A THEORETICAL ROADMAP FOR OPTICAL LITHOGRAPHY OF PHOTONIC BAND GAP MICROCHIPS

by

Timothy Y. M. Chan

A thesis submitted in conformity with the requirements for the degree of Doctor of Philosophy
Graduate Department of Physics
University of Toronto

Copyright © 2008 by Timothy Y. M. Chan
Abstract

A Theoretical Roadmap for Optical Lithography of Photonic Band Gap Microchips

Timothy Y. M. Chan
Doctor of Philosophy
Graduate Department of Physics
University of Toronto
2008

This thesis presents designs and fabrication algorithms for 3D photonic band gap (PBG) material synthesis and embedded optical waveguide networks. These designs are suitable for large scale micro-fabrication using optical lithography methods. The first of these is a criss-crossing pore structure based on fabrication by direct photo-electrochemical etching in single-crystal silicon. We demonstrate that a modulation of the pore radius between pore crossing points leads to a moderately large PBG. We delineate a variety of PBG architectures amenable to fabrication by holographic lithography. In this technique, an optical interference pattern exposes a photo-sensitive material, leading to a template structure in the photoresist whose dielectric-air interface corresponds to an iso-intensity surface in the exposing interference pattern. We demonstrate PBG architectures obtainable from the interference patterns from four independent beams. The PBG materials may be fabricated by replicating the developed photoresist with established silicon replication methods. We identify optical beam configurations that optimize the intensity contrast in the photoresist. We describe the invention of a new approach to holographic lithography of PBG materials using the diffraction of light through a three-layer optical phase mask (OPM). We show how the diffraction-interference pattern resulting from single beam illumination of our OPM closely resembles a diamondlike architecture for suitable designs of the phase mask. It is suggested that OPML may both simplify and supercede all previous optical lithography approaches to PBG material synthesis. Finally, we demonstrate theoretically the creation of three-dimensional optical waveguide networks in holographically
defined PBG materials. This requires the combination of direct laser writing (DLW) of lines of defects within the holographically-defined photoresist and the replication of the microchip template with a high refractive index semiconductor such as silicon. We demonstrate broad-band (100-200 nm), single-mode waveguiding in air, based on the light localization mechanism of the PBG as well as sharp waveguide bends in three-dimensions with minimal backscattering. This provides a basis for broadband 3D integrated optics in holographically defined optical microchips.
Acknowledgements

I would first like to thank my advisor, Professor Sajeev John, for his guidance and support during my graduate studies. I am deeply grateful for his advice, insight, perspective, motivation, and encouragement. Neither I nor this thesis would be the same without his supervision.

I would also like to thank Professor G. A. Ozin and Professor J. H. Thywissen of my supervisory committee for keeping watchful eyes on my progress, both in the context of my work and my development as a graduate student.

I have been fortunate to have been surrounded by a diverse cast of colleagues in Professor John’s research group and scattered throughout the physics department. Our interactions, whether or not related to physics, have truly been enriching, and I wish each of these friends the best. I am particularly indebted to Dr. Ovidiu Toader and Dr. Alongkarn Chutinan for numerous helpful discussions and pieces of advice.

Finally, I thank my family for their enduring love, encouragement, and understanding. I especially thank my wife Karen for being my steadfast partner and for her sacrifice and support.

Contents

1 Introduction 1
   1.1 Photonic Band Gap Materials 1
   1.2 Design and Fabrication of 3D PBG Materials 6
   1.3 Outline 14

2 Photonic Band Gap Synthesis by Photo-electrochemical Etching 16
   2.1 Introduction 16
   2.2 Photonic Band Structure of Kielovite and Optimization of the PBG by Pore Modulation 18
   2.3 Robustness of the PBG to Structural Parameter Modifications 21
   2.4 Discussion 25

