layer, the placement of the QWs and the thickness of the cavity can be fine-tuned to optimise
emission into specific states. This allows optimisation of total extraction efficiency or particular guided modes for directional emitters. However, there is a limitation as these parameters do not allow independent control of the extraction length at the same time, since increasing the air filling fraction decreases the interaction of guided modes with the PhC. If the fabrication challenges can be addressed, it may be possible to produce PhCs with a graded $A_{FF}$ to overcome this issue, where the $A_{FF}$ is increased towards the GaN buffer layer, providing a region with low $A_{FF}$ next to the cap layer to extract the modes well, and a high $A_{FF}$ further away to confine the modes. To confine guided modes to the capping layer, a PQC thicknesses over 300nm and air filling fraction over 30% are required for blue light, which is quite achievable with modern fabrication techniques. To confine optical power to the guided and radiation modes of the capping layer, much higher air filling fractions are expected to be required. The experimental samples with $A_{FF}$≈33% appeared to go some way towards this goal, but the confinement was nowhere near complete, even for very thick ($≈1300$nm) PhC layers.

For high light extraction, a buried PhC with low $A_{FF}$ acting in the coupled configuration is the most likely candidate to overcome the competition between absorption and extraction lengths (see equation (3.2)), given current fabrication technology. Within the coupled configuration, there is freedom to optimise the PhC parameters for best extraction without changing the behaviour. To achieve extraction efficiencies much larger than 50%, additional mechanisms for extracting light lost to substrate modes or preventing their excitation must be applied. This figure compares well with the best reported results of 46% unencapsulated and 54% encapsulated [181] extraction efficiency for buried PhC LEDs. The requirements for extracting light lost to the substrate are not exactly the same as for extraction from planar LEDs, as a reflective substrate surface, or a dielectric mirror inserted in the structure may perform well—light is reflected back towards the PhC above for diffraction and/or extraction from the top surface.

### 7.7 Conclusion

The underlying physical mechanisms and behavioural trends which produce the features in the far-field intensity data from LEDs with buried PQC slabs have been demonstrated and experimentally validated. The work presented confirms buried photonic quasicrystal LEDs can be represented well by the 1D-2D model, a combination of an independent 1D model, comprising the vertical device design, and 2D model, comprising the tiling of the PQC itself. The 1D model determines the nature of guided optical modes which can be predicted to a good level of accuracy using a slab waveguide model, with the PQC layer represented by a homogeneous dielectric medium. These modes are diffracted out
of the LED by the 2D PQC structure into the emission cone in directions which can be controlled by the reciprocal lattice and pitch of the PQC. Depending upon the air filling fraction and PQC layer thickness chosen, the device can operate in one of two ways.

If the depth and filling fraction of the PQC are small enough, the overlap with high order guided modes can be increased to optimise the extraction of light trapped in these states. In this case, controlling the ultimate destination of optical power either emitted directly to or diffracted to substrate modes is the limiting factor to achieving extraction efficiencies much above ≈50% for buried photonic crystal LEDs, comparable to the best reported results in the literature of 46% unencapsulated extraction. To achieve better results, a reflective substrate surface is likely to be necessary to redirect light otherwise lost to substrate modes.

Alternatively, buried photonic crystals are able to confine a substantial proportion of the light emitted in a device to a small set of modes guided in the capping layer above the PQC, which the 2D device design can then diffract as desired, as required for directional emitters. The decoupled case is unlikely to allow for improved extraction efficiency as it requires high PhC air filling fractions, which will reduce the interaction between the PhC and the guided modes, increasing the extraction length. If it is possible to produce a graded filling fraction in the PhC, the overlap of the modes with the PhC can be controlled, allowing increased interaction whilst maintaining the decoupling effect. For the decoupling effect to be strong for guided modes, the PQC layer thickness and air filling fraction must be higher than for optimum device extraction efficiency. These parameters are easy to achieve with modern nanofabrication techniques, as the PQC layer needs to be ≈300nm thick or greater for blue wavelengths, with an air filling fraction of at least 30%. Fabricated devices have been shown to exhibit these decoupling properties experimentally and the decoupled regime is a good candidate for applications which require good control and extraction of guided modes, such as for highly-directional LEDs. Further work is required to investigate the feasibility of photonic crystals operating in the diffractive regime for directional emitters, which is considered in chapter 9.

The modelling methods, experimental tools and trends developed and identified in this chapter can be applied to predict the behaviour of devices with different PhC and PQC configurations, reducing the need in product development for fabrication of initial test devices.
Chapter 8

Photonic crystal effects in nanorod and core-shell LEDs

8.1 Introduction

Nanorod and core-shell LED designs have been shown to exhibit many advantages over their planar counterparts, as was discussed in §4.3. When etched through strained quantum wells, as is typical in planar InGaN/GaN LEDs, strain relief of the quantum wells has been observed, leading to reduction of the quantum-confined Stark effect and a corresponding increase in internal quantum efficiency. Core-shell LEDs allow a much larger active region for the size of the device as they make use of the area of the sidewalls of nanorods, offering a potential avenue to mitigate efficiency droop. When grown on c-plane templates, core-shell structures produce non-polar quantum wells on the nanorod sidewalls which are in principle completely devoid of the QCSE and with potentially much lower defect densities due to the lateral growth and small structures where strain is much reduced.

When created in regular arrays, nanorod and core-shell structures exhibit in-plane periodicity and so should display photonic crystal effects. The extent to which this is possible has not been the subject of much investigation and no detailed experimental studies in the III-nitrides are known to the author on the photonic crystal behaviour of embedding the emitting layers within a periodically structured region. A theoretical study has suggested that they may operate in the ‘strong’ or Bloch regime [214], where the photonic states supported in the structure are significantly modified by the presence of the periodicity, in contrast to the ‘weak’ or diffractive regime, where a photonic crystal acts as a diffraction grating. The aim of this chapter is to investigate the nature of photonic crystal effects in III-nitride nanorod structures with embedded emitters experimentally, to investigate what factors affect whether they operate in the strong or the weak photonic regime and to develop models to predict their behaviour.
8.2 Sample fabrication and luminescent properties

Arrays of both core-shell nanorods and nanorods containing a quantum disc were fabricated from c-plane template wafers grown on a planar sapphire substrate. All the samples were patterned with a nickel mask through nano-imprint lithography (NIL) using copies from the same master plate, containing a hexagonal tiling at a pitch of 600nm. Figure 8.1 displays a top-down planar SEM image of one of the core-shell samples after fabrication, showing a slightly distorted hexagonal tiling which is consistent across all the samples. Referring to the figure, there is approximately a 10% stretch perpendicular to the direction labelled ‘a’, giving a pitch in the ‘b’ direction of \(\approx 648\) nm and in the ‘c’ direction \(\approx 653\) nm, measured using average measurements from several calibrated SEM images.

![Figure 8.1: Plan-view SEM of a core-shell nanorod array after regrowth steps.](image)

After the NIL process, the quantum disc samples were fabricated by Cl\(_2\)/Ar ICP etching of MOVPE planar templates containing a single InGaN quantum well surrounded by \(\approx 600\) nm GaN above and \(\approx 5000\) nm below, provided by Osram GmbH. The shape and sidewall profile of the nanorods were controlled by varying the etch temperature [254], and the height controlled by varying the etching time.

The core-shell samples were fabricated by Dr E. Le Boulbar using a ‘top-down’ approach of epitaxial overgrowth on bare GaN nanorods etched into a \(\approx 6\) \(\mu\)m thick MOVPE template. Figure 8.2 summarises the fabrication process, which has been published and is described in detail in ref. [202]. To prevent regrowth at the base of the rods, they were passivated by spinning on and curing a hydrogen silsesquioxane (HSQ) layer that fills the regions between the nanorods to \(\approx 20\) nm thickness. A significantly thinner layer of HSQ covers the part of the nanorod sidewalls, which can be removed by a carefully timed buffered oxid etch (BOE) process. A short GaN growth recovers \{1\bar{1}0\} \(m\)-plane facets on the sidewalls of the nanorods which is followed by a period of InGaN growth and finally a GaN capping layer. Figure 8.3 shows an oblique SEM image of a representative core-shell sample, showing the non-polar \(m\)-plane facets on the rod sidewalls and the
formation of \{10\bar{1}1\} \textit{r}-plane semi-polar facets creating a pyramid at the top of the rod. The core and shell epitaxial layers described can be resolved in the TEM image shown in figure 8.4. Several high aspect ratio core-shell nanorod samples with a height of \(\approx4000\text{nm}\), along with a shorter sample with height \(\approx850\text{nm}\) on a thinner template were fabricated by varying the initial ICP etch time.

The PL emission for an excitation wavelength of 405nm was measured and is shown in figure 8.5 for one tall and one short core-shell sample as well as a representative quantum disc nanorod sample. Quantum well emission centred at 445nm is observed from the quantum disc nanorods. Also, there is intense yellow band emission at wavelengths longer than 500nm, which is typical in GaN and is usually attributed to deep level states in the band gap from Ga vacancies in n-doped GaN [255], possibly additionally introduced during the etching of the rods. The core-shell nanorods emit broadband PL over visible
wavelengths, with a wide blue-green peak around 450-550nm, merging into a yellow-red emission band 575-700nm for the tall core-shell sample. It is not clear why there is no significant yellow band emission from the short core-shell nanorods, but it is thought to be because the template used was unknowingly not Si doped. The high intensity doublet feature observed around 694nm is attributed to the ‘ruby’ lines of the sapphire substrate from luminescence of Cr$^{3+}$ ion impurities [256].

The luminescence was resolved with position in the rod using cathodoluminescence (CL) hyperspectral imaging measurements at a resolution of $\approx 20$nm [257] by Dr P. Edwards at the University of Strathclyde. This experiment was performed by repeatedly measuring the spectrum emitted when an electron beam is directed at the sample for different positions and so the CL measurements are spatially resolved only in the sense of where the electron beam hits the sample. A 5kV accelerating voltage was used during the measurements to allow probing of the lower band gap InGaN layer inside the GaN capping layer while limiting the loss of spatial resolution due to electron scattering to an acceptable level. Figures 8.6a and 8.6b show SEM images of the tall and short core-shell structures respectively with a real-colour representation of the emission from the rods overlaid, determined by calculation of the chromaticity coordinates from each spectrum taken.

The two separate emission peaks observed in the PL are also seen in the CL measurements; the blue-green band originates from near the intersection of the $r$-plane pyramids and $m$-plane sidewalls where higher In incorporation has occurred due to the conditions...
of the InGaN growth step, and the yellow band is emitted from everywhere. Whilst it is not evident in the figures, as they cover the visible range only, the emission occurred with decreasing intensity into the near UV part of the spectrum down the core-shell nanorods away from the pyramids. This was as a result of the InN mole fraction decreasing towards the base of the nanorods. Due to the below bandgap wavelength of the exciting laser for these regions, UV emission cannot be observed in the PL experiments on these samples.

This behaviour is not precisely representative of all the core-shell samples due to the incorporation of different indium mole fractions. However, all the samples are qualitatively similar, with blue or blue-green emission coming from a region near the top of the rods and yellow band emission from everywhere. Similar CL measurements were performed on a quantum disc nanorod sample to confirm that the blue emission originates from the quantum well and the yellow band is emitted from all regions, behaving comparably to the core-shell samples.
8.3 Angular luminescence observations from emissive nanorods

Angular luminescence experiments have been used to investigate the behaviour of arrays of emissive nanorods, using the experimental system described in chapter 6. The spectra were taken at a resolution of 0.1° for horizon-to-horizon scans at fixed azimuth, and at a resolution of 0.25° when scanning over both azimuth and incline. The samples were aligned to the in-plane tiling in azimuth by matching diffraction features with the 2D lattice for data collected at a fixed inclinal angle while varying azimuth over 180°.

![Figure 8.7](image)

**Figure 8.7:** Effect of a stretching distortion on the reciprocal lattice of a hexagonal tiling. The first-order reciprocal lattice points are shown by the gray circles, the first Brillouin zone (FBZ) as a solid black line, the irreducible Brillouin zone (IBZ) as a solid gray line and the outline of the hexagonal rods shown in figure 8.1 are shown as dashed red lines. Compared to a hexagonal lattice, the edge of the IBZ no longer contains directions uniquely definable as \( \Gamma K \) or \( \Gamma M \) in the conventional sense.

The stretching distortion of the lattice leads to a lifting of the degeneracy between the three directions, a, b and c, and consequently it is not possible to define a unique \( \Gamma K \) or \( \Gamma M \) reciprocal lattice direction as in a perfect hexagonal lattice. Instead, the irreducible Brillouin zone (IBZ) covers 180°, except in the special case when the stretching distortion is perpendicular or parallel to one of the lattice directions thereby giving a reflective translation in the reciprocal lattice and an IBZ of 90°. Referring to figure 8.7, the directions are defined for the purpose of formalism as \( \Gamma K_i \), where \( i \) specifies the closest corresponding spatial lattice direction a, b or c, and \( \Gamma M_j \), where \( j \) specifies the corresponding reciprocal lattice direction, labelled \( ab' \), \( bc' \) or \( ca' \). The horizon-to-horizon data was collected along \( \Gamma K_a \) when not stated otherwise and in the case of the stretching present in the experimental samples, this aligns about 0.5° away from the ‘a’ direction in figure 8.1.
8.3.1 Quantum disc nanorods

Nanorod arrays with the dimensions described in table 8.1 were fabricated, and are shown schematically in figure 8.8a. The ICP etch conditions used produced nanorods with a slight vertical taper, where the diameter increases marginally from the tip towards the base at the GaN buffer layer. The air filling fraction $A_{FF}$ was estimated from plan-view SEM images, such as that shown in figure 8.10b.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Nanorod height (nm)</th>
<th>GaN buffer depth (nm)</th>
<th>$A_{FF}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NR1</td>
<td>850</td>
<td>4750</td>
<td>0.69</td>
</tr>
<tr>
<td>NR2</td>
<td>1200</td>
<td>4400</td>
<td>0.70</td>
</tr>
<tr>
<td>NR3</td>
<td>1700</td>
<td>3900</td>
<td>0.72</td>
</tr>
<tr>
<td>NR4</td>
<td>2300</td>
<td>3300</td>
<td>0.73</td>
</tr>
<tr>
<td>NR5</td>
<td>3050</td>
<td>2600</td>
<td>0.75</td>
</tr>
<tr>
<td>NR6</td>
<td>4600</td>
<td>1000</td>
<td>0.77</td>
</tr>
</tbody>
</table>

Table 8.1: Dimensions of the tapered quantum disc nanorod structures after fabrication.

Angular PL measurements were made on the sample with the shortest nanorods (NR1) and are plotted in a k-space projection in figure 8.9a, where a rich array of features can be seen. In the plan-view SEM image of the sample in figure 8.9b, there are some thin membrane-like sheaths of material around the bases of the nanorods, which will cause light to be scattered randomly, reducing the contrast of the periodic effects in the angular PL. Etching the samples for 20 minutes in a warm (40°C) 1 Molal (mol kg$^{-1}$) potassium hydroxide (KOH) solution removes the majority of the sheaths, and also has the effect of smoothing the sidewalls to a degree due to the high selectivity of the etch to non-polar facets. It can be seen in figure 8.10a that the contrast of the features in the angular PL
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is increased markedly compared to the results before etching, and so the 20 minute warm KOH process was applied to all the samples.

Several families of features are discernible in these measurements, including Fabry-Pérot fringes in the background, most clearly seen near normal incidence \((k_{||}=0)\) for the blue emission \((k_0 \approx 1.35 \times 10^7 \text{m}^{-1})\) as broad, slightly curved, near-horizontal bands. Additionally, there are large rounded regions of low or high intensity which are caused by the far field pattern of optical fibre-like modes propagating along the vertical axis of the nanorods [258]. The final and most prominent family of features is the multitude of sharp diagonal lines originating from diffraction of guided slab waveguide modes. The seeming abundance of the latter comes about foremost from the highly multi-moded behaviour of the structures and also due to the distortion in the lattice providing three different periodicities for extraction of the light. These are in groups of approximately parallel lines, with each group representing diffraction from one reciprocal lattice point, a process described in detail in §3.2.1. An attempt was made to investigate the polarisation of the diffracted modes in these structures with the buried photonic quasicrystal nanohole structures presented in chapter 7, but due to the higher pitch, multi-moded nature of the structures, distortion of the hexagonal lattice and lower brightness of the emission, no useful data could be collected.

The guided modes have effective refractive indices \(n_{\text{eff}}\) between \(\approx 1.8\) (sapphire) and 2.5 (GaN), determined by using a method based on that discussed in §7.3.1, which shows that they are guided in a layer containing GaN – although measurement of precise values was prevented by the large quantity of the far-field features. The modes with lowest \(n_{\text{eff}}\) (crossing normal incidence at higher \(k_0\) within the family from each reciprocal lattice point) are broader, suggesting they are the most lossy and the modes with higher \(n_{\text{eff}}\) appear narrower and fainter, such as the faint features with a negative gradient around \(k_{||}=1.1 \times 10^7 \text{m}^{-1}\) and \(k_0=1.28 \times 10^7 \text{m}^{-1}\) in figure 8.10a. This suggests that the modes are guided in the GaN buffer layer as the lower order modes will be more confined away from overlap with the nanorod layer, reducing their loss to diffractive effects and vice versa. This assumption is confirmed by analysing the emission from taller nanorod structures which have a much thinner GaN buffer layer, shown in figure 8.11 for sample NR5 and figure 8.12 for sample NR6. The quality of the surfaces after etching becomes poorer with increasing ICP etch time, which is partially responsible for the lower contrast in the features, and the potency of the optical fibre-like modes increases due to the increased length of the nanorods.

For these taller structures, there is a significant difference in behaviour between the blue quantum well emission \((k_0 \approx 1.33-1.48 \times 10^7 \text{m}^{-1})\) emitted at the top of the rods away from the GaN buffer and the yellow band emission \((k_0 \lesssim 1.32 \times 10^7 \text{m}^{-1})\) which originates
Figure 8.9: Sample NR1 with 850nm high nanorods.

(a) Angular PL collected along ΓK_a.

(b) Plan view SEM.

Figure 8.10: Sample NR1 with 850nm high nanorods after 20 minute etch in 40°C 1mol kg⁻¹ KOH solution.

(a) Angular PL collected along ΓK_a.

(b) Plan view SEM.
(a) Angular PL collected along $\Gamma K_a$.

(b) Cross section SEM

**Figure 8.11:** Sample NR5 with 3050nm high nanorods.

**Figure 8.12:** Angular PL collected along $\Gamma K_a$ for sample NR6 with 4600nm high nanorods.

**Figure 8.13:** Angular PL collected along $\Gamma K_a$ for sample NR1 with 850nm high rods using 1200l/mm grating.
from all the structure. The slab modes guided in the buffer layer are only observed for the yellow band emission and not observed for the blue emission, showing that the guided slab modes are evanescent in the nanorods and only couple weakly with the quantum wells. The poor contrast of the guided modes for yellow emission in figure 8.12 is attributed to a decreased proportion of the yellow emission originating near or from the buffer layer, as well as an increase in scattered light from the rougher surfaces. The decrease in the number and corresponding increase in the spacing of the modes with increasing etch depth provides further confirmation that the nanorod structures have no more than a perturbative effect on light guiding in the GaN buffer layer.

This finding implies that these structures may be beneficial for light extraction as they are able to diffract light emitted into guided slab modes and, in the case of the tall rods, light emission into GaN slab modes is inhibited; although light may still be emitted from the QW into the continuum of substrate modes, not all of which will be evanescent in the nanorods. The thin diagonal dark lines (for example, near normal incidence for \( k_0 \approx 1.32 - 1.4 \times 10^7 \text{m}^{-1} \) in figure 8.13) within the range of the blue QW emission for the sample with the shortest rods (NR1) suggest that the opposite process may occur under some conditions, where light emitted into the continuum of useful radiation modes is diffracted away into slab modes.

In sample NR1 with the shortest rods, there is significant coupling of the QW emission into the guided slab modes, likely due to strong evanescent coupling as the QW is only \( \approx 250 \text{nm} \) from the GaN buffer layer. However, for this blue emission, the intensity plot appears to show a different ‘texture’ when compared with the yellow emission. It is not clear if this is due to superposition of the large number of features which are not well resolved at the highest available angular and spectral resolution (shown in figure 8.13 using a higher resolution grating), or due to some interaction with the periodic medium creating possible anti-crossing-like features between some of the modes; a process observed previously in nanohole surface photonic crystal LEDs [170]. The change in behaviour between the blue and yellow bands seems particularly clear for the tallest rods (NR6, shown in figure 8.12), where the periodic medium could cause a perturbation of the vertical Fabry-Pérot resonances. In this case, the rods are much longer, so light trapped in these lossy Fabry-Pérot states will interact more with the periodic medium before exiting the surface.

### 8.3.2 Core-shell nanorods

Several core-shell nanorod samples were fabricated using different growth conditions for a different investigation; samples which are informative in this discussion of photonic crystal effects were selected and are summarised in table 8.2. The tall core-shell samples
Chapter 8. Photonic crystal effects in nanorod and core-shell LEDs

CS2-CS4 are quite similar, but slight differences are seen between the cross-section SEM images of the samples presented later.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Rod height (nm)</th>
<th>GaN buffer depth (nm)</th>
<th>$A_{FF}$</th>
<th>BOE etch (sec)</th>
<th>InGaN growth (nm)</th>
<th>Temp (°C)</th>
<th>Pressure (mBar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CS1</td>
<td>850</td>
<td>1650</td>
<td>0.50</td>
<td>80</td>
<td>750</td>
<td>300</td>
<td></td>
</tr>
<tr>
<td>CS2</td>
<td>4000</td>
<td>2250</td>
<td>0.50</td>
<td>30</td>
<td>750</td>
<td>300</td>
<td></td>
</tr>
<tr>
<td>CS3</td>
<td>4000</td>
<td>2250</td>
<td>0.50</td>
<td>20</td>
<td>750</td>
<td>500</td>
<td></td>
</tr>
<tr>
<td>CS4</td>
<td>4000</td>
<td>2250</td>
<td>0.50</td>
<td>20</td>
<td>700</td>
<td>500</td>
<td></td>
</tr>
</tbody>
</table>

Table 8.2: Summary of the core-shell samples investigated.

The short core-shell sample (CS1) was found to behave in a similar way to the quantum disc nanorod samples investigated previously, and angular PL measurements are presented in figure 8.14. Fabry-Pérot fringes, the diffraction of guided slab modes with $n_{eff}$ between $\approx 1.8$ and $2.5$ and evidence of the vertical optical fibre-like modes, albeit less pronounced, presumably due to the pyramidal tips, were again observed. In addition, the data shows distinct triangular regions delineated by step changes in intensity which were much less clear in the quantum disc results. The intensity steps align with band folding of the edges of the air and sapphire extraction cones. Due to the thickness of the sapphire substrate, a near-continuum of modes exists within the sapphire extraction cone and are too closely spaced to be individually resolved. This light and the continuum of light inside the air cone also undergo diffraction. Competition between the different diffraction orders causes the discontinuities in the intensity of the light at the boundaries of the folded extraction cones observable in the data. The process acts on all the light including that in the discrete guided slab modes, which can be seen most clearly along the line $k_0=0.9-1.1 \times 10^7 \text{m}^{-1}$ and $k_\parallel=0.9-0.5 \times 10^7 \text{m}^{-1}$ in figure 8.14a. The power is distributed between the various extraction routes and so the far-field intensity changes because, as each mode passes into a region folded to an extraction cone, another route becomes available for its diffraction. The features imply that, compared to the quantum disc nanorods, there appears to be a substantial quantity of light in the continuum of the extraction cones or an increase in the diffractive effect on this light; but it is not clear what might cause this as there are many physical differences between the samples.

Figures 8.15-8.17 show angular PL measurements next to cross section SEM images of samples CS2-CS4 respectively. These tall core-shell nanorod arrays behave in a profoundly different way compared to CS1; the light is emitted in a small number of broad bands which interact through both crossing and anti-crossing-like features. Sample CS2 will initially be considered in detail to understand the origin of the behavioural change, since the contrast of the features over the background emission before normalising the data for

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Angular PL data were collected over azimuth and inclinal angle for both CS1 and CS2 to compare their behaviour further, and are displayed projected into in-plane reciprocal space at wavelengths chosen to best illustrate the differences in their behaviour in figure 8.18. It is clear that the sharp white lines in sample CS1 form arcs in the far field pattern, indicating that there is no azimuthal variation of $k||$ (the radius) within each mode and so the sample demonstrates conventional diffractive behaviour well described by trapped light propagating in slab waveguide modes. In contrast, figure 8.18b clearly shows that this is not the case for sample CS2, where the features vary in a pattern which correlates with the reciprocal lattice of the nanorod tiling. This correlation of the broad bands with the tiling of the nanorods shows that they originate from Bloch modes with a strong periodic component\(^1\). The far-field features are a result of these strongly periodic modes folded into the air cone. The experimental results show that these samples are operating in what has been referred to as the strong or Bloch photonic crystal regime discussed in §4.1.

8.3.3 Shaped nanorods

There are a number of physical differences between CS1 and CS2 which may cause the change in behaviour, namely the height of the core-shell nanorods and additionally the sidewall shape. Sample CS1 contained short nanorods with near-vertical sidewalls, whereas CS2 contained tall nanorods with an ‘undercut’ sidewall profile where there is a wider region near the tips. The quantum disc nanorod samples NR1-NR6 investigated in §8.3.1 have a ‘tapered’ sidewall profile, where the diameter increases from the tip towards the base of the rods. It is not clear how important the effect of nanorod height is on the behaviour as in the tallest quantum disc sample NR6 (figure 8.12), there was perhaps some evidence of a change in behaviour compared to the shorter samples (figures 8.10a and 8.11a). There is therefore no information available about the effect of the sidewall profile on the behaviour which is independent of the nanorod height.

The effect of varying the sidewall profile independently of the nanorod height was investigated by fabricating further quantum disc nanorods, but with an undercut sidewall by changing the temperature during the ICP etching step. Two samples with etch depths approximately matching the heights of NR3 (shown in figure 8.20 for comparison) and NR5 (see figure 8.11) were fabricated at a higher etch temperature. The increased temperature caused the nanorod sidewalls to have the undercut profile that is displayed in the cross-

\(^1\)It should be made clear at this point that whilst strictly the diffracted slab modes could be defined as Bloch modes as they contain a small periodic component responsible for the diffractive effect, the meaning here only refers to modes with a significant periodicity, changing the nature of the dispersion from that of a slab waveguide mode.
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(a) Angular PL collected along $\Gamma K_a$.  

(b) Cross section SEM

Figure 8.14: Sample CS1 with 850nm high core-shell nanorods.

(a) Angular PL collected along $\Gamma K_a$.  

(b) Cross section SEM

Figure 8.15: Sample CS2 with 4000nm high core-shell nanorods and 30sec BOE etch after passivation.
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Figure 8.16: Sample CS3 with 4000nm high core-shell nanorods and 20sec BOE etch after passivation.

Figure 8.17: Sample CS4 with 4000nm high core-shell nanorods and 20sec BOE etch after passivation with a lower growth temperature.
Chapter 8. Photonic crystal effects in nanorod and core-shell LEDs

(a) Sample CS1 with 850nm high core-shell nanorods at 600nm
($k_0=1.05\times10^7\text{m}^{-1}$).

(b) Sample CS2 with 4000nm high core-shell nanorods at 530nm
($k_0=1.19\times10^7\text{m}^{-1}$), 180° of data have been collected and tiled.

Figure 8.18: Single frequency intensity variation, projected into reciprocal space, where $k_x$ is parallel to the $\Gamma K_a$ direction.
section SEM images in figures 8.19b and 8.19d. The heights of the nanorod array in the
two undercut samples were measured to be 3175nm and 1800nm, in comparison to 3050nm
(NR5) and 1700nm (NR3) for the tapered samples.

The angular luminescence in figure 8.19 from the samples with an undercut sidewall
profile shows Bloch mode formation for the blue light emitted from the quantum wells
\( k_0 \approx 1.33 - 1.48 \times 10^7 \text{m}^{-1} \), as well as diffractive behaviour, most clearly seen for the yellow
emission \( k_0 \lesssim 1.32 \times 10^7 \text{m}^{-1} \). The variation of the strength of the features due to diffrac-
tion of slab modes in the undercut samples with distance from the GaN buffer layer is due
to the same process as in the tapered nanorods discussed in §8.3.1. None of the nanorods
with a tapered profile investigated showed such clear evidence of Bloch mode formation
as in the undercut rods.

### 8.3.4 Summary

Strong photonic crystal effects have been shown to arise in arrays of both core-shell and
quantum disc nanorods. The initial observations above suggest that they depend upon
the shape of the sidewalls of the nanorods; those with a tapered profile, where the rod is
narrowest at the time and increases in diameter towards the base, do not show any clear
evidence of Bloch mode formation, whereas those with an undercut profile, where there is
a region of higher dielectric fill near the top of the rods, do show strong photonic crystal
effects. The remainder of this chapter investigates the conditions which are required for the
strong or Bloch operating regime and discusses why the undercut sidewall profile causes
Bloch mode formation.
Figure 8.19: (top) 3175nm and (bottom) 1800nm high nanorods with undercut sidewalls.

Figure 8.20: Sample NR3 1700nm high quantum disc nanorods with tapered sidewalls.
8.4 Analysis of Bloch mode formation

This section discusses the factors that can lead to the strong photonic crystal behaviour using the experimental observations, and provides a model to fit the dispersion of the Bloch modes.

The origin of the strong photonic crystal behaviour in the Bloch regime clearly originates from the interaction of the light with the periodic medium, as described in §3.2.2. However, understanding why it does not occur in all devices which contain a periodic medium requires consideration of the confinement of the light to this periodic medium for sufficient interaction to manifest the strong effects.

The behaviour of light in a finite 2D slab containing a periodic refractive index variation in a plane \( \mathbb{P} \) perpendicular to the \( z \)-direction, can be written as

\[
H_k(\mathbb{R}) = e^{i\hat{k} \cdot \mathbb{R}} u_k(\mathbb{P}, z) \quad (8.1)
\]

where \( H_k(\mathbb{R}) \) represents the field pattern over a space \( \mathbb{R} \), for each wavevector \( \hat{k} \) and the function \( u_k(\mathbb{P}, z) \) represents the wavevector and space dependent interaction of light with the medium. In an ideal lossless structure in which the slab comprises a homogeneous layer and a photonic crystal layer, the function \( u_k(\mathbb{P}, z) \) can be split into two terms – a term \( W(z) \) representing the homogeneous slab layers and a periodic Bloch term \( B(\mathbb{P}, z) \) for the layers with in-plane periodicity. The interaction of light with the overall structure is illustrated by applying a wavevector dependent coefficient \( \alpha_k \) or \( \beta_k \) to each constituent part of the overall medium using first-order perturbation theory [259], giving approximately

\[
u_k(\mathbb{P}, z) \approx \alpha_k W(z) + \beta_k B(\mathbb{P}, z) \quad (8.2)\]

When \( \beta \) is sufficiently large compared to \( \alpha \), the Bloch term \( B \) dominates, causing \( u_k(\mathbb{P}, z) \) to give solutions for \( \hat{k} \) which resemble that of a completely periodic medium as observed in figure 8.18b for the tall core-shell nanorods, operating in the strong or Bloch regime. In the weak or diffractive regime, the slab-like contribution to \( u_k(\mathbb{P}, z) \) dominates and \( \beta \) is only large enough to cause diffraction of guided slab modes (for example, as seen in figure 8.18a for the short core-shell nanorods), leaving the fields closely resembling those of a homogeneous slab. When \( \alpha \) and \( \beta \) have comparable influence on \( u_k(\mathbb{P}, z) \), a combination of both slab and Bloch-like behaviour dependent on \( \hat{k} \) and wavelength is expected, which is the situation observed in the shaped quantum disc nanorod samples shown in figure 8.19.

The size of \( \alpha \) and \( \beta \), representing the magnitude of interaction with the homogeneous and periodic parts of the structure respectively, clearly depend on the overlap of the field.
profile with that part of the medium. Therefore, the strength of the effect will depend upon the proportion of optical energy confined to each region for each allowed value of \( \hat{k} \) or photonic state\(^2\). The interaction with the periodic medium of all the possible states will vary, but by placing the source inside or near the periodic medium, the states which have a reasonable degree of field overlap with the periodic medium will be selectively excited over those which do not; offering the best chance of creating predominantly Bloch-like behaviour for all the emission.

In a practical structure with surface roughness and imperfections that are not periodic from which light scatters, an additional competing process is present to redirect light away from the periodic terms to non-periodic terms. For example, the effect of incoherent scattering of trapped light is qualitatively illustrated by including a third term in (8.2) containing all the random imperfections in the medium with its own interaction coefficient\(^3\). It should also be stated that optical absorption is considered a negligible effect in the experimental samples investigated when compared to the diffractive and random scattering, but will have an analogous influence to surface roughness – increasing the influence of non-periodic terms whilst reducing that of the periodic terms.

In the same way a photonic band gap arises, as described in §3.2.2, the occurrence and size of the anticrossing or ‘miniature band gap’ features observed in the samples can be considered\(^4\). Adding just a weak periodicity to a waveguide is enough to lift the degeneracy between certain values of wavevector by coupling parts of reciprocal space to each other through band folding, creating a frequency gap referred to here as an anticrossing. The size of the resulting frequency gap is determined, to a first order approximation, by the optical field energy in the medium for the states either side of the anticrossing. This will in turn depend upon the proportion of the total field energy in the periodic region for which a difference in the overlap of the field energy with dielectrics of different refractive index can occur, leading to the difference in frequency between the two bands. A band gap will always occur where these states meet no matter how weak the periodicity is [137], although it may be too small to resolve experimentally. Small interactions of this nature are likely to be responsible for the apparent change in behaviour of the Fabry-Pérot fringes in the blue emission in the taller nanorods, such as that seen most clearly in sample NR6 in figure 8.12. It is assumed that if of opposite polarisation after folding, the states will

---

\(^2\)Here, the energy from a guided state which is diffracted or folded to e.g. the air cone is represented by a corresponding increase of its energy in the non-periodic air region, which will increase with extraction efficiency, acting to increase \( \alpha \).

\(^3\)Strictly, it breaks the in-plane translational symmetry required in the definition of (8.1) and so cannot be directly included, but it does illustrate the effect of these processes.

\(^4\)Although these features do not arise from the same interactions which lead to anticrossings between e.g. light and heavy holes in the valance band of a quantum well, they are conventionally referred to as anticrossings for ease of description. They are purely a consequence of the periodicity and the resulting opening of band gaps in frequency and/or reciprocal space.
cross as a degeneracy remains.

In summary, the presence of the Bloch modes in the samples is due to field overlap with the periodic regions of the device structure.