3 PBG Templates Using Optical Interference Lithography 27
   3.1 Introduction 27
   3.2 Structure Description 29
   3.3 Design of holographic structures which exhibit photonic band gaps 32
      3.3.1 Face Centered Cubic 34
      3.3.2 Body Centered Cubic structure 42
      3.3.3 Simple Cubic 45
   3.4 Generalized tetragonal structures 48
   3.5 Robustness of holographic photonic crystals 50
### 4 Optical Phase Mask Lithography: A New Paradigm for Photonic Band Gap Synthesis

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.1 Introduction</td>
<td>63</td>
</tr>
<tr>
<td>4.2 Diffraction of light by optical phase masks</td>
<td>64</td>
</tr>
<tr>
<td>4.3 Optical Phase Mask Architecture</td>
<td>69</td>
</tr>
<tr>
<td>4.4 Photonic Band Gap Formation</td>
<td>72</td>
</tr>
<tr>
<td>4.4.1 Direct Structures</td>
<td>73</td>
</tr>
<tr>
<td>4.4.2 Inverse Structures</td>
<td>82</td>
</tr>
<tr>
<td>4.5 Proposed OPML Configurations</td>
<td>87</td>
</tr>
<tr>
<td>4.5.1 SU-8 photoresist</td>
<td>89</td>
</tr>
<tr>
<td>4.5.2 As$_2$S$_3$ photoresist</td>
<td>90</td>
</tr>
<tr>
<td>4.6 Discussion</td>
<td>91</td>
</tr>
</tbody>
</table>

### 5 Circuits for Light in Holographically Defined Photonic Band Gap Materials

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1 Introduction</td>
<td>94</td>
</tr>
<tr>
<td>5.2 Design Parameters</td>
<td>96</td>
</tr>
<tr>
<td>5.2.1 Computational Methods</td>
<td>97</td>
</tr>
<tr>
<td>5.3 Waveguide Design</td>
<td>98</td>
</tr>
<tr>
<td>5.4 Waveguide Bends</td>
<td>108</td>
</tr>
<tr>
<td>5.4.1 Horizontal Type I Waveguide Bends</td>
<td>108</td>
</tr>
<tr>
<td>5.4.2 Horizontal Type II Waveguide Bends</td>
<td>111</td>
</tr>
<tr>
<td>5.4.3 Horizontal Hybrid Waveguide Bends</td>
<td>114</td>
</tr>
<tr>
<td>5.4.4 Vertical Bends from Type I Waveguides</td>
<td>114</td>
</tr>
<tr>
<td>5.4.5 Vertical Bends from Type II Waveguides</td>
<td>115</td>
</tr>
<tr>
<td>5.5 Discussion</td>
<td>119</td>
</tr>
</tbody>
</table>

### 6 Discussion and Conclusions

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6. Discussion and Conclusions</td>
<td>121</td>
</tr>
</tbody>
</table>
List of Tables

3.1 Global intensity contrast ...................................................... 55
List of Figures

1.1 Partially infiltrated inverted opal structure ............................... 7
1.2 Diamond lattice of air spheres .............................................. 8
1.3 Slanted pore photonic crystal .............................................. 10
1.4 Woodpile photonic crystal .................................................. 11
1.5 Square spiral photonic crystal .............................................. 12

2.1 (a) First Brillouin zone and (b) photonic band structure of Kielovite . . . . 18
2.2 (a) Representation of Kielovite and (b) Side view of pore with radius modulation 20
2.3 Band structure of Kielovite with pore radius modulation and dependence of PBG on dielectric contrast ................................................. 20
2.4 Effect of the modulation amplitude $A$ on the PBG ........................ 21
2.5 Effect of the modulation width on the PBG ................................ 22
2.6 Effect of the bare pore radius on the PBG ................................ 22
2.7 Photonic band edges as functions of changes in the structural parameters .... 23
2.8 Dependence of the PBG on the healing length of step modulations ......... 24

3.1 Reciprocal space of a simple cubic lattice .................................... 33
3.2 Iso-intensity surfaces of the FCC interference pattern ....................... 36
3.3 Beam configuration for diamond interference pattern with (a) elliptically polarized and (b) linearly polarized beams ............................... 39
3.4  (a) Iso-intensity surface generated by FCC intensity pattern with $\xi = \pi/2$ and
(b) corresponding photonic band structure .......................... 40

3.5  Beam configuration which generates the non-inversion symmetric FCC structure 41

3.6  Optimized BCC iso-intensity pattern ................................. 43

3.7  Beam configuration for BCC interference pattern with (a) elliptically polarized
and (b) linearly polarized beams ....................................... 44

3.8  Optimized Si structure for SC HLPC ................................. 46

3.9  Beam configurations generating the SC intensity pattern using (a) elliptically
and (b) linearly polarized beams ....................................... 47

3.10 PBG size as a function of the angle between target vectors ............... 49

3.11 Photonic band structure of a generalized Tetragonal photonic crystal .... 50

3.12 Volume solid fraction versus intensity threshold ........................ 51

3.13 PBG vs. solid volume fraction ....................................... 53

3.14 Photonic band structure diagrams for optimized structures ................ 54

3.15 PBG size as a function of the refractive index contrast ................... 55

3.16 (a) Average intensity contrast factor and (b) Minimum intensity contrast as
functions of solid volume fraction ..................................... 57

3.17 Changes in photonic band gap edges as beam amplitudes are perturbed 58

3.18 Changes in photonic band gap edges as elliptical polarization components are
perturbed ............................................................... 59

3.19 Changes in photonic band gap edges as elliptical polarization phases are per-
turbed ............................................................... 60

3.20 Changes in photonic band gap edges as linear polarization angles are perturbed 60

4.1  Schematic representation of the optical phase mask .................. 70

4.2  Target intensity pattern ............................................... 71

4.3  Iso-intensity surface created by optical phase mask .................. 73

4.4  Solid volume fraction and resulting PBG as functions of threshold iso-intensity 75
Chapter 1

Introduction

1.1 Photonic Band Gap Materials

Photonic crystals are periodically ordered, artificial, dielectric microstructures that facilitate the localization of light with wavelengths comparable to the lattice periodicity of the structure [1]. When the Bragg scattering resonance from the periodic lattice and the microcavity resonances from the individual dielectric “atoms” in a single unit cell are tuned appropriately through careful engineering of the photonic crystal structure, electromagnetic waves of a certain spectral region, referred to as the photonic band gap (PBG), are forbidden from propagating in any direction in the crystal. The presence of the PBG in the electromagnetic density of states leads to the possibility of strong light localization [2], inhibition of spontaneous emission [3], and other quantum electrodynamical effects due to the formation of a photon-atom bound state [4].

From a practical point of view, one of the most exciting potential applications of photonic crystals is in the area of information processing. Traditionally, electron transport mechanisms in semiconductors have been used to perform the computing, storage, and transfer tasks required in this technology. However, these electronic mechanisms suffer from high heat generation and significant cross-talk between channels due to the interactions between electrons, shortcomings that become increasingly important as the size of information processing com-
ponents decreases. On the other hand, photons do not in general interact with one another, except in nonlinear processes significant only under specific conditions. In addition to limiting cross-talk, this allows for increased bandwidth in multi-wavelength photonic channels. The amount of heat generated in a photonic crystal-based optical device is also low, due to low absorption of light in the material. Already, photons in optical fibers are the information carrier of choice for transport over distances from about one meter, interconnecting multiple computers to form clusters, to hundreds of kilometers, creating international communications networks. At shorter length scales, the unique characteristics of PBG materials make them an attractive and robust platform for integrating active and passive devices in an all-optical microchip.