### 8.4.1 Fit with infinite nanorod model

The freely available software package MIT Photonic Bands (MPB) [260], which uses the plane wave expansion technique to solve Maxwell’s equations with periodic boundary conditions for specified in-plane wavevectors, was used to characterise the behaviour further and attempt to provide a model for the Bloch mode dispersion. In this software, a periodic geometry can be set in up to three dimensions, with the non-periodic dimensions set to be invariant, making simulation of an infinitely periodic structure very simple and fast. For structures such as the finite nanorods under consideration, there is periodicity in the two dimensions parallel to the slab ($xy$), but no periodicity and the medium is not invariant in the direction perpendicular to the slab ($z$). As a result, full simulation of photonic crystal slab structures is not possible as MPB tiles the slab and its surrounding medium in the $z$-direction as well as the desired in-plane directions. This stacking of the simulation geometry means that MPB cannot produce meaningful results for light which is not completely guided in the $xy$-plane, such as the extracted light observed in the experimental far-field angular PL.

The structure of sample CS2 was modelled as a two-dimensional array of infinitely long nanorods using the planar SEM image in figure 8.1 to reconstruct the in-plane cross section of the nanorods. A birefringent model was used, with the refractive index of the ordinary and extraordinary rays given in ref. [248]. To take into account the variation of the refractive index with wavelength, a first order perturbative model was used to modify the frequency of the bands [261]

$$k_0 = k_{0s} \left(1 + E \left(\frac{n_s - n(k_{0s})}{n_s}\right)\right)$$

(8.3)

where $n_s$ is the refractive index used for the simulation, $k_{0s}$ is the frequency of the simulated solution and $n(k_{0s})$ the refractive index at $k_{0s}$ from [248]. $E$ represents the proportion of the electric field energy in the dispersive dielectric, which can be calculated by MPB.

An overlay of the simulation is shown for sample CS2 in figure 8.21, which produces a consistent fit and shows that the structures behave very similarly to an ideal 2D photonic crystal comprising infinitely long nanorods. To achieve this fit, the simulated dielectric fill fraction was varied slightly to allow for the uncertainty of the effect of its variation with vertical position in the rod. As a consequence, it is not known if there is an upwards shift in frequency of the bands caused by increased overlap with air for light near the top...
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Figure 8.21: Angular PL collected along $\Gamma K_a$ fitted with an infinite rod model produced by MPB.

of the rods or a downwards shift caused by increased interaction with the GaN buffer in the measured sample when compared to ideal, infinitely long nanorods. In either case, the shape of the bands shows good agreement between the simulated dispersion and the experimental measurements. It is clear that the Bloch term is highly dominant in sample CS2 and that there is substantial confinement of the optical power to the nanorod region. The possible mechanisms for this confinement will now be considered.

8.4.2 Effective medium index guiding

In the weak or diffractive regime the behaviour of periodic structures can be well represented by considering the 2D in-plane PhC properties and 1D vertical slab waveguide structure separately. For the purpose of the 1D vertical analysis, the periodic region is replaced by a bulk dielectric with an effective refractive index $n_e$, where the effective bulk refractive index of a nanostructure is between the values given by the expressions (7.7) and (7.8) from [249].

The vertical variation in effective refractive index can be calculated for the shaped nanorods (illustrated schematically in figure 8.22a) by measuring the air filling fraction at different positions in the nanorod array ($A_{FF}(z)$), such as those shown in in figure 8.22b using the model for the electric field parallel to the interfaces (equation (7.7)) at a vertical resolution of $\approx 20\text{nm}$ ($\ll \lambda$). $A_{FF}(z)$ was determined by measuring the variation in diameter of nanorods on cross-section SEM images ($D(z)$). To minimise the effect of systematic

$^5$See, for example, chapter 7 [262] or ref. [181].
errors in the SEM the diameter considered representative of the filling fraction measured previously from top-down images was used to relate $D(z)$ to $A_{FF}(z)$. The nanorods with an undercut vertical profile which show evidence of a significant Bloch term have a region of higher dielectric fill near the tops of the rods, and a section of lower fill separating the underlying GaN buffer layer from this region. Thus the index of the medium is higher near the top of the undercut rod profile, and lower in the underlying region of the rods, forming an effective waveguiding structure similar to a suspended photonic crystal slab in this consideration. This waveguide provides a mechanism for optical confinement to the periodic regions for nanorod arrays with an undercut sidewall profile, leading to the formation of Bloch modes. This hypothesis will now be investigated.

The effective bulk refractive index model should be able to provide an indication of the degree of optical confinement to the periodic and non-periodic layers in the vertical direction, but can only give a qualitative description for the Bloch regime as it does not take into account the effect of the periodicity on the effective index and in-plane wavevector for different azimuthal directions.

Figure 8.22c shows the field profiles of the TE modes with the strongest first order resonance in the nanorods for the undercut and tapered structures. These were calculated using the slab waveguide model described in chapter 5, and include a large, but finite sapphire substrate layer to force discretisation of modes with $n_{eff}<n_{sapp}$. For the tapered quantum disc nanorods, which did not show Bloch effects, there were no modes without a significant field overlap with the non-periodic regions, examples of which are shown in curves iv) and v) of figure 8.22c where the first order TE resonance with the largest field in the nanorods is displayed.

For the undercut structures which did show evidence of Bloch effects, modes with their field profile confined almost entirely to the periodic region by index guiding exist, confirming the formation of a quasi-suspended slab region, shown in curves i)-iii) of figure 8.22c. The quasi-suspended photonic crystal slab is located near the top of the rods where the blue QW emission originates from in the quantum disc nanorod samples. The QW will therefore have a good coupling strength with this effective guiding region. This is the cause of the Bloch effects in the blue emission of the undercut nanorod samples in figure 8.19. On the other hand, the yellow emission is not localised to the effective slab region, but mostly comes from the underlying homogeneous slab or the lower parts of the rods and as such cannot couple as strongly to the confined Bloch modes. The same conclusion is reached when repeating the process using the lower limit to the volume-averaged refractive index

\[ n_{eff} < n_{sapp} \]

Although it is thought that the 1D consideration will provide a good quantitative analysis at least for weaker Bloch effects as light must first be confined to the periodic medium for these effects to be significant, and at their onset they will only be perturbative.
of the nanorod layer (given by equation (7.8) for the electric field perpendicular to the interfaces). At least one mode is confined entirely to the periodic region for the undercut nanorods, but not in the tapered structures.

Curve vi) in figure 8.22c shows that the small separation from the buffer layer and minimal undercut of the short core-shell nanorods is not sufficient to confine light in the nanorods. Also, the regularity of the shape of the short core-shell nanorods is poor compared to the other samples, with the effect that scattering may inhibit the formation of strong Bloch modes.

In the tall core-shell samples CS2-CS4 with a similar undercut and separation from the GaN buffer, no clear evidence of slab modes is seen in the angular PL measurements presented in figures 8.15a-8.17a for the blue-green emission ($k_0 \gtrsim 1.1 \times 10^7 \text{m}^{-1}$ for CS2, $k_0 \gtrsim 1.15 \times 10^7 \text{m}^{-1}$ for CS3, $k_0 \gtrsim 1.12 \times 10^7 \text{m}^{-1}$ for CS4) originating from the top of the rods. This is well explained by the index guiding mechanism as, due to the large undercut and separation by the region of lower dielectric fill, the source cannot couple to the GaN buffer slab modes. In the cross section SEM image of sample CS4 shown in figure 8.17b, the index guiding region of higher dielectric fill is seen to be rougher than in the other samples, which will decrease the effect of the periodicity through random scattering. This mechanism is considered to be responsible for causing the Bloch features to be less distinct in the angular PL in figure 8.17a, but they survive as the scale of the roughening is small compared to the wavelength of the light.

Figure 8.22: Transfer matrix modelling of nanorods showing (top) Bloch and (bottom) slab behaviour. i) 3175nm and ii) 1800nm high rods with undercut sidewalls, iii) sample CS2, 4000nm tall core-shell nanorods, iv) sample NR5, 3050nm and v) sample NR3, 1700nm high rods with tapered sidewalls and vi) sample CS1, 850nm tall core-shell nanorods.
The index guiding mechanism explains the Bloch effects seen for localised emission in the quasi-suspended slab, such as the blue-green emission from the core-shell samples or the blue emission from the quantum disc samples. However, some of the experimental observations are not explained. The yellow emission in sample CS2 is dominated by Bloch behaviour (figure 8.15a), which is not expected by this index guiding mechanism as such emission occurs throughout the whole structure, notably the lower parts of the nanorods and the underlying buffer layer. In contrast, Bloch mode formation in this spectral range does not occur in sample CS3 (figure 8.16a); only diffraction from slab modes is visible for the yellow emission. Referring to the cross-section SEM images of the tall core-shell samples CS2 and CS3 in figures 8.15b and 8.16b, the guiding region at the top of the rods, from which the blue-green emission originates, is very similar but there is a clear difference in contrast between the high contrast Bloch features seen in CS2 and the much weaker features in CS3 at these emission wavelengths. As a consequence of these differences, index guiding is unlikely to be solely responsible for the behaviour of the structures.

To investigate further the effect of the nanorod shape on the index guiding, finite-difference time-domain (FDTD) simulations were performed for hexagonal arrays of nanorods of the same pitch and approximate height as sample NR3 with 1800nm high rods and the 1700nm high undercut quantum disc nanorods. The FDTD method gives a full 3D simulation of structures, and models the interaction of light in a medium by calculating the solutions to Maxwell’s equations for discrete time steps inside a discrete spatial mesh to approximate the medium [263]. The sidewalls were kept straight, but the angle was varied from negative (undercut profile) to positive (tapered profile), as shown in figure 8.23. The overall volume of dielectric in the nanorod array was kept constant between the simulations, and a perfectly matched layer (PML) was placed a short distance below the nanorods so that only resonances associated with confinement to the nanorod layer are seen. All the FDTD simulations presented in this thesis were performed by Dr S. Lis.

The band structures were determined by thresholding of the field amplitudes to detect resonances at each $k_{||}$ value and are shown in figure 8.23. The tapered (2.25° and 0.91°) and undercut (-2.25°) nanorods follow the trend expected from the experimental data and the index guiding mechanism, where there is little evidence of Bloch effects for a positive (tapered) sidewall angle and Bloch effects are seen for the negative (undercut) angle. The effects disappear quickly with an increasing sidewall angle; for example, little remains with a positive 0.91° sidewall and there is no band formation with a positive 2.25° sidewall. However, the nanorods with the vertical sidewalls also clearly exhibit Bloch-like behaviour, which cannot be due to index guiding in the nanorod region, as there is no spacer region of lower dielectric fill, so must be due to a different mechanism.
8.4.3 Lossy Fresnel reflection

Previous theoretical simulations of nanorod arrays in GaN with vertical sidewalls have suggested operation in a Bloch-like regime [214]. In ref. [214], the confinement mechanism is ascribed to non-total or ‘lossy’ Fresnel reflection at the interfaces above and below the nanorod region, leading to enough field overlap with the nanorods for the Bloch term to become dominant. This can arise in two ways: in both, the optical confinement requires lossy Fresnel reflection at the interface between the nanorods and the higher index GaN buffer slab, but at the upper interface between the nanorods and the superstrate the reflection could be lossless due to total internal reflection or it could be lossy from Fresnel reflection. The confinement arising from the lossy Fresnel reflection mechanism will therefore critically depend upon the reflectivity of the interface at the base of the nanorods. In theoretical work, such as the FDTD results presented in figure 8.23 and those in ref. [214], all the interfaces (including the nanorod sidewalls) are ideal with no surface roughness to reduce their reflectivity, which will prevent any losses from scattering. The experimental samples investigated have varying degrees of roughness in different parts of the structure, particularly at the interface between the nanorods and the underlying GaN buffer region.

In order to examine whether this lossy Fresnel reflection mechanism can cause Bloch
mode formation, a process was developed for fabricating arrays of quantum disc nanorods with as little roughness as possible. A sample was fabricated on a wafer fragment, and two regions of the sample are shown in the oblique SEM images in figure 8.24. To create this sample, a nanorod array was patterned and ICP etched to a depth of \( \approx 1800 \text{nm} \) using the method described above and then wet etched for 6 hours in a solution of 25\% AZ400K (a buffered KOH based developer) and 75\% water by volume. The solution was heated to 60\(^\circ\)C in a vessel submerged in an oil bath to minimise disturbance of the solution by convection currents. It was found that disturbance of the solution, through stirring or from the temperature gradient present when heating with a planar hot plate beneath, produced tapered nanorods. This process produced regions of nanorods with sidewalls very close to vertical, such as that shown in figure 8.24a, which varied towards a more tapered shape in other regions, as in figure 8.24b. Whilst the interface between the nanorods and the GaN buffer slab is faceted, it is quite smooth. Angular PL revealed a feature very similar to a slab mode with \( n_{\text{eff}} \approx 1 \) in figures 8.25 and 8.26, but with anticrossing features indicative of Bloch effects, shown in the insets. This mode was only present for the blue quantum well emission from the region with vertical sidewalls and not observed for the yellow emission, which in such narrow nanorods (diameter \( \approx 40-50 \text{nm} \)), predominantly comes from the slab. This mode was not present in the tapered nanorod regions, supporting the conclusions of the FDTD simulations in figure 8.23.

For the mini gap between the two bands producing the anticrossing to appear, there must be a difference in the overlap of the optical field with the dielectric when compared between the fields of the two bands. As the dielectric fill fraction is so low, of the order of 2.5\%, this anticrossing shows that there must be a significant overlap of the associated Bloch mode with the periodic region to produce this change in the overlap with the dielectric between the two bands – the dispersion of a Bloch mode of infinite nanorods with a fill fraction this low is very close to that of a homogeneous slab mode with \( n_{\text{eff}} \approx 1 \). Indeed, a good fit with an infinite 2D MPB model (described above) for these thin nanorods was achieved, demonstrating that the sample behaves in a strongly Bloch-dominant regime for the blue emission. The structure likely provides very good conditions for Fresnel confinement as the light trapped in the Bloch mode will have a phase velocity close to parallel with the effective slab interfaces of the nanorods because the slab-approximate \( n_{\text{eff}} \) of the mode is close to the volume-averaged refractive index of the material. There is a high refractive index contrast between the volume-averaged nanorods and the GaN buffer layer, which will produce a favourable Fresnel coefficient for light meeting the interface at angles near 90\(^{\circ}\) to normal incidence. Unfortunately, experiments on nanorod arrays with a higher fill fraction to investigate this effect were not possible as a shorter wet etch time could not produce rods which were as vertical or as smooth for reasonable comparison. It
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(a) Vertical sidewalls.  
(b) Tapered sidewalls.  

**Figure 8.24:** Oblique SEM images of slow-etched quantum disc nanorods.  

**Figure 8.25:** Angular PL collected along (left) $\Gamma M_{ca'}$ and (right) $-10^\circ$ from $\Gamma K_a$ from the vertical-sided quantum disc nanorod array.  

**Figure 8.26:** Single frequency intensity variation at 437.5nm ($k_0=1.44\times10^7\text{m}^{-1}$), projected into reciprocal space, where $k_x$ is parallel to the $\Gamma K_a$ direction from the vertical-sided quantum disc nanorod array. The white oval feature is due to direct diffraction of the long wavelength tail of the exciting laser.
is not clear if the mode undergoes total internal reflection at the nanorod-air interface, but it seems likely due to the low refractive index contrast, which will lead to a low reflection coefficient if above the critical angle.

The light cannot be confined by index guiding at the interface between the nanorods and GaN buffer layer owing to the nanorod shape and the observed Bloch mode is only present for light emitted from the quantum well inside the nanorods. Therefore, these results provide strong experimental evidence that the lossy Fresnel reflection mechanism can confine light sufficiently to the periodic region for Bloch effects to become apparent when the surfaces are smooth enough, although it is not clear to what extent this is possible for higher dielectric fill fractions.

8.4.4 Discussion

Both the index guiding and lossy Fresnel reflection mechanisms for confinement of light to the nanorod region are required to fully explain all the experimental observations from the core-shell devices. The band structure for the blue-green emission originating from the top of the rods in sample CS3 (figure 8.16a) is very similar to that of CS2 (figure 8.15a), and is caused by confinement of the blue-green light to the periodic nanorod array. The blue-green light is emitted near the top of the rods, where it is confined by index guiding to the periodic region of higher dielectric fill, thus forming Bloch modes. The yellow light is emitted from all regions of the nanorods, and will not primarily originate from within the index guiding region near the top of the rods, but the Bloch effects remain in the yellow only for CS2 and not for CS3. The only difference between these samples which can be discerned is that the different passivation process applied to each before growth has led to the base and lower part of the nanorods being much rougher in CS3 than in CS2, seen in figures 8.15b and 8.16b respectively. This would critically affect the reflectivity of the interface between the nanorods and the GaN buffer layer in these samples and therefore the efficacy of confinement through lossy Fresnel reflection. The lossy Fresnel reflection mechanism is therefore considered to be responsible for the difference in the behaviour of the yellow emission between CS2 and CS3.

Some slab-like effects are visible in the background of the data, for example around \(k_0 \approx 0.95 \times 10^7 \text{m}^{-1}\) and \(k_\parallel \approx 0.4 \times 10^7 \text{m}^{-1}\) in figure 8.15a, and it is likely that these primarily Bloch-like modes may have some overlap with the slab region [214] as well as significant overlap with the regions at or near the base of the rods. This explains why only homogeneous slab behaviour is seen for the yellow emission in CS3 in figure 8.16a, as any modes with significant overlap with the lower part of the nanorods will also overlap the rough region and undergo more scattering. There is therefore a high loss factor and so no far-
field Bloch features to observe for the yellow light. The contrast enhancement techniques applied will instead reveal the much lower contrast features from diffraction of homogeneous slab modes for CS3, which are assumed hidden behind the higher contrast Bloch features from CS2. It is also possible that a larger proportion of the yellow light in CS3 originates from the slab region which can readily couple to the homogeneous slab modes – the rougher interface may scatter a significant amount of the exciting laser light into guided slab modes where it can be absorbed over a much larger distance.

The Bloch features for CS3 (figure 8.16a) for the blue-green emission are of much lower contrast than CS2 (figure 8.15a). This is thought to be due to increased scattering and decreased reflectance by the rough interface at the bottom of the rods of downward-directed light which has been folded out of index-guided states and is destined for extraction. There may also be some increased Fresnel confinement of the blue-green light in CS2, particularly for those states which are not index guided, although this is thought to be insignificant as the behavioural change seen for the yellow emission between the two samples is much more substantial. CS4 (figure 8.17) has a very rough region near the area of high dielectric fill, causing scattering from the guided modes and also reducing the contrast of the features compared to CS2. There are still Bloch effects present in CS4 for the blue-green emission even with this roughness, suggesting that the index guiding mechanism is more resilient to roughness than the lossy Fresnel reflection mechanism.

8.4.5 Summary

Experiments were performed which show that both the index guiding and lossy Fresnel reflection mechanisms can lead to the optical confinement required for Bloch mode formation. The difference in behaviour between otherwise comparable quantum disc nanorod structures both experimentally (figures 8.19 and 8.20) and using FDTD simulations (figure 8.23) shows that index guiding is able to provide a mechanism for formation of Bloch modes. A slab waveguide model using a volume-averaged index for the nanorod region is able to determine if there is likely to be enough confinement for Bloch mode formation. Bloch modes were also observed in FDTD simulations (figure 8.23) and experimentally in samples with vertical sidewalls (figure 8.25), where the index guiding mechanism cannot be present. The dispersion of the Bloch modes formed in the core-shell structures was fitted without requiring a complex 3D model of the structures, instead using a simple 2D infinite-nanorod model run with freely available software.
8.5 Core-shell LEDs with a confining underlayer

To make use of both the index guiding and lossy Fresnel reflection confinement mechanisms, a second generation of top-down core-shell devices was fabricated by Dr E. Le Boulbar and Dr P-M. Coulon using a similar process to that described above, but employing a different passivation process. The structure of the planar GaN wafer before patterning is shown on the right side of figure 8.27. It consists of a bulk GaN layer with ≈200nm graded AlGaN and then pure ≈200nm AlN underlayers grown on a silicon substrate. The AlN and AlGaN layers exist as a nucleation layer optimised for allow growth on the silicon substrate, but will double as an index guiding layer due to the lower refractive index of AlN and AlGaN compared to GaN. The nanorods were etched through to the silicon substrate before the overgrowth of the shell layers and the as-etched silicon surface is smooth. Figure 8.27 shows a cross section SEM image of a representative sample, which shows that the regrown facets on the sidewalls are highly vertical and smooth, which will minimise scattering losses, and the tops of the nanorods are flat. Notably, the horizontal surfaces between the nanorods are very smooth to form a reflective silicon substrate, which will act to maximise confinement of light through the lossy Fresnel reflection mechanism when the light is not totally internally reflected. Additionally, the nucleation/confining layers are seen to have a lower dielectric fill than the rest of the rod as lateral regrowth was inhibited on the AlN and AlGaN layers as well as the silicon. An estimate of the volume-averaged refractive index profile was calculated from the SEM images using (7.7) and is shown in figure 8.27. It is clear there is a wide region of higher refractive index in the nanorods for index guiding to occur. In other words, both mechanisms for optical confinement to the periodic nanorod layer should operate in these structures.

![Cross section SEM and volume averaged refractive index profile of the core-shell samples grown on a silicon substrate.](image-url)
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The PL spectrum at normal incidence is shown in blue in figure 8.28 where there are significant peaks seen over the background emission. These resonances dominate the PL spectrum, in contrast to the previous core-shell samples where no such sharp peaks are observed, shown in dashed red on the figure for reference. The origin of these peaks becomes apparent upon examination of the angular PL from this core-shell structure presented in figure 8.29, where an abundance of bands of Bloch modes is observed, correlating with the large peaks in the spectrum measured at normal incidence. These Bloch features appear sharper than those previously observed, for example in figure 8.15a, indicating lower loss from the Bloch modes. The data show that the core-shell LEDs with the confining underlayer and smooth silicon substrate support substantially stronger Bloch resonances than previously achieved with the shaped rods. This performance is remarkable given that the confining layer used was optimised for its performance for GaN growth on the silicon substrate, rather than designed specifically for its waveguiding properties. The sharpness and intensity of the features is likely due to the increased confinement offered by the combination of the index-guiding layers, the reflective silicon substrate and the smoothness of the physical structures. It may also be as a result of the high verticality of the sidewalls. With the more variable fill fraction that arises with lower verticality, such as that seen previously in sample CS2 (figure 8.15b), the resonance of the Bloch mode may be weakened and more spread out in frequency due to a variation of the optical field energy overlap with the dielectric with vertical position.

Angular PL taken over both varying inclination and azimuth for a single wavelength is shown in figure 8.30a and bears a remarkable resemblance to that predicted by David et al. [214], yet there are two significant differences. First, the nanorod array has a completely different pitch and the states observed experimentally are viewed inside the air cone. The ring-like feature around the centre of the plot which is interrupted by anticrossings and has a slab-equivalent $n_{\text{eff}}$ of approximately 0.75 (a radius of 75% that of the air cone), correlates with what is termed a quasi-guided mode confined through lossy Fresnel reflection with $n_{\text{eff}} \approx 1.6$ in the study by David et al. at the pitch they investigated. Figure 8.30b shows a frequency where there is a similar mode but with a much reduced radius ($\approx 0.05$). Here, the feature is ellipsoidal due to the distortion in the hexagonal lattice, and there are many other states which do not display similar slab mode-like properties. An interpretation of these circular features to be slab-like modes implies that the lossy Fresnel confinement mechanism is significant even inside the air cone for their $k_\parallel$ within the first Brillouin zone. This seems unlikely as there will not be total internal reflection at the nanorod-air interface and the angle of propagation at the base of the nanorods will be too close to normal incidence for a strong Fresnel reflection. Additionally, light
Figure 8.28: Photoluminescence at normal incidence observed from the core-shell structures grown on silicon, compared with sample CS2, excited with a 405nm laser diode.

Figure 8.29: Angular PL from the core-shell sample on a silicon substrate along (left) $\Gamma M_{bc'}$ (right) $\Gamma K_a$ with MPB simulation of infinite nanorods.
Figure 8.30: Single frequency intensity variation of the core-shell sample on a silicon substrate, projected into reciprocal space, where $k_x$ is parallel to the $\Gamma K_x$ direction. 180° of data have been collected and tiled.
trapped in the mode with the very small radius in figure 8.30b will be travelling very close to vertical in the structure, all of these factors leading to small coefficients of Fresnel reflection. Indeed, in figure 8.30a, there appears to be a Fabry-Pérot fringe visible as a broad ring of higher intensity about halfway between the centre and the edge, suggesting that these resonant states travelling close to vertical are present and very lossy. It is likely that in these structures the slab-mode-like states are vertically confined to the nanorods in other Brillouin zones outside the air cone due to the large pitch in comparison to the wavelength, before becoming observable after a proportion of the trapped optical power is folded to the air cone. This shows that these ring-like features are due to the properties of the 2D tiling, and only act as a helpful example for illustrating the vertical confinement mechanism rather than representing the typical behaviour.

The fit with an infinite nanorod array model using MPB is shown in figure 8.29. This model cannot include any vertical resonance effects, and once again aligns closely with the modes present. As a result, it seems that the dispersion in these tall nanorod array structures is defined by the tiling itself. Whilst the vertical resonances in the structure provide the mechanism for the Bloch modes to form, they do not provide more than a perturbation of the frequency of the Bloch modes, without affecting the amplitude of the in-plane wavevector.

The fit with the simulated infinite nanorod array is excellent, apart from a replica of the features at a slightly higher frequency in the experimental data. This replica is believed to be due to a higher order vertical resonance in the experimental structure; that is, a field pattern in the vertical direction with a larger number of antinodes than the features which are well fitted, but with the same in-plane field pattern that gives rise to the dispersion of the Bloch mode. For these higher order replicas, the field is less well confined in the vertical direction, leading to an increased overlap with air at the top of the nanorods which in turn produces the observed increase in frequency.

In order to examine this further, FDTD simulations were performed to investigate the effect of increasing the height of vertically sided nanorods, and the results are shown in figure 8.31. In the shortest rods, no sign of replicas is seen, but as the height is increased, a second copy of the fundamental band begins to appear. The appearance of a higher frequency replica of the resonances is found only in the taller structures, which are expected to be able to support more vertical resonances. There is also a decrease in the frequency of the fundamental for each band with increasing nanorod height as the vertical field overlap with the dielectric will increase for resonances with more energy confined to the nanorods. These simulations provide further evidence that vertical resonances in structures only supporting lossy Fresnel confinement just act to perturb the band structure rather than defining where the resonances appear.
To investigate further the band structure of the Bloch modes, another set of growths was performed. The filling fraction was varied by varying the growth time of the outer GaN capping layer with an additional 15, 30 or 60 minutes extra, along with a control sample with no extra growth. The vertical structure of the 0, 15 and 30 minute samples were very similar and the nanorod diameters were measured to be $\approx 318\,\text{nm}$ for the control and $\approx 338\,\text{nm}$ for the sample with 30 minutes extra growth, corresponding to $A_{FF}$ around 0.7. Angular PL measurements along the $\Gamma \mathbf{K}_a$ direction from the 0 and 30min samples are shown in figure 8.32a and the spectra at normal incidence of the two samples after normalisation is compared in figure 8.32b. The wavelength of one of the bands at normal incidence for all three samples is shown in figure 8.33. It is clear that the bands of the Bloch modes are shifted downward in frequency and the resonances at normal incidence upward in wavelength with the extra growth (decreasing $A_{FF}$), caused by an increase in the overlap of the modes with the higher volume of dielectric. Thus, the dispersion of the Bloch modes in these structures can be designed using a simple and fast 2D model, and then tuned to the desired location by controlling the fill fraction carefully to take into account factors not present in the model.

The extra growth on the sample that underwent an additional 60 minute growth time
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(a) Angular PL taken along $\Gamma K_a$ for (left) no extra growth (right) 30mins extra growth.

(b) Normal incidence spectrum, after normalisation as described in chapter 6.

**Figure 8.32**: Effect of filling fraction on the band structure of the Bloch modes for 0min and 30min extra growth time of the outer GaN capping layer.

**Figure 8.33**: Effect of extra growth time on the wavelength of the resonance at $k_0 \approx 1.3 \times 10^7 \text{m}^{-1}$ at normal incidence.

(a) Angular PL collected along $\Gamma K_a$.  

(b) Cross section SEM

**Figure 8.34**: Sample with 60min extra growth time of the outer GaN capping layer.
for the GaN capping layer produced nanorods with less vertical sidewalls due to the emergence of another facet towards the AlGaN layer, shown in cross section in figure 8.34b. There was increased growth on the AlGaN and AlN nucleation layers, which led to rougher surfaces at the base of the nanorods. These structural changes are reflected in the angular PL shown in figure 8.34a, where the bands are much less distinct than those with the smoother and more vertical sidewalls (figure 8.32a). The change in shape with the new facet will vary the fill fraction with vertical position in the nanorod, leading to a broadening of the resonances, and the increased roughness will increase scattering losses of the Bloch modes. For best performance, an optimised fabrication procedure therefore needs to maintain vertical sidewalls over the confinement region and smooth facets in addition to strong index guiding at the lower interface of the quasi-suspended slab formed by the nanorods.
8.6 Conclusion

Arrays of nanorod LEDs have shown significant photonic crystal effects, operating in a Bloch-mode dominated regime, and have been shown to fit well with the modes supported by a simple infinite two-dimensional dielectric-rod structure. The Bloch effects dominate when there is sufficient vertical confinement of the optical field to the region with in-plane periodicity compared with homogeneous slab regions. When there is not sufficient confinement to the nanorod region, arrays of nanorod and core-shell LEDs operate in the diffractive regime. The confinement necessary for Bloch mode formation can be achieved through index guiding, lossy Fresnel reflection at at least one interface, or both index guiding and lossy Fresnel reflection acting together. Once there is sufficient optical confinement, the source can be placed inside the periodic region to preferentially excite the Bloch modes supported by the structure.

Index guiding can be achieved where a layer of higher dielectric fill with a higher volume-averaged refractive index creates a quasi-suspended photonic crystal slab separated from any planar regions by a layer of lower dielectric fill. For example this occurs in a nanorod array with shaped sidewalls, or when a layer of a lower refractive index material is added, or a combination of both. Shaping the sidewalls presents significant advantages to practical devices in the III-nitrides, as it does not require compromising the optimised epitaxial layer structures necessary for fabricating high performance devices, e.g. by adding mismatched layers of a different refractive index. However, if the epitaxial structure does contain a layer of lower refractive index such as epitaxial AlN nucleation layers on silicon, these can be used to create the necessary index profile.

Lossy Fresnel reflection refers to the situation where there is not true waveguiding through total internal reflection, but instead the Fresnel reflection coefficients are high enough to confine a significant proportion of optical power to a layer in a quasi-guided mode. This operating mechanism has been predicted previously and by FDTD simulations performed as part of this work, but it is more challenging to implement in practice due to the high reliance on the smoothness of the Fresnel interface and the detrimental impact of roughness on the reflectivity.

Surface roughness and variation of the vertical profile of the nanorods in the confinement region has been experimentally observed to lead to broadening and reduced contrast of the Bloch modes. Further, FDTD simulations have shown that even a slightly tapered sidewall profile causes the Bloch effects to disappear. These non-ideal characteristics must be controlled or accounted for to create structures which perform as expected.

The findings from this investigation show that it is possible to manifest Bloch effects
previously only observed in suspended air-hole photonic crystal membranes over large areas of dielectric rod-in-air structures which cannot be suspended. These nanorod structures allow electrical contacting, good heat dissipation and high utilisation of the substrate via their large surface area-to-footprint ratio, giving scope for future exploitation in practical devices.
Chapter 9

Directional emission from photonic crystal LEDs

9.1 Introduction

Previously, photonic crystals (PhCs) have facilitated more directional emission than alternative light extraction techniques, as was discussed in §4.4. The mechanism of choice for previous attempts to improve the directional emission from PhC LEDs is through control of the optical slab modes in the device, with the PhC lattice chosen to preferentially diffract light to surface normal. For ideal operation, this design requires a thin waveguide containing the active emitting region to confine the light to a single slab mode, and practical devices have relied upon a metallic reflector on one side of the guide [217, 264]. As shown in chapter 7, the buried PhC configuration offers a way to confine light to specific guided modes which does not rely on an absorptive reflector and may provide an alternative way to exploit the design. §9.2.1 of this chapter considers whether the buried PhC configuration is suitable for use to create directional emitters in the weak regime.

The best published results for directional emission from experimental photonic crystal LEDs operating in the diffractive regime (≈12% of power within 30° of normal incidence) [112] fall short of the theoretical maximum performance (50% within 30°). They offer only slightly improved performance for étendue-limited applications over the best encapsulated surface-roughened devices exhibiting Lambertian emission at high extraction efficiency. The theoretical maximum value of 50% may be unrealistic as it is reached by a simple calculation which only considers a single emission frequency and assumes that all light trapped in a mode can be extracted by the desired diffraction order and PhC lattice. The practical constraints on the maximum performance possible in the diffractive regime are considered in §9.2.

Operation in the Bloch regime has been shown to be possible in large-area devices in chapter 4.1 by creating a quasi-suspended PhC slab, and may allow the design proposed by Fehrenbach et al., which operates in the Bloch regime, to be realised [218]. This
design was predicted to extract 80% of the emitted power inside a half angle of 0.2° from normal incidence for a single frequency. The latter part of this chapter considers whether the design proposed by Fehrembach et al. can be implemented in the III-nitride material system using quasi-suspended photonic crystal slabs, and compares the performance of this approach with the diffractive regime.

9.1.1 Étendue

The étendue (\( \hat{E} \)) of a component describes the spatial and angular limits of the light which the component or system emits or collects and is therefore closely related to the area (\( A \)) and numerical aperture (\( NA = n \sin \theta \)) of the component. It is given by

\[
\hat{E} = \pi An^2 \sin^2 \theta
\]

(9.1)

for rotationally symmetric emitters, where \( n \) is the refractive index of the entrance/exit medium of the component and \( \theta \) the half-angle of collection [265]. The total luminous flux throughput (\( \Phi \)) of an optical system is related to the luminance (\( L \)) and étendue by

\[
\Phi = \eta_{sys} L \hat{E}
\]

(9.2)

where \( \eta_{sys} \) represents the efficiency of the transfer of optical power through the system [87]. The luminance of the source will therefore affect the quantity of optical power which can be coupled through the system; a source with the same area but higher luminance will emit more light which can be made use of.