A fundamental requirement for an all-optical microchip is the existence of waveguides to transport light throughout various points in the chip. Traditionally, dielectric guides based on total internal reflection have been used to guide light at visible and near infrared wavelengths\(^1\). This scheme for light transport is restricted by radiation loss as light is guided around sharp bends with radii of curvature on the order of the wavelength of the guided light. On the other hand, by making use of strong light localization stemming from the existence of a PBG, photonic crystal waveguides can have sharp, low-loss bends. This is achieved by introducing defects into the periodic structure of the photonic crystal, allowing for localized modes with frequencies inside the PBG. When the defects are created by the removal of dielectric material from the photonic crystal, these localized modes are “air modes” with the majority of the electromagnetic field concentrated in the regions of low dielectric constant (typically air) in the structure [5]. A waveguide can then be formed by carving a linear defect in the photonic crystal. Light in the waveguide is confined to the vicinity of the line defect as the presence of the PBG forbids propagation in the unaltered regions of the photonic crystal. Since the localized mode is concentrated mainly in air, the loss from absorption is low, and therefore the main source of loss can be only from reflection at the end of the waveguide. As a result, it is possible in a photonic crystal to guide light through micron-scale, single-mode waveguide

\(^1\)Metallic pipes can be used to guide microwaves but are lossy in the optical regime.
channels with sharp, low-loss bends [6–9]. Extending the waveguide network to all three spati-
dial dimensions [10, 11] provides an opportunity to create an all-optical microchip with high
density. Furthermore, the inclusion of point defects in the photonic crystal forms resonant cav-
ities in the optical network, leading to the possibility of other passive optical devices such as

The existence of a PBG can also facilitate frequency selective control over spontaneous
emission of light from individual atoms in the photonic crystal circuit. It has long been rec-
ognized that the spontaneous emission rate is not an intrinsic property of atoms, but rather an
effect that depends on the interaction between atoms and their environment [14]. If the den-
sity of available photon modes in the frequency range of interest is high relative to the free
space density of states, the spontaneous emission rate will be enhanced. Conversely, sponta-
neous emission is suppressed when the electromagnetic density of states is lower than in free
space [15]. Prior to the introduction of the PBG concept, experimental work on the enhance-
ment and inhibition of spontaneous emission focused on metallic cavities in the microwave
regime [16–18]. This paradigm is not well suited to optical frequencies since metallic cavities
become lossy. On the other hand, photonic crystals fabricated using dielectric materials can
offer significant deviation from the free space density of states in the optical regime. Intro-
ducing a defect into a photonic crystal so that only a single desired mode is supported and
other spontaneous emission modes are suppressed can lead to the realization, in the ideal case,
of “thresholdless” lasers [19, 20]. The same concept can be used to increase the extraction
efficiency from light-emitting diodes [21].

In order to reap the benefits of photonic crystal-based optical microchips it is crucial to
develop efficient, low-cost methods for micro-fabrication of high quality, wafer-scale materials
with large and robust, three-dimensional (3D) PBGs centered around 1.55 \( \mu m \), the wavelength
of choice in optical telecommands. The lattice constant for the photonic crystal scales with
the wavelength of the band gap, and hence structures with optical PBGs must have submicron
lattice constants. Synthesizing such structures with high accuracy and low cost has been a
major scientific and technological challenge over the past two decades. In this context, a major focus of this thesis is the design of photonic crystals with large, robust, 3D PBGs and the invention of novel methodologies for microfabrication. A specific highlight of this thesis is the introduction of a method that we refer to as “Optical Phase Mask Lithography” (see Chapter 4). This method should greatly simplify the task of fabricating 3D PBG materials on a large scale and possibly enable the very low cost, mass production of PBG-based optical microchips.

The conventional wavelength window for fiber-optic communications spans the range 1.53–1.57 $\mu$m (a frequency bandwidth of approximately 2.6% of the center frequency), and recently optical fibers have been developed exhibiting low loss over the wavelength range 1.30–1.65 $\mu$m (corresponding to a relative frequency bandwidth of approximately 24% of the center frequency) [22]. These bandwidths can be considered the current and foreseeable future requirements for a PBG-based system. In practice, the actual PBG in a synthesized structure must withstand degradation from fabrication-related imperfections. Therefore, it is important to design 3D photonic crystal structures with large and robust bandgaps.