For application-specific optical systems, the étendue of the light source (\( \hat{E}_{src} \)) should be matched to the optical system to use the light emitted optimally [87, 265, 266]. There are likely to be specific components in the optical system, for example, the imager in a projector, which limit the étendue of the system due to physical, operational or cost constraints on their construction. The efficiency of the light source in the application will be impacted if \( \hat{E}_{src} \) is higher than that of the optical system, as light will be emitted which cannot be coupled through the system and is therefore wasted. In the opposite case where \( \hat{E}_{src} \) is lower, there is more flux throughput available due to (9.2). As a consequence, the performance of the system can be improved by increasing \( \hat{E}_{src} \) up to the system étendue and further then only by increasing the luminance \( L \) of the source. For an LED source of fixed size, increasing \( L \) is in principle possible simply by increasing the drive current to increase the total light output. This comes at the cost of increased heatsinking requirements, further complicated by efficiency droop, leading to a practical upper limit to \( L \) through increasing drive current and compromising the system efficiency for a given source.
From (9.1), the source area, refractive index and half-angle of collection of the source emission by the optical system will all impact the ability to use the light emitted as they determine $\mathcal{E}_{\text{src}}$. Changing the source area provides the most straightforward way to match the source with the system étendue to get best flux throughput ($\Phi$) performance. Unintuitively, hemispherical encapsulation to increase total light extraction offers only a disadvantage – the encapsulation will act to effectively magnify the source area from the point of view of the optics, increasing $\mathcal{E}_{\text{src}}$ by a factor of $n^2$ for an encapsulant with refractive index $n$. Reducing the half-angle of collection allows $\mathcal{E}_{\text{src}}$ to be decreased, allowing a corresponding increase in the emitting source area $A$ which can be used, but obviously does not make use of any light which is not collected. For a Lambertian emitter, the luminance is constant at all viewing angles for fixed drive current and so no flux advantage can be gained by either encapsulation or reducing the collection angle, even at the expense of efficiency. However, the luminance is not constant for a directional emitter – it will be higher for at least some values of $\theta < 90^\circ$ than for all the emission and so therefore directional emission allows improvement to be made through the increase in $L$ for forward directions and the $< 90^\circ$ collection angles of optics in practice.

Typical collimation optics used are unable to collect at 100% efficiency up to $\theta = 90^\circ$ [266] and they must be made large compared to the source to collect from large half-angles [267], adding cost and bulk to the end system. With increased forward luminance it becomes more practical to use a smaller collection angle as less light is wasted, allowing collection losses and the size of optics to be reduced, considerations of particular interest to miniature optical systems such as compact and battery powered projectors. Where product size is not a concern, higher flux performance can be achieved with directional emitters by increasing the emitting area while still matching the étendue of external optics due to the reduction of the collection angle, instead of needing to increase the size of expensive components such as imagers in projection systems.

### 9.1.2 Quantifying directional emission

When considering the optimisation of a device for applications requiring highly directional emission there are two figures-of-merit that are useful to consider. The first is the directivity ($D$) which expresses the ratio of the light power emitted to the air cone ($P_{<\theta}$) within a given angle $\theta$ from normal incidence to the total light emitted to the air cone ($P_{\text{air}}$),

$$D = \frac{P_{<\theta}}{P_{\text{air}}}$$  \hspace{1cm} (9.3)

Directivity is a useful measure only for applications requiring minimum spill outside the desired emission where using an aperture is not possible, but it is widely used as a figure-
of-merit for the performance of directional devices because it is easily measured from polar intensity patterns.

The second quantity is the total power emitted within the given half angle, $P_{\theta}$, which is more challenging to measure directly and depends on the wall plug efficiency and the drive power, but gives a direct measure of the useful optical power available and can be related directly to radiance\(^1\). Due to the dependence on the drive power, the efficiency of emission $\eta_{\theta}$ within half-angle $\theta$ is referred to below as $P_{\theta}$ normalised to the total power ($P_{\text{total}}$) under consideration, for example just the power in a single guided mode, or all the power emitted in the device, including that which does not escape.

$$\eta_{\theta} = \frac{P_{\theta}}{P_{\text{total}}}$$

(9.4)

For applications which require control of all the light emitted, the directivity is a useful measure as it provides information about all the emitted power, but in the case of applications such as projection, which require the power at normal incidence to be maximised and can make use of apertures in the optical system to block unwanted light flux, $\eta_{\theta}$ is a much more useful parameter. Control of both the directivity and the power within a half-angle from normal incidence are discussed below.

\(^1\)Which can then be converted to luminance using the photopic luminosity function.
9.2 Diffraction of guided modes for directional emission

In the ideal and most basic case, a single-moded slab waveguide is set up adjacent to a PhC, with the PhC pitch $a$ chosen to diffract the mode to normal incidence at first order,

$$k_\parallel = \frac{2\pi}{a}$$  \hspace{1cm} (9.5)

producing a single wavelength far-field emission pattern similar to the reciprocal space projection shown in figure 9.1 for a hexagonal PhC. The PhC operates in the weak or diffractive regime, where the behaviour of the slab waveguide is not affected significantly by the presence of the PhC and so the guided modes are diffracted as arcs in reciprocal space. This is due to the circular in-plane rotational symmetry of the waveguiding medium and is discussed in §3.2.1. As an additional consequence of this symmetry, there will be an equal amount of power guided in the mode in each in-plane azimuthal direction, so the energy emitted inside an area of interest in reciprocal space, such as the air cone, will be proportional to the angle subtended by each arc inside that space. It can also therefore be seen that the proportion of power inside an area of interest is independent of the order of rotational symmetry of the PhC as this relation applies to diffraction from each reciprocal lattice point.

![Figure 9.1: Ewald construction for a single mode with $k_\parallel = \frac{2\pi}{a}$ chosen to diffract to normal incidence in a hexagonal PhC lattice, shown in red. The green circle represents the air cone and the blue dashed circle 30° from normal incidence in air.](image)

9.2.1 Experimental directivity enhancement in photonic crystal LEDs

The buried photonic crystal device arrangement considered experimentally in chapter 7 confines light to guided modes, which are then diffracted to the air cone. When the pho-
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tonic crystal is made deep enough, light is confined in a small number of modes in the cap layer above the photonic crystal. These cap layer modes combined with diffraction by the photonic crystal offer the mechanism for enhancing the directivity of emission discussed above and so existing experimental samples allow some investigation of the approach.

The experimental device with the 600nm thick cap layer and 1300nm deep photonic crystal is chosen as it was shown to offer the most confinement to the cap layer modes. Figure 9.2 shows the polar emission measured from electroluminescence after integration over wavelength and 30° of azimuth, where the behaviour is close to Lambertian, but with slightly enhanced emission at ≈±10° from normal incidence due to the presence of diffracted guided modes at the emission wavelengths. The optimal situation shown in figure 9.1 is not satisfied for the device emission, which is centred at approximately 455nm, but is satisfied for diffraction of the second order mode for emission at 485nm, as shown in figure 9.3. Using the algorithm described by equation (6.3), the wavelength dependence of the emission can be removed and convolution with the desired emission then performed to give an indication of the performance of a practical device emitting at this optimal wavelength. Figure 9.4 shows the effect of this process on the polar emission for Gaussian emission with 30nm FWHM, which is similar to the original emission width of the experimental sample, and for 10nm FWHM, chosen to represent an upper limit of what it might be possible to realise. At 30nm FWHM, an intensity enhancement of ≈5% at normal incidence is observed in the polar emission in figure 9.4a when compared with the experimental pattern, which is a small, but potentially useful increase. For a narrower QW peak of 10nm FWHM, then this enhancement could be much greater as in figure 9.4b.

The polar emission plots in figure 9.4 show two features, which are the combination of a Lambertian pattern from emission directly to air and a pronounced peak at normal incidence due to the diffraction of guided modes. The photonic crystal is not optimised for best extraction and the second order mode is diffracted to the air cone by multiple diffraction orders, limiting the power in the pronounced peak and the enhancement to the directivity. In an optimised device with a thinner cap layer designed so that only a single mode is significantly excited, along with a photonic crystal pattern tailored for a higher extraction efficiency; it is expected that the power in this peak can be increased substantially.

This experimental sample was not designed to represent the ideal case and its effectiveness is limited as a result, but despite this, improvement in directivity over Lambertian emission is seen, showing that the buried photonic crystal device design is a likely candidate for enhancing directivity through controlled extraction of guided modes by diffraction.
Figure 9.2: Polar emission integrated over all azimuthal directions for an LED with a 1300nm deep buried photonic crystal.

Figure 9.3: Single wavelength emission at 485nm for a device with a 1300nm deep buried photonic crystal and 600nm capping layer. The second order cap layer mode is diffracted to normal incidence.

Figure 9.4: Polar emission integrated over all azimuthal directions for an LED with a 1300nm deep buried photonic crystal. Emission peak modelled at 485nm centre wavelength with varying FWHM.
9.2.2 Performance limitations

For the performance of both directivity \( D \) and the extraction efficiency inside a half-angle from normal incidence \( \eta_{<\theta} \), the emission of power into substrate, superstrate and guided modes must be considered. For \( D \), emission of power into states other than the desired guided mode must be minimised to avoid diluting the directional emission pattern created by diffraction of the guided mode. The overall extraction efficiency will have no effect on \( D \) as only the light which is extracted is considered. In contrast, the extraction efficiency is a significant concern for \( \eta_{<\theta} \) because as much as possible of the total power emitted in the device needs to be extracted inside \( \theta \). Any power not emitted to the intended mode is power which cannot be extracted through the optimal channel, so the power emitted into the ideal mode must be maximised. However, power emitted from other origins is not wasted as that inside \( \theta \) will contribute to \( \eta_{<\theta} \). In both cases, the ratio of the total power emitted into the guided mode and the extraction efficiency of that mode are significant limiting factors. Due to the many possible device configurations, the performance of the ideal case of a single slab mode is considered for the diffractive approach, leading to an upper limit of what might be achievable to \( D \) and \( \eta_{<\theta} \). The upper limit to \( D \) in a multi-moded approach has previously been considered in detail to be \( \approx 32.5\% \).

The directivity that can be achieved using the weak regime to diffract light from a single mode is limited as power from slab modes with azimuthally-invariant \( k_{||} \) will always be diffracted to all angles from normal incidence, as can be seen in figure 9.1. This is discussed by Wiesmann et al. who consider the ideal case for a single mode \[ D_{\max} \approx \sin \theta \] (9.6) where the directivity function \( D \) is given by the ratio between the arc length within the half-angle of interest and the total arc length inside the air cone, as discussed above. \( \eta_{<\theta} \) requires consideration of power which is not in the air cone, and will be discussed later – (9.6) sets an upper limit to the maximum \( \eta_{<\theta} \) achievable if all the power in the mode can be extracted. Figure 9.5a compares the ideal situation of (9.6) with Lambertian emission graphically from e.g. a surface roughened device where \( D = \sin^2 \theta \).

The relation (9.6) gives a figure that makes a number of simplifications about the operation of the device in order to produce an upper limit and so how a practical implementation might impact the performance will now be considered. The ideal case makes several assumptions: a single mode is present, a single emission wavelength is considered, there is no loss to other diffraction orders and there is no emission directly to the air cone, all of which will be highly dependent on the device configuration and so the feasibility of
which will be specific to the device design. However, it is possible to consider the likely
effect of other modes and non-zero emission linewidth in general.

In the ideal case, the PhC is designed so that the mode is diffracted to normal incidence.
This situation will only be accurate for a single frequency as both components defining
the radius of the mode’s diffraction arc \( k_{\|} = n_{\text{eff}} k_0 \), where \( n_{\text{eff}} \) is the effective index of
the mode, will change with frequency. An example of the consequence of detuning the
emission from the ideal frequency is shown in red in figure 9.5a for a radius 90% of the ideal
\( k_{\|} \), where the effect is most detrimental to extraction near normal incidence. To cause
this change in practice, \( n_{\text{eff}} \) will vary slightly as the confinement of the mode changes and
due to material dispersion, but the significant variation will be from the variation of \( k_0 \)
directly with frequency and so \( \Delta_0 \) and \( \eta_{<\theta} \) will be directly affected by the linewidth of the
emission. The solid lines in figure 9.5b show \( \Delta_0 \) for Gaussian emission with three values of
FWHM, where 30nm is considered representative of typical InGaN QW emission, centred
about a wavelength of 450nm. The dashed lines include the effect of dispersion of \( n_{\text{eff}} \) for
the first order mode in a 250nm thick GaN slab to give an indication of its possible effect.
The performance is only affected significantly within about 15° of normal incidence and so
dispersion and the variation of \( k_0 \) must be considered for highly-directional devices, but a
substantial improvement over Lambertian emission (≈3-fold within 15°) is certainly still
available for practical emission linewidths. The presence of additional guided modes will
also degrade the performance of \( \Delta_0 \) or \( \eta_{<\theta} \), particularly for smaller \( \theta \), in a similar fashion
by allowing emission to other channels which will reduce the proportion of the optical
power in the desired mode.

Only the order of diffraction used for extraction of the mode to normal incidence can
be allowed to diffract the mode to the air cone for ideal operation; lower or higher orders
will result in additional energy extracted at oblique angles impacting the performance. To
avoid this situation, the magnitude of the reciprocal lattice points \( |\hat{G}_{m_N}| \) of the order
\( (m_N) \) performing the diffraction of the mode to normal incidence \( (k_0 n_{\text{eff}} = |\hat{G}_{m_N}|) \) must
not be within \( k_0 \) of the magnitude of any other reciprocal lattice point,

\[
k_0 < ||\hat{G}_i| - |\hat{G}_{m_N}|| \quad \forall \; i \neq m_N
\]

referring to the notation defined in §3.2.1, specifically equation (3.5). Equivalently, if the
air cone is placed centred about any of the reciprocal lattice points of order \( m_N \), it must
not circumscribe any reciprocal lattice points of a different order. This can be expressed
more generally by removing the dependence on pitch \( a \) and \( k_0 \) using (9.5), which leaves a
constraint on \( n_{\text{eff}} \) to a minimum value for the mode specific to the chosen order \( m_N \) of
any reciprocal lattice

\[
n_{\text{eff}} > \frac{m_N}{m_i - m_N} \quad \forall \; i \neq N
\]

(9.8)
Choosing \( m_i \) to give the smallest denominator of (9.8) defines a maximum value for the right side of (9.8) for each order \((m_N)\), giving the lower limit for \(n_{eff}\) of the mode which can avoid diffraction of other orders degrading the performance of \(D\). Evaluating (9.8) for the Euclidean lattices shows this condition is very restrictive to low order modes in GaN slabs, where typically \(n_{eff}\) is between 2.1 and 2.5. Only the first order can be used for both Euclidean lattices; square lattices are a possibility for highly confined modes with \(n_{eff} > 2.44\), but the hexagonal lattice provides a good option as the condition is satisfied for \(n_{eff} > 1.37\) and it has good diffraction efficiency at the first order [164]. For quasicrystals, it is not possible to satisfy this condition completely due to the high density of weak intensity points in the reciprocal lattice, but once the strength of these points is taken into account and scaled for a given fill fraction, some tilings may be feasible. Once a suitable tiling is chosen, the pitch \(a\) is then set to diffract the mode directly to normal incidence according to

\[
a = \frac{\lambda_0 m_N}{n_{eff}}
\]  

(9.9)

For \(\eta < \theta\) performance, the constraints on the 2D lattice chosen for the diffraction are lifted somewhat because emission at oblique angles does not have such a detrimental effect as it does to directivity. This leads to a relaxation of the constraint (9.8) – diffraction due to other reciprocal lattice points of different order can now be allowed to diffract the mode into the air cone, as long as they, or points of the same order, do not diffract the in-plane directions within the half-angle from normal incidence to the air cone outside \(\theta\). More simply, a single route for diffraction from each in-plane propagation direction (before
diffraction) of the guided mode to inside \( \theta \) is required to avoid diverting power away from the intended extraction direction. Figure 9.6a shows how the maximum value of the angle from normal incidence \( \theta \) for which this condition is satisfied for the hexagonal tiling of the plane with reciprocal points \( m_N \) still depends upon a minimum value of \( n_{eff} \). This allows a broader choice of \( m_N \), which is less restrictive for smaller values of \( \theta \) as adjacent diffraction orders tend to be rotated in the reciprocal lattice.

However, for considering \( \eta<\theta \), all the power in the mode, whether extracted or not, must be accounted for – any power which cannot be extracted is lost and limits the performance. Recalling figure 9.1, the proportion of the in-plane propagation directions which can be extracted to the desired location due to each reciprocal lattice point is given by the ratio of the arc length within that location to the whole circumference of the mode in reciprocal space. The proportion of the in-plane directions which can be extracted, and so ultimately the proportion of the power \( (\eta<\theta) \), is therefore limited and defined by the order of rotational symmetry of the lattice. Figure 9.7 graphically shows how this ratio for \( n_{eff} = 2 \) and 2.5 changes with rotational symmetry, suggesting that photonic crystals with more rotational symmetry should produce better results for modes propagating in GaN layers. However, as the order of rotational symmetry is increased to increase \( \eta<\theta \) by this method, the angle of rotation between adjacent diffraction orders becomes smaller and avoiding the restrictions imposed by the single diffraction route condition becomes highly limiting. The effect is illustrated in figure 9.6b for the 12-fold \((3^6; 3^2.4.3.4; 3^2.4.3.4)\) quasi-crystal tiling described previously in figure 7.3.

### 9.2.3 Summary

The buried photonic crystal configuration operating in a decoupled regime is a promising vertical device structure as it is able to confine light to a small number of controllable guided modes without interaction with absorbing reflectors and may offer some small improvements as a result. However, an ideal single-moded device is likely to be challenging to realise as the confining waveguide would need to be very thin (\( \approx 100\)nm) and contain all of the active region to couple to the mode.

In the diffractive regime, the waveguide modes behave as if they are in an azimuthally-invariant medium, with no dependence of the in-plane wavevector on the photonic crystal tiling. As a result of this, guided light will propagate in all in-plane directions, leading to unavoidable extraction of power outside the desired location. This mechanism fundamentally limits the proportion of the power which can be extracted inside the half-angle \( \theta \) from normal incidence to \( \sin \theta \). The ideal performance of \( D<\theta = \sin \theta \) assumes that the device is single-moded and operates only at a single wavelength. For non-zero linewidth, the variation with emission frequency of the wavevector of the mode which the PhC extracts to normal incidence leads to lower directivity, especially for \( \theta<15^\circ \). Likewise, the spread
Figure 9.6: Maximum half-angle $\theta$ for which no in-plane direction of a guided mode diffracted inside $\theta$ is also diffracted to a different location in the air cone outside $\theta$. The guided mode satisfies (9.9) and has an effective index $n_{\text{eff}}$.

Figure 9.7: Limit to $\eta_{<\theta}$ of optical power emitted into the ideal mode as a function of PhC lattice rotational symmetry, assuming regular polygons in reciprocal space.
of wavevectors in a multi-moded approach will lead to a further reduction in performance, suggested to allow \( \approx 32.5\% \) emission inside \( \theta < 30^\circ \) after optimisation in ref. [112].

To avoid power in a single guided mode being extracted by another order away from the intended destination close to normal incidence, there is a minimum \( n_{\text{eff}} \) of the mode being extracted. This constraint limits the choice diffraction order to the first order for modes in GaN layers, and only the first order of the hexagonal lattice is able to extract a wide range of modes. In addition, the ability to realise high-performance devices by diffraction of slab modes is significantly limited by constraints on the geometry of the PhC lattice, which only allow a small range of \( n_{\text{eff}} \) of guided modes to be extracted optimally without dilution of power through diffraction to angles away from normal incidence. For a mode with \( n_{\text{eff}} = 2.5 \), only \( \approx 75\% \) of the power emitted into the mode can be extracted to air with a hexagonal lattice.

9.3 Ultra-directional LEDs: exploiting strong photonic crystal effects

The fundamental limitation of slab modes is not applicable in the strong photonic operating regime, as the in-plane wavevector is no longer constrained to an azimuthally-invariant value for each guided mode or photonic band, as demonstrated experimentally in chapter 8 and shown in figure 9.8. Highly directional emission was initially suggested by Fehrembach et al. using this approach in theoretical work considering very thin GaAs suspended nanohole PhC membranes [218]. Exploitation of the strong photonic regime to create highly directional LEDs and whether improvements to performance are possible over the weak regime for practical devices will be investigated in this section.

9.3.1 Principles of operation – breaking the weak limit

2D hexagonal lattice PhCs with infinite length can be designed to support either TE or TM band gaps (or no gap) through the choice of air holes or dielectric rods respectively, but complete gaps are not supported for GaN as a dielectric because the refractive index contrast between air and GaN is too low [137]. With finite size in the third dimension, as in PhC slabs, there cannot be frequency band gaps for all states as there will always be a continuum of states in the medium surrounding the slab (radiation modes), but frequency gaps for the guided states can exist. Figure 9.9 shows the band structure for a hexagonal air-hole PhC slab surrounded by air, where the \( y \)-axis represents the frequency by normalising the freespace wavelength \( \lambda \) to the pitch \( a \) and the \( x \)-axis represents the in-plane wavevector \( k_{||} \) around the edges of the irreducible Brillouin zone (IBZ), \( \Gamma \text{KM} \). The continuum of states in air are outside the black line, and the allowed states in-plane
Weak or diffractive regime showing diffracted slab modes.

Strong or Bloch regime showing azimuthally-dependent modes.

Figure 9.8: Experimental single wavelength plots of photonic crystal LEDs acting in the Bloch and diffractive regimes.

are shown in blue or red according to their polarisation state, which is discussed in more detail later, along with the details of the model used to generate the result.

Figure 9.9: Band structure around the edge of the IBZ for a 0.6\(a\) thick slab of dielectric \(\epsilon = 12\) with a hexagonal tiling of air holes of radius 0.3\(a\) suspended in air. The guided states exhibit a TE-like band gap; those not confined to the slab exist outside the black lines and are not shown.

The design suggested by Fehrembach et al. uses a suspended slab which is impractically thin (0.06\(\lambda\)) with a high refractive index (\(n = 3.5\)). The reason for a slab this thin is to create a complete band gap in-plane for all polarisations by cutting off the TM modes. Due to the suppression of TM emission for guided light in InGaN/GaN QWs, as discussed in §5.2.4, it should be possible to realise a device with a practical thicker PhC slab which
supports only a TE band gap, but still operates effectively under the same principle. The
design as presented by Fehrembach et al. also used a homogeneous dielectric substrate with
a significantly lower refractive index ($n = 1.5$) to confine the light in this slab. Though
this substrate is not likely to be feasible in an InGaN/GaN device as it will interfere with
the epitaxial layers and make electrical contacting highly challenging, the results from
chapter 8 demonstrate that it is possible to create a practical quasi-suspended photonic
crystal slab over a large area through from careful design of the PhC structure to confine
light in the periodic region. The experimental results were from arrays of nanorods, but
the optical confinement mechanisms will also be valid for arrays of nanoholes with the aim
of supporting a TE band gap.

Considering only the TE polarisation shown in blue, it can be seen from figure 9.9
that the highest frequency of the lowest band is where $k_{||} = K$, which is because it has
the largest magnitude of $k_{||}$ within the IBZ. At this frequency, this is the only available
photonic state trapped in the slab and so all TE-polarised guided light will be confined to
the K-point. Therefore, to manipulate the situation for emission out of the slab at normal
incidence ($\Gamma$ in reciprocal space), the state $k_{||} = K$ needs to be diffracted to $\Gamma$. Applying
this constraint to the vector form of the Bragg equation (3.4) gives

$$ \Gamma = K + \hat{G}' $$

(9.10)

The required diffraction can be achieved by a new grating with unit reciprocal lattice
vectors $\hat{G}'$ equal to the $\Gamma K$ vectors of the primary lattice, which can be seen when $\Gamma$ is
set to zero in (9.10) above\(^2\). As a result, this new secondary lattice to extract the light at
normal incidence shares the hexagonal symmetry of the primary one, but is rotated by $30^\circ$
and the pitch increased by a factor $\sqrt{3}$. The secondary lattice overlays the original one
as shown in figure 9.10 and so its periodicity can be applied by introducing a distortion
where these lattices coincide. For a single frequency, Fehrembach et al. predicted that as
much as 80% of the optical energy emitted could be collected in a cone of half width $0.2^\circ$
from surface normal, creating the secondary lattice by decreasing the size of every third
hole in the primary lattice by 20%.

For practical implementation, the PhC tiling must be designed to exhibit a suitable
TE band gap near the emission frequency of the quantum wells to produce the state at
$K$, and the vertical structure must be designed to decouple this state from the epitaxial
layers below. Figure 9.11 schematically illustrates a proposed design, where the emitting
region is embedded in a PhC near the top of the device with an undercut region of lower
dielectric fill fraction below to create the quasi-suspended PhC slab. This design and its
potential performance will now be discussed.

\(^2\)as $\hat{G}' \equiv -\hat{G}'$
9.3.2 Modelling quasi-suspended photonic crystal slabs

The experimental work on nanorod arrays in chapter 8 showed that a 2D simulation produces a good fit to the observations, but without further experiments, investigation of any frequency shift due to the finite nature of the nanorods was not possible due to uncertainty in measurement of the air filling fraction. The software package MIT Photonic Bands (MPB) previously described is not able to model three-dimensional finite structures fully as it tiles the simulation cell in all three dimensions, but it will be able to model states which are confined only to the slab such as those of interest for the primary lattice. Setting the simulation supercell size in the $z$-direction suitably large to avoid coupling interactions between light guided in the stacked slabs disturbing the result allows these states to be considered. Figure 9.9 is a reproduction of a band diagram presented on page 137 of [137] produced by the model used for this work and was used to validate the simulation method, using a supercell size of $z = 8a$.

The polarisation of the light states in a PhC slab cannot be described as purely TE and TM due to the restricted symmetry created by the in-plane periodicity – the refractive index is not invariant in any direction. However, for a PhC slab which is symmetrical about the $z=0$ plane, parallel to the plane of the slab, the states can be described as having even
Figure 9.12: Asymmetrical slab.

Figure 9.13: Structure with underlying GaN substrate.
or odd symmetry about this plane and at \( z = 0 \), this corresponds exactly to TE and TM polarisations respectively. The fields away from \( z = 0 \), but within a short distance, remain principally consistent with TE or TM polarisation and so the states can be considered and are often referred to as TE-like or TM-like [137]. When this \( z=0 \) symmetry constraint is broken, such as for the proposed design of a PhC slab on a substrate shown in figure 9.12a, the states can no longer exhibit perfectly odd or even symmetry, but MPB can calculate the parity about the central plane in the simulation supercell, corresponding to \( z=0 \). The parity value provides a measure of the degree of symmetry present in the form of an expectation value between 1 and -1, defining perfectly even and odd (≈TE and TM) behaviour respectively.

Figure 9.12b shows the dispersion of the asymmetric structure shown in figure 9.12a, where a hexagonal nanohole PhC with hole radius 0.4\( a \) is bounded by air above, and a homogeneous substrate with \( n = 1.22 \) below. In the band diagram (figure 9.12b), the parity about the \( z=0 \) plane is shown by the colour of the line, with blue representing TE-like even symmetry and red TM-like odd symmetry. The states confined by the volume-averaged substrate to the PhC layer (those inside the inner black lines) have parities either very close to 1 or -1. This shows polarised behaviour which is only slightly perturbed from a symmetric slab. The states which are not confined mostly have parities near zero, and so no reasonable approximation of the polarisation is possible in this context.

It would be impractical to set up a full simulation of the proposed design shown in figure 9.11, which includes the GaN underlayer and a large enough air gap to avoid coupling between vertical cells, as the computation time scales as an increasing function of the volume of the supercell. Additionally, the full structure supports many more modes and so a much larger number of bands must be computed. The parity of the states provides a mechanism for easy recognition of the decoupled states localised in the quasi-suspended slab and gives information about their polarisation if the slab is placed centred about \( z=0 \). This can be understood simply, as the field pattern of the confined modes will have little energy outside the symmetrical suspended slab and so have parities near to ±1, whereas the states with significant field energy in the substrate and the PhC layer will have parity closer to 0. A simulation was performed which includes a thick GaN underlayer (\( n \approx 2.49 \)), a PhC slab with thickness \( a \) and hole radius 0.4\( a \), and a confining PhC layer of larger air holes (radius 0.5\( a \)). The geometry is shown in figure 9.13a and the results of the simulation in figure 9.13b.

The minimum information required to inform the proposed design shown in figure 9.11 is the dispersion of the lowest two TE-like bands inside the decoupled PhC layer at the device surface. It is suggested here that this information can be approximated by modelling...
the quasi-suspended PhC slab above a homogeneous substrate, as in figure 9.12a. The effective index of this homogeneous medium represents the confining PhC region of higher dielectric fill below the quasi-suspended PhC slab. A hole radius of 0.5a in GaN is used and the refractive index calculated using the parallel volume-averaging method in (7.7), where the air fill fraction ($A_{FF}$) of a hexagonal lattice is given by

$$A_{FF} = \frac{2\pi r^2}{a^2\sqrt{3}}$$

for $r \leq 0.5a$

where $r$ is the radius of the hole. The results are shown in figure 9.12b and took only a few minutes to produce on the available resources. In contrast, computation of the bands in the full structure including the GaN underlayer shown in figure 9.13b took approximately 36 hours. The results compare closely for the strongly polarised bands below the light line of the guiding PhC layer and indistinguishable for the lowest TE-like band, demonstrating that the approximation can be used to obtain accurate information. This result was confirmed for other substrate hole radii and using equation (7.8). The many unpolarised bands present in the full simulation are those with significant energy outside the PhC slab, likely confined below the guiding layer in the GaN. At present, it will be assumed that the GaN layer is suitably decoupled from the source to neglect excitation of these modes and the decoupling of such states from a source in the quasi-suspended PhC slab will be investigated later.

### 9.3.3 Photonic crystal and vertical structure design

The volume-averaged approximation such as that in figure 9.12a is used to allow investigation of how the frequency of the lower band and the width of the gap varies for a range of parameters within feasible computational timescales. Figure 9.14 shows the frequency of the lowest band at the $K$-point and size of the TE-like gap for guided light relative to the mid-gap frequency as a function of the PhC slab thickness ($x$-axis) and the hole radius ($y$-axis) for several substrate volume-averaged hole sizes. The upper bounding frequency of the gap was determined to be the lowest frequency which could not be considered as TM-like by a parity less than -0.5. Where this point was not confined to the slab, the upper frequency was set to the highest frequency guided in the slab.

Decreasing the PhC slab thickness leads to an increase in the frequency of the lowest band, as a thinner slab will act to push the fields out of the slab and increase their overlap with the bounding regions of lower refractive index either side. This larger overlap with

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3Interestingly, using the perpendicular volume-averaging equation (7.8) produces a result which is much less accurate for the TE-like modes, but does fit the upper TM-like band in figure 9.13b well but is cut off when using the parallel method (7.7) shown in figure 9.12b. This suggests that for TE polarised light, (7.7) is most valid, and for TM polarised light (7.8) should be used.
(a) K-point frequency for a volume averaged substrate of $0.5a$ radius holes.

(b) Gap width for a volume averaged substrate of $0.5a$ radius holes.

(c) K-point frequency for a volume averaged substrate of $0.4a$ radius holes.

(d) Gap width for a volume averaged substrate of $0.4a$ radius holes.

(e) K-point frequency for a volume averaged substrate of $0.3a$ radius holes.

(f) Gap width for a volume averaged substrate of $0.3a$ radius holes.

Figure 9.14: (left) frequency map of the K point of the lowest TE-like band and (right) TE-like band gap map as a function of the quasi-suspended PhC slab hole radius and thickness.
areas of lower refractive index causes the increase in frequency of the band. Similarly, as
the hole radius in the PhC slab or the substrate is decreased, the frequency decreases due
to the smaller volume of air in the structure.

As discussed in §3.2.2, the emergence of a band gap is due to the change in energy
introduced between two initially degenerate bands when a periodic variation of the refrac-
tive index is added. As the energy of each band is determined by the field overlap with
the dielectric, the width of the energy gap between the two bands will depend upon the
contrast in this overlap. The contrast is reduced for smaller hole radii and also once the
strips of dielectric between the air holes become sufficiently small for large radii, giving a
narrower or no band gap. This is illustrated in figures 9.14b and 9.14d where there is an
optimum hole radius, with a decreased gap size either side of the optimum. Increasing the
refractive index of the substrate will also reduce the contrast between the bands, which
is responsible for the reduction in the gap width seen from the \( r = 0.5a \) to the \( r = 0.4a \)
substrate holes.

The gap in the guided states can be formed either when the second TE band is cut off
from the PhC slab or when the first band is at a lower frequency than all the states in the
second band. The former case can have little significance when the lower band is close to
the light line, such as for the situation in figure 9.15a, and it is responsible for the small
size of the gaps observed when the substrate holes have \( r = 0.3a \) in figure 9.14f. Conse-
quently, the lower band will not have a high density of states as desired to concentrate
emission as there is only a small region of the IBZ near to \( K \) in the gap for which the states
are confined below the light line of the substrate, making it of little use. However, for
larger substrate holes, the gap in guided states is opened for a much larger portion of the
IBZ due to the increased frequency of the substrate light line and the greater frequency
difference possible between the two bands for higher air fill fractions (for example in figure
9.15b). When the PhC slab thickness is small, the second band is cut off and the first
band has a high frequency, giving a small gap. As the slab thickness increases, the gap
size increases sharply due to increasing confinement of the lower band leading to reduced
frequency. Once the slab is sufficiently thick, the second band is no longer cut off from
the slab and as the rate of decrease of the frequency of the first band slows, so the gap
width decreases and closes.

A reasonable range of parameters are available to form an in-plane gap in these struc-
tures, but under the assumption that the confining layer below the quasi-suspended PhC
slab fully confines the guided states. This assumption relies on the confining PhC layer
with larger air holes being of sufficient thickness and high enough air fill to decouple the
suspended PhC slab from the GaN underlayer below. The ratio of the TE power lost from
states in the quasi-suspended PhC slab to the the total TE power for all states evanescent
(a) $r=0.3a$ radius holes as a volume averaged substrate, $0.25a$ radius suspended PhC holes, $1a$ suspended PhC thickness.

(b) $r=0.4a$ radius holes as a volume averaged substrate, $0.25a$ radius suspended PhC holes, $1a$ suspended PhC thickness.

**Figure 9.15**: Dispersion of the TE-like states in the first 6 bands. The shaded areas indicate an in-plane band gap for guided light.

(a) $r = 0.5a$ radius guiding PhC layer holes.

(b) $r = 0.4a$ radius guiding PhC layer holes.

**Figure 9.16**: Ratio of TE power lost from PhC layer to total TE power for all states evanescent in the confining PhC layer for a suspended PhC slab thickness of $1.5a$. The refractive index of both PhC layers was volume averaged, calculated with (7.7), and the source emitting at a frequency of $0.3\lambda/a$ was positioned 0.75 of the PhC layer thickness from the device surface.
in the underlying confining PhC layer is shown in figure 9.16 as a function of underlayer thickness and PhC hole radius, which was found using the slab waveguide model discussed in chapter 5. Equation (7.7) was used to determine an effective homogeneous refractive index for the PhC layers as it gives the worst-case scenario and appears to give the best fit for the TE-like modes in these structures.

The blue areas of figures 9.16a and 9.16b show where there is high decoupling of the useful guided states for 0.5$a$ and 0.4$a$ confining PhC hole radii, without considering the 0.3$a$ holes as they do not allow a suitable band gap to form. The quasi-suspended slab PhC holes must be sufficiently smaller than in the confining PhC layer underneath and the thickness of the layer is estimated to need to be a wavelength thick to be sure of decoupling the PhC slab. With consideration of the gap maps in figure 9.14, decoupling the quasi-suspended slab is unlikely to place any additional restrictions on the PhC hole size.

9.3.4 Device performance

Once multiple frequencies of emission are taken into account, the maximum directivity $D$ or extraction efficiency $\eta_{<\theta}$ within half angle $\theta$ which could be achieved is constrained by the locus of the band about the $K$-point over the frequencies of interest. Figure 9.18a shows the dispersion of the first TE-like band around the edge of the IBZ for the structure with the widest gap which was found for 0.4$a$ radius guiding PhC layer holes. As the frequency decreases, the band moves away from the $K$-point and therefore away from normal incidence once diffracted by the secondary lattice. For a practical source, the directivity is thus dependent upon the linewidth of the emission due to this variation of $k_{||}$ with frequency.

For the effect this has on $D$ and $\eta_{<\theta}$, it is no longer adequate to just calculate the frequency of the band around the edge of the IBZ, as all the states inside the IBZ will contribute to the emission. Instead, the location of the band in in-plane $k$-space as a function of frequency must be calculated, and is shown in blue in figure 9.17 at a frequency of 0.295$a/\lambda$, where the band is not extracted to the air cone at all. Once folded by the secondary tiling which maps $K$ to $\Gamma$, all the emission at this frequency can be inside the air cone close to normal incidence, shown by the red line, giving a high value of $D$ as there is no emission at angles far from normal incidence.

In contrast to the azimuthally invariant slab modes, for which the excitation is not dependent on the direction of emission, there will be variation of the excitation of the states in the band with their azimuthal direction. This excitation is proportional to the density of states (DOS)\(^4\), which can be calculated for delocalised excitation from the inverse group

\(^4\)It should be made clear that throughout this section, the DOS refers to the number of states per unit
velocity for each band by

\[ N_i(\omega) = \int_{\text{EFS}_i} \frac{1}{\omega} \left\| \frac{d\vec{k}}{d\omega} \right\| ds \]  

(9.11)

where \( \left\| \frac{d\vec{k}}{d\omega} \right\| \) is the inverse group velocity resolved to the direction normal to the surface element \( ds \) of the equifrequency surface (EFS)\(^5\) of the band \( i \) \([268]\). For the two dimensions of the in-plane space of a 2D PhC, the EFS for each band is represented instead as a contour, such as the lines in figure 9.17. With discretisation of the contours, (9.11) can be evaluated using the trapezium rule, with \( ds \) approximated by the Euclidean distance between adjacent in-plane states. This method was validated against figures 3 and 4 of ref. [269] using group velocity values produced by MPB and is shown for the first band of the test structure in figure 9.18b for arbitrary units normalised to the peak value.

For considering emission by an embedded 2D QW layer, the delocalised DOS is a suitable model as the emission is also predominantly delocalised in-plane – the emission is only localised in-plane to the region of dielectric fill, which carries the vast majority of the field energy in the first band. The in-plane regions with most of the field energy of the band align well with the in-plane position of the QW. This assumption will not be valid for core-shell-type structures in nanoholes or nanorods as the emission is localised in-plane.

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\(^5\)Analogous to a Fermi surface for semiconductor states.
Chapter 9. Directional emission from photonic crystal LEDs

In-plane wave-vector $k_{\parallel}$

Frequency $a/\lambda$

$\Gamma \quad \Delta \quad \Lambda \quad \Gamma$

0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

(a)

Figure 9.18: Dispersion and DOS of the first TE-like band for 0.4$a$ radius guiding PhC holes, 0.25$a$ radius suspended PhC holes with a thickness of 1.5$a$.

Figure 9.19: Ratio of power in the first TE-like band emitted inside half-angle $\theta$ for a frequency of 0.3035$a/\lambda$, close to the band gap for 0.4$a$ radius guiding PhC holes, 0.25$a$ radius suspended PhC holes with a thickness of 1.5$a$.

Figure 9.20: DOS of the first TE-like band weighted by a Gaussian emission peak to represent QW emission centred at 470nm with 30nm FWHM for 0.4$a$ radius guiding PhC holes, 0.25$a$ radius suspended PhC holes with a thickness of 1.5$a$.
Considering the $z$-direction perpendicular to the suspended PhC slab, the QW source will be localised in position, but the medium does not vary with $z$ position inside the PhC slab. The $z$ position is therefore unlikely to affect the relative excitation of in-plane states to each other and their variation with frequency significantly within the lowest band. This will preserve the important information about how the excitation varies around the $\mathbf{K}$-point and simplifies the model accordingly.

By integrating the EFS of the band within the half angle $\theta$ from normal incidence around the $\mathbf{K}$-point, the DOS as a function of $\theta$ can be found and, once normalised to the DOS at the frequency and assuming no losses, $\eta_{i<\theta}$ is found. Figure 9.19 shows $\eta_{i<\theta}$ for a single frequency close to the band gap, corresponding to $0.3035 a / \lambda$, and the emission is extremely directional for this single-frequency as expected, with all the power emitted inside $1^\circ$ of normal incidence. To take into account multiple emission frequencies, the DOS is weighted by a Gaussian emission profile after converting the frequency so the edge of the band gap lies at 450nm. Figure 9.20 shows an example of how the DOS varies with wavelength for an emission peak to represent QW emission, centred at a wavelength of 470nm with a FWHM of 30nm, and normalised to its peak value. Integrating over both angle and frequency after weighting allows investigation of the directional characteristics of the emission,

\[
N_i(\theta) = \int_\omega \int_0^{|\mathbf{k}'| \leq k_0 \sin \theta} \frac{d\mathbf{k}}{d\omega} \| d\mathbf{k} \| ds \, d\omega \quad \forall \mathbf{k} \in \text{EFS}_i
\]

(9.12)

where $\mathbf{k}' = \mathbf{k} - \mathbf{K}$.

The result of (9.12) is shown in figure 9.21a for an emission peak of 30nm FWHM and a range of centre wavelengths. The data shows optimal performance occurs when the centre wavelength is not centred at the edge of the band gap. At longer wavelengths, the total power which is extracted reduces as a proportion of the mode can no longer be folded to the air cone, but the source of the performance reduction at shorter wavelengths is less clear. Referring to figure 9.20, the tail of the peak is cut off sharply by the band gap, where there can be no emission into the mode – emission at wavelengths shorter than 450nm can only occur into states unguided by the slab and cannot contribute directly to the directional enhancement desired. In a device with negligible non-radiative recombination, this may give a slight advantage for a small overlap with the gap as it will increase the emission into the highly directional states that occur just above 450nm wavelength, although a larger overlap will cause an increase in the proportion of the light emitted to less useful places, such as straight to the air cone. In a more practical device limited by the non-radiative recombination rate, the corresponding decrease in the radiative recombination rate will
result in potentially much lower quantum efficiency [156]. This effect has been included in the calculation in figure 9.21a by subtracting the proportion of power of the Gaussian peak for which no emission can occur into this mode and is responsible for the poorer performance as the centre wavelengths moves closer to the band gap. Consequently, it is optimal for the emission peak to be located such that the band gap does not overlap with the emission significantly to avoid this detrimental effect to performance.

\[ \eta' < \theta \]

Figure 9.21: Ratio of total power emitted into the first TE-like band which is extracted inside the half angle \( \theta \) from normal incidence for 0.4\( a \) radius guiding PhC holes, 0.25\( a \) radius suspended PhC holes with a thickness of 1.5\( a \) after weighting by Gaussian emission. The proportion of the emission power which is inhibited by the band gap has been subtracted, giving \( \eta'_<\theta \) as a lower limit for 100% extraction of the band.

9.3.5 Comparison with the diffractive regime

Figure 9.21b shows the effect of varying the FWHM and locating the emission peak to achieve the most emission within 30\( ^\circ \), and is compared with the upper limit of performance which could be achieved for just a single frequency using weak photonic crystal behaviour. For these parameters, it should be possible to extract \( \approx 76\% \) of the power emitted into the PhC mode within 30\( ^\circ \) of normal incidence in a device with a practical emission linewidth with 30nm FWHM and 92\% of the power inside 30\( ^\circ \) for 20nm FWHM. In contrast, the upper limit offered by the weak regime is for a hexagonal lattice extracting a single slab mode in GaN with \( n_{\text{eff}} \approx 2.4 \) at first order is \( < 40\% \) power inside 30\( ^\circ \) for a single frequency of emission.

In practice, the best performance achieved to date with the weak regime of \( D \approx 0.33 \) and \( \eta' < \theta \approx 13\% \) within 30\( ^\circ \) used multi-moded operation due to the challenges associated with creating a single-moded slab adjacent to a PhC [112]. A single-moded GaN slab in air must be no more than 100nm thick (at 450nm wavelength) as avoiding significant exci-
tation of the second order mode in such a thin slab is not possible with a MQW structure. In contrast, the quasi-suspended slab in the example above operating in the Bloch regime is 200nm thick with room for increase whilst maintaining single-moded operation, giving much more space for a practical MQW structure. Indeed, figure 9.14d shows that the gap remains open up to a slab thickness of more than 2.5\(a\) (>300nm thick for 450nm operating wavelength).

The performance achievable in a realised device operating under either the weak or strong regime will ultimately be limited by the ratio of the power which can be emitted into the ideal mode and the efficiency at which that mode can be extracted from the device. In the weak approach, engineering good overlap with the PhC to give good extraction gives a trade off between the confinement required to trap the light in the intended mode and the overlap of that mode with the PhC. However, in the quasi-suspended PhC slab approach operating in the strong regime, the overlap between the mode confined in this slab and the secondary grating which diffracts the mode close to normal incidence will be very high, leading to very good extraction efficiency. Due to the high overlap with the extracting PhC, it is expected that the extraction efficiency of the mode in the strong regime will be higher than in the weak regime. This high extraction efficiency will enable resilience to absorptive processes through material absorption and photon recycling losses (when \(\eta_{IQE}<100\%\)) which will compete with extraction in practice.

The matter of the ratio of total power which can be emitted into the ideal mode to undergo directional extraction is rather more complex to compare quantitatively between the two approaches as the simplifying assumptions made in the simulations may prevent direct comparison. Finding this ratio would require calculating the excitation of all the states, which is not possible for states propagative outside the slab with the MPB model due to tiling in the third dimension. As a result of the effect of the PhC on the density of states, a 1D slab model with volume-averaged layers to predict the excitation of the guided states would not be representative. Some comparative comments can however be made based upon consideration of the mode only, which are of use if it is assumed that the emission into radiation modes is mostly unaffected by the PhC [214]. When below a band gap, the first band of the PhC slab in the Bloch regime will have a high overlap with the dielectric, as is obviously the case for a low order mode in a homogeneous GaN slab in the weak approach, suggesting that qualitatively the excitation in each operating regime will be of comparable magnitude – the states will ‘feel’ a similar dielectric constant. Speculatively, this comparison goes even further, as the small quantity of energy in air for the first state in a PhC slab is akin to the overlap with air either side for low order modes in a thin slab. Quick MPB simulations of the delocalised density of states for a homogeneous GaN slab found to give best ratio using a 1D model provide some support...
for this approximation, although this does not provide rigorous proof. It is therefore con-
sidered likely that, in a practical device, a similar ratio of the total emission power can be
confined in the intended mode in both the strong and weak approaches. This mode will
be better extracted from the PhC slab in the Bloch regime due to the high overlap with
the extracting photonic crystal, allowing the direct comparison in figure 9.21 and table 9.1
to be representative and possibly pessimistic of the substantial performance improvement
offered by the proposed design.

To compare the possible performance improvement offered by the proposed design,
the flux throughput (Φ) through a system of fixed unit étendue, source area and source
emission power is considered in table 9.1 for a few different scenarios. In table 9.1, a
system which only uses light emitted within 30° of normal incidence is considered, and
the flux is calculated using (from (9.1) and (9.2))

\[
\Phi = \frac{\eta_{\text{ext}} \eta_{\text{mode}} \eta_{<30^\circ}}{n_{\text{encap}}^2}
\]

where \( \eta_{\text{ext}} \) is the extraction efficiency, \( \eta_{\text{mode}} \) is the ratio of the power which is emitted into
the desired mode for directional emission and \( n_{\text{encap}} \) is the refractive index of the encapsulant. Note that this calculation ignores any power emitted directly to the superstrate inside 30° from normal incidence and so are expected to be a slight underestimate for the
PhC devices, except for the best published PhC device, as the experimental measurements
include this effect.

For étendue-limited systems, table 9.1 shows that exploitation of strong photonic crys-
tal effects is estimated to nearly double the flux throughput of a realistic estimate of a
best-case practical device operating in the weak regime, and more than double the perform-
ance of currently available devices.
### Table 9.1: Flux throughput ($\Phi$) of various emitters through a system with fixed unit étendue, source area and source emission power.

*Based on 73% best published unencapsulated extraction efficiency for a PhC LED [88].

<table>
<thead>
<tr>
<th>Scenario</th>
<th>$\eta_{ext}$</th>
<th>$\eta_{mode}$</th>
<th>$\eta_{encap}$</th>
<th>$\eta_{&lt;30^\circ}$</th>
<th>$\Phi$</th>
<th>Enhancement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perfect Lambertian emitter (encapsulated)</td>
<td>1</td>
<td>1.41</td>
<td>0.25</td>
<td>0.125</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Best published Lambertian emitter [113]</td>
<td>0.9</td>
<td>1.41</td>
<td>0.25</td>
<td>0.113</td>
<td>0.9</td>
<td></td>
</tr>
<tr>
<td>Best published PhC device [112]</td>
<td>0.39</td>
<td>1</td>
<td>0.31</td>
<td>0.121</td>
<td>0.97</td>
<td></td>
</tr>
<tr>
<td>Weak PhC limit (0nm FWHM)</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.5</td>
<td>5</td>
<td>4</td>
</tr>
<tr>
<td>More realistic weak PhC estimation (0nm FWHM)</td>
<td>0.75*</td>
<td>0.5</td>
<td>1</td>
<td>0.4</td>
<td>0.76</td>
<td>1.2</td>
</tr>
<tr>
<td>Ideal strong PhC - this work (20nm FWHM)</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.92</td>
<td>0.92</td>
<td>7.36</td>
</tr>
<tr>
<td>Realistic estimation of strong PhC - this work (30nm FWHM)</td>
<td>0.75*</td>
<td>0.5</td>
<td>1</td>
<td>0.76</td>
<td>0.29</td>
<td>2.28</td>
</tr>
</tbody>
</table>
9.4 Conclusion

Two approaches utilising photonic crystal effects have been considered for highly directional emitters for étendue-limited applications. The first approach, which has been investigated previously, ideally confines light to a single mode in a homogeneous slab, which is then diffracted by a carefully designed adjacent PhC to optimise directional emission. The performance of this approach is limited due to the azimuthal invariance of the slab mode, causing emission at all inclinal angles, and some of the power carried in the mode cannot be extracted at all without considerable restrictions on the design of the vertical and PhC structures. The performance in the weak regime is expected to offer $\approx 1.2 \times$ performance enhancement over an encapsulated Lambertian emitter with 100% extraction efficiency. In practice, ideal single-moded operation is unlikely to be achievable as it requires the active region to be fabricated inside a waveguide of $\approx 100\text{nm}$ thickness.

Exploitation of strong photonic crystal effects using a quasi-suspended photonic crystal slab provides a promising alternative approach to overcome the performance limitations of the weak regime. With a suitable PhC design, light can be confined to an azimuthally directional Bloch mode guided in a slab of practical thickness, which can all be extracted close to normal incidence by a secondary grating created by perturbing every third element of the primary lattice. This approach also relies on the quasi-suspended PhC slab remaining single-moded, but in this case, the slab supports a single Bloch mode for thicknesses $>300\text{nm}$. For an example device, which has not undergone extensive optimisation, $2.28 \times$ performance enhancement over an encapsulated Lambertian emitter with 100% extraction efficiency is expected.

The performance of both the approaches depends upon both the ratio of the total power which is emitted into the desired waveguide modes for directional emission, and the ratio of the power in the desired modes which is extracted from the device. The former is considered to be comparable for both approaches as there will be a similar overlap of the emitting region with the vertical mode profiles in both cases, and the latter favourable for the strong regime as the overlap between the mode and the extracting PhC will be higher, giving a shorter extraction length. If both these ratios are set to 100% for the strong device, and a 20nm FWHM linewidth achieved, the upper limit of performance enhancement over a Lambertian emitter is $7.36 \times$.
Chapter 10

Conclusions

LEDs have seen rapid uptake for applications in space lighting, but the low brightness and high étendue of commercially available devices compared with arc and filament lamps restricts their use as sources in étendue-limited optical systems such as projectors and headlamps. In order to enable the uptake of LEDs for these applications, sources with more directional emission than those available at present are required as not all the light emitted from the source can be projected onto, for example, the viewing screen or road. Only 5% of the light emitted in a GaN LED is emitted from the top surface of the device due to total internal reflection, and so light extraction techniques are necessary to improve this performance. Light extraction techniques which provide the best overall efficiency performance in commercial devices of ≈90% use surface-roughening to scatter light trapped in the LED [113], offering no control over the direction of light emission, and encapsulation, which increases the source étendue by the square of the refractive index of the encapsulant. Surface-roughened devices show a Lambertian emission pattern, where only 25% the extracted power is emitted with $30^\circ$ of normal incidence.

Photonic crystals extract light from LEDs through diffraction, and have been able to provide the highest reported unencapsulated light extraction efficiency of 73% [88]. Diffraction is a coherent process, so photonic crystal LEDs can have a non-Lambertian emission pattern. However, experimental photonic crystal devices have produced results only slightly better than the best surface-roughened devices, despite their much higher potential upper limit of 50% in the diffractive regime [112], or close to 100% in the Bloch operating regime [218] emitted within $30^\circ$ of normal incidence. This thesis has investigated whether photonic crystals can be used to improve the performance of InGaN/GaN LEDs as sources in étendue-limited optical systems over present results, and what the limits to performance might be in practical devices.
Efficiency droop provides a further performance limit for high-brightness blue LEDs, as the efficiency of InGaN quantum wells is observed to decrease for high drive currents as a function of increasing current density. Core-shell LEDs use a 3D device geometry where the InGaN active quantum well region is grown on the sidewalls of nanorods etched into the GaN, enabling a larger emitting surface area for the LED device area. As a result, the current density in the active region is lower, allowing operation to higher device currents before the onset of efficiency droop. Core-shell LEDs can be fabricated in regular arrays, and therefore should show photonic crystal effects, but there are no detailed experimental studies of their behaviour, even though a theoretical study [214] has suggested they may operate in the strong or Bloch regime, where the periodicity of the photonic crystal dominates the optical properties. Chapter 8 of this thesis has studied the behaviour of nanorod and core-shell LEDs and has shown experimentally, possibly for the first time, that these devices can operate in the Bloch regime as well as the diffractive regime.

Previously, Bloch mode formation has only been observed in small-area suspended slab structures in the III-nitrides, which are not suitable for high brightness devices of a practical size and do not allow dielectric rod-in-air structures to be possible. In this work, periodic arrays of core-shell and quantum disc nanorods have been observed experimentally to operate in the Bloch regime using angular luminescence measurements. Bloch modes can therefore manifest in devices which are suitable for large-area fabrication with practical routes to electrical contacting and good heat dissipation, so this finding will enable future research wishing to exploit strong photonic crystal effects for new applications, such as for highly directional light sources.

The Bloch regime requires a mechanism to confine light to the photonic crystal layers and random scattering losses from surface roughness and imperfections must be minimised. In practice, it was shown that creating a quasi-suspended photonic crystal slab could readily facilitate Bloch mode formation. In this mechanism, the optical confinement for Bloch mode formation is achieved using index guiding by introducing lower-refractive index layers in the photonic crystal, specifically, regions of lower dielectric fill (and therefore lower volume-averaged refractive index). The apparent strength and sharpness of the Bloch features correlated with sidewall roughness – the Bloch features were sharper with a higher contrast over the background for core-shell nanorods with regrown crystal facets on the sidewalls than visibly rougher quantum-disc nanorods fabricated only by etching – and verticality – core-shell structures with a less consistent fill fraction in the vertical direction showed broader Bloch mode features.

The mechanism of lossy Fresnel reflection, where non-total internal reflection either side of the photonic crystal provides a high enough field overlap for the periodic behaviour
to emerge, has also been shown to enable Bloch mode formation in this work, confirming past prediction of this effect for light propagating at large angles from surface-normal, close to parallel with the interfaces [214]. The experiments performed were not able to confirm how applicable this mechanism is for air fill fractions much less than 1, where light will propagate at shallower angles, as the experimental structure operating by lossy Fresnel confinement took many attempts to fabricate. The test sample which did provide results was not consistent over all the wafer fragment and required a lot of material to be etched away before vertical sidewalls were achieved. In order to have a reasonable area available for the active region, an air fill fraction much less than 1 would be required in a practical design to provide a reasonable emitting area and thus lower current density to mitigate the effect of efficiency droop. During the fabrication process, the confinement was found to be highly sensitive to roughness at the interfaces and surfaces – nanofabrication of practical devices is unable to create perfectly smooth structures. Further study may wish to attempt fabrication of nanorod structures with highly smooth interfaces at lower air fill fractions to investigate if the lossy Fresnel mechanism could be useful in practice and arise for shallower propagation angles, and attempt to quantitatively understand the operational limits to interface roughness.

In ref. [214], it was suggested that the Bloch modes could be considered as a perturbation of quasi-guided modes similar to homogeneous slab waveguide modes due to the vertical confinement in the structures; i.e. that the 1D Fabry-Pérot resonances for light propagating at large propagation angles from surface normal defined their approximate properties. This work has provided evidence to the contrary, as the experimental measurements of comparable far-field features from arrays of core-shell nanorods could be modelled by a 2D structure with no variation (and therefore no confinement) in the vertical direction. The comparable features were due to modes with a wide range of effective refractive index, including those with an angle of propagation close to surface normal. The fit between the 2D model and the experimental data shows that the dispersion in the experimental structures was due primarily to the 2D periodicity, and was only perturbed by the vertical structure. However ref. [214] only refers to the lossy Fresnel mechanism, but it was not clear by which mechanism these experimental structures performed as they contained both a region of lower dielectric fill to enable index guiding and an underlying smooth silicon substrate to promote the lossy Fresnel mechanism.

These best performing experimental devices, displaying very strong Bloch resonances, were highly vertical core-shell nanorods with a lower index material and a lower dielectric fill fraction between the active InGaN region and a smooth and reflective silicon substrate. These devices fit well with the simple 2D model of infinitely-tall nanorods, and control of the frequency dispersion of the Bloch modes was shown by varying the fill fraction, which offers a process for further work to engineer the dispersion in such structures.
is not conclusive whether the variation in the fill fraction and refractive index, allowing
index guiding, or the smooth silicon surface, leading to lossy Fresnel reflection, is primarily
responsible for the strong behaviour, but future work could investigate this by adding a
step to roughen the silicon to see how the Bloch modes change.

This study of these effects shows experimentally, possibly for the first time, that core-
shell and nanorod LEDs in regular arrays can operate in the Bloch regime, but much more
work is required for deeper understanding. This study was almost entirely qualitative, and
unable to provide quantitative details of how the device parameters affect the formation of
Bloch modes, which is required for future exploitation. The core-shell samples mentioned
in this thesis were a subset of available samples created with the purpose of investigating
the fabrication of core-shell structures and the initial observation of the strong effects was
by chance. A lot of samples were measured as there was little control over the design of the
structures, and those providing single-variable changes most informative to this work were
selected for more detailed experimental investigation. No choice of the vertical structure
design was available due to the layer stack of pre-fabricated devices and substrates, but
the possibility of varying these parameters provides scope for future investigation of the
confinement effect, as samples with different vertical structures could be compared. The
quantum-disc nanorod structures with different sidewall shapes were fabricated specifically
for this work, but were also limited to the distorted hexagonal lattice with a pitch of
600nm due to availability of nano-imprint masks and so it was not possible to investigate
other pitches or crystal lattices. Further research would do well to study smaller pitches,
of particular interest as the frequency density of Bloch modes supported decreases with
pitch and most suggested methods of exploiting Bloch modes rely on the lowest-order
modes.

**Buried photonic crystal LEDs**

The majority of previous work into photonic crystal LEDs has etched the photonic
crystal into the surface of the LED, with the photonic crystal design optimised to diffract
light trapped in homogeneous slab waveguide modes efficiently, overcoming the competi-
tion with optical absorption processes. The extraction of the guided mode is proportional
to the overlap of the mode field with the extracting photonic crystal, which is poor for
surface photonic crystals and low-order guided modes. The buried photonic crystal LED
configuration places the photonic crystal away from the surface where the overlap with
the low-order modes is greatly increased, and has been demonstrated to provide an unen-
capsulated light extraction efficiency of 46% [181], but has not been widely investigated.
Chapter 7 sought to investigate if this performance could be improved. It was also hoped
that this study would be able to provide insight into the effect of the buried photonic crys-
tal on the electrical properties of the LED, but the the passivation mask used to prevent overgrowth on the nanohole sidewalls prevented a good contact being made to the n-GaN after etching the mesa.

Buried photonic crystal LEDs have been experimentally shown to operate in two ways; firstly in a decoupled case, where the slab modes in the cap layer above the buried photonic crystal are optically decoupled from the guided modes below by a photonic crystal with a high enough air filling fraction and thickness, and secondly in a coupled case where the photonic crystal has a low enough air filling fraction or thickness to allow optical coupling of slab modes.

It has been shown that the commonly-used ‘1D-2D’ model to simplify operation of a photonic crystal LED structure into a separate 1D slab waveguiding structure and 2D crystal tiling provides a good method for predicting the behaviour of buried photonic quasi-crystals LEDs by comparing simulations with experimental data. Representing the photonic crystal layer with a refractive index in the 1D model requires an effective medium model, which is achieved in other studies of photonic crystal LEDs by volume-averaging the dielectric constant without justification. However, a theoretical study [249] suggests that this conventional method provides an upper limit for the refractive index, and provides an expression for the lower limit, stating these apply to media with periodicity less than \( \frac{1}{10} \) the wavelength of the light under consideration. This study cannot provide any justification for use of either the upper or lower limit in practice due to the experimental error as both models provided a fit the data within the error bounds, but did suggest the method presented in [249] is at least useful outside the suggested physical limits for periodicity greater than \( \frac{1}{10} \) the wavelength. It was not possible to reduce these errors or produce more devices to investigate in more depth, but further work using a range of different photonic crystal layers could be carried out to consider this. Future work should consider carefully the choice of expression for representing the photonic crystal layer.

The coupled case has been previously considered to provide good overlap of guided modes with the photonic crystal and therefore studied for high extraction efficiency. In the coupled case, this study found using waveguide simulations that techniques to extract the light diffracted or emitted into the substrate modes is required to obtain an extraction efficiency much greater than 50%. The simulations used to reach this conclusion performed a partial parametric search, but the computational resources available were not capable of providing a thorough multi-variate analysis to see if a substantial amount of the power in the device could be emitted directly to the air superstrate. The 50% estimation agrees with other published work which produced experimental devices in the coupled case with light extraction of 46% after an optimisation process [181], which provides some further evidence that the 50% estimation is reasonable. More research could provide insight
into this conclusion by investigating whether using a polishing step and/or a depositing a reflective material on the substrate underside provides performance enhancement over a rough substrate surface, and whether this technique might produce devices with an unencapsulated light extraction efficiency greater than 73%.

Simulation work has predicted that 90% of the guided power in a buried photonic crystal LED can be confined to guided modes in the cap layer in the decoupled case when the thickness and air filling fraction are greater than 300nm and 0.3 respectively. This approach provides a possible path to reduce the metal absorption in directional photonic crystal LEDs by replacing the lossy metallic mirror used to create a cavity in previous designs with a buried photonic crystal. Increasing the air filling fraction further to decouple the substrate was also considered for improving the light extraction by preventing loss of diffracted power to the substrate. This investigation could not show whether decoupling the substrate would improve redirection of diffracted light towards the superstrate but the air filling fraction (at least 0.5-0.8) required is likely too high. The high air fill will reduce the overlap between the photonic crystal and the low order modes carrying a significant proportion of the optical power, leading to an extraction length too high to compete with the optical absorption [181]. Further experiments on samples with air filling fraction greater than 0.33 could determine what effect this has on substrate and radiation modes, and to what extent they can be decoupled. By shaping the nanoholes, it may be possible to use a graded air filling fraction, which increases with distance from the cap layer, to provide a high overlap with some of the photonic crystal for low order modes whilst maintaining the decoupling effect for the substrate modes.

**Pathway to highly directional emission**

Previous experimental attempts to use photonic crystals in LEDs for étendue-limited applications have produced comparable performance to the best encapsulated surface-roughened LEDs. Due to their encapsulation and Lambertian emission, a conventional device with 90% extraction efficiency is only able to couple ≈11.25% of the optical power through a system with fixed étendue and acceptance angle of 30°. The best result achieved by a photonic crystal LED improves this figure to 12.1%, despite the 50% limit suggested in the diffractive regime [112], and close to 100% potentially available by exploiting the Bloch regime for a GaAs emitter [218]. Chapter 9 of this thesis sought to understand what performance could be achieved in a practical device operating in the diffractive regime by considering the implications of the assumptions made to reach the 50% figure. In light of the findings from chapter 8, showing that the Bloch regime is available for exploitation in photonic crystal LEDs, chapter 9 also investigated whether the Bloch regime can be exploited in the III-nitrides to create highly directional emitters and what performance
Directional devices operating in the diffractive regime confine a single mode or group of modes to a homogeneous slab, which is then diffracted preferentially to normal incidence by a suitably-designed PhC. The stated performance limit of 50% for the diffractive regime makes several assumptions to produce an absolute upper limit, which are not achievable in practice. In particular, the limit relies upon single-moded operation, which requires the active region of the LED to be embedded within an optical cavity of no more than \(\approx 100\text{nm}\) thick, presenting a significant challenge for fabrication. Even if fabrication were possible, it was shown that significant constraints are placed on the photonic crystal lattice to avoid dilution of power by different diffraction orders or away from the intended emission direction by rotation of the same order. For example, only \(\approx 75\%\) of the total optical power emitted into a low order mode in GaN with an effective refractive index of 2.5 can be extracted to all angles in air by a hexagonal lattice.

The 50% performance limit of the weak or diffractive approach is fundamentally due to the lack of selectivity of in-plane propagation direction of the slab waveguide mode, and so light is diffracted out of the device at all angles. Using the Bloch operating regime to confine light in Bloch modes with specific in-plane propagation directions allows this fundamental limit of the weak approach to be overcome. The dispersion of the Bloch mode is controlled by a photonic band gap of the photonic crystal, and then extracted by diffraction through a second photonic crystal overlaid by slightly distorting some elements of the first. This study has shown that it is possible to create quasi-suspended nanohole photonic crystal slabs in GaN which can support Bloch modes suitable for directional emission. Instead of requiring a band gap for both polarisations, the TE emission polarisation of \(c\)-plane GaN requires only a TE-like band gap in the slab for the same effect. This is provided by a nanohole photonic crystal slab containing an emitting region, with a supporting layer of lower dielectric fill below to confine light in the photonic crystal.

Although this approach relies upon single-moded operation, the TE-like band gap remains open up to a thickness of over 300nm, allowing enough space to form a multi-quantum well active structure. The overlap of the Bloch mode with the extracting photonic crystal will be high due to the confinement to the photonic crystal region necessary for the Bloch mode to form, and so the diffraction efficiency of the intended mode is expected to be better than in the weak approach, where the diffracting photonic crystal is adjacent to the slab where the light is confined. It was not possible to compare the proportion of the total emitted power which excites the intended mode between the diffractive and Bloch regimes, but this is considered to be similar between the two for a quasi-suspended photonic crystal slab containing a quantum well due to the similar field profiles (and therefore overlap with the active region) in the direction perpendicular to the slab. Parameter optimisation was
not attempted, but it was shown that at least 76\% of the power in the Bloch mode could be emitted inside 30° from normal incidence for an emission linewidth of 30nm FWHM. For étendue-limited applications, exploitation of the Bloch regime is expected to offer at least double the performance of devices currently available, with the potential for up to 7×.

The design presented for a highly-directional LED exploiting strong photonic crystal effects shows the potential for significant performance improvement over results to date based on simulations of photonic crystal and waveguiding effects. The basis for the simulation techniques was established from the fit between experimental measurements and simulations in chapters 7 and 8. Unfortunately, these techniques used were not able to quantitatively investigate the proportion of the light which could be emitted into the desired Bloch mode and the efficiency at which this could be extracted in the desired direction. The primary limitation of the investigation is its consideration of a photonic crystal containing a quantum well, which is required for the use of the delocalised density of states to be justifiable when calculating the emission into the Bloch mode. This quantum well would have material removed when etching the photonic crystal, thus reducing the emitting area therefore increasing the effects of efficiency droop. To mitigate this, a core-shell approach would be advisable as it allows the whole area of the sidewalls to be used to increase the active area, but to investigate the performance in more detail, the simulation would need to consider the effect of localising the active area to the sidewalls on the excitation of the Bloch mode.

There is a wide potential for future research into the practical feasibility and performance of this design as it has not been demonstrated experimentally, and there are several unexplored variables. A nanohole structure was chosen as it supports a TE-like band gap, as the emission from InGaN quantum wells is expected to be TE polarised for guided modes. This assumption should be tested, as dielectric rod-in-air photonic crystal slabs can support a TM-like band gap to increased thickness over a nanohole slab [150] and Bloch mode formation in such structures has been demonstrated experimentally. In a realised device, it is very likely that the nanoholes would be hexagonal in shape due to the crystal facets of the GaN, which has not been taken into account here. The scale of the distortion required to the primary grating in order to form the secondary grating which extracts the light has not been considered.

To realise the design, the region of lower dielectric fill to confine light to the slab must be formed, the interfaces and sidewalls must be made smooth to minimise scattering losses and any etch damage must be recovered. A core-shell approach is considered most likely to provide a feasible path as it will produce smooth sidewalls, the lower dielectric fill could be formed by inhibiting regrowth in these regions and it mitigates the effect of losing emitting area when forming the photonic crystal.
This thesis has shown that photonic crystal emitters operating in the strong photonic regime may offer a pathway to meeting the performance challenges facing LEDs for étendue-limited applications, if they can be realised. Confinement of light to periodic structures has been shown to manifest Bloch modes, and a design presented which is estimated to offer more than double the performance limit possible using available devices, and maybe as much as $7\times$. This design also offers the potential to mitigate efficiency droop using a core-shell approach which gives a large active area-to-device footprint ratio, allowing a lower active area current density for the device planar current density.

The work presented in this thesis has concentrated specifically on photonic crystals in to blue InGaN/GaN LEDs. Whilst the quantitative details are not applicable to other material systems with different refractive indices, the behavioural trends will apply to any other material system, and may be even more potent in materials with higher refractive indices.
Published work

Peer-reviewed journal


International conference


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C.J. Lewins


Dept. Electronic & Electrical Eng. 239 University of Bath