The difficulties in large-scale micro-fabrication of 3D architectures have led some scientists to study simpler 2D photonic crystals [23,24]. These materials are characterized by periodicity in two dimensions and (for membranes) finite thickness in the third dimension. Their simpler architectures lend them to more conventional semiconductor micro-lithography [25]. The drawback is the loss of PBG-based confinement along the third dimension. Finite-thickness 2D photonic crystal “membranes” rely on conventional total internal reflection (index guiding) to confine light in the third dimension [26]. This is accomplished by using a thin, high refractive index photonic crystal layer surrounded by a low index homogeneous background [27–30]. The high index contrast enables specific modes with frequencies inside the 2D PBG to be confined without leakage through total internal reflection. By restricting operation to these modes below the light line, it is possible to achieve 3D confinement of light. However, this confinement, which is lossless in principle, is compromised by disorder and surface roughness causing scattering into the third dimension. As the scattering losses scale with the cube of the differ-
ence in dielectric constant, \((\Delta n)^3\) [31], robustness to disorder is particularly relevant to high index contrast slabs. Losses as low as 5 dB/cm have been reported for straight waveguides in silicon 2D photonic crystal membranes with 3 nm surface roughness [32]. In comparison, thin (100 nm thick) silver plasmonic waveguides have exhibited losses of approximately 1.2 dB/\(\mu m\) [33]. An alternative to 2D photonic crystal membranes for index guiding in 2D photonic crystal slabs is the use of a three-layer structure consisting of a high index core surrounded by lower index cladding regions. In this paradigm, 2D periodicity extends throughout the core and cladding layers [36]. For small index contrast between the core and cladding layers (typically \(\Delta n \approx 0.2\)), the radiation leakage into the third dimension is small even though the modes operate above the light line (weak confinement) [37]. However, this phenomenon relies on large aspect ratios for the periodic features in the cladding layers, making fabrication more arduous in general. In both of the above 2D photonic crystal paradigms, the 3D electromagnetic density of states is non-zero due to degenerate modes that are not bound by total internal reflection. As a result, the inhibition of spontaneous emission in 2D photonic crystal slabs is not as strong as that in 3D PBG materials. On the other hand, 2D-3D PBG heterostructures, consisting of 2D photonic crystal layers surrounded by 3D PBG cladding layers that provide PBG-based confinement in the third dimension, have been predicted to guide light without radiation leakage [38, 39].

A particularly successful application of 2D photonic crystals has been in the control of dispersion and guidance of light in air in so-called photonic crystal fibers (PCF) [40,41]. These are a novel class of micro-structured fibers consisting of finite-size 2D photonic crystals with an axial defect. Light propagates along the fiber axis but is transversely localized in the defect by the photonic crystal structure. For an appropriately designed “hollow core” PCF, it is possible to achieve guidance in air [42]. This effect depends crucially on light localization within the 2D PBG, and is not possible with index guided fibers.

---

Plasmonic waveguides are subject to a tradeoff between mode size and propagation size [34]. As a result, infinitely wide plasmonic thin slab waveguides have shown attenuation on the order of 10-0.1 dB/cm [35].
1.2 Design and Fabrication of 3D PBG Materials

In this thesis we present a novel route to the microfabrication of 3D PBG materials. However, the optical lithography methods that we describe were preceded by numerous efforts utilizing more conventional semiconductor microlithography. In this section we review some of the history of PBG microfabrication.

The first proposals of the PBG concept suggested that structures with face centered cubic (FCC) Bravais lattice symmetry might have full 3D PBGs [2, 3]. This is because the first Brillouin zone (BZ) of the FCC lattice exhibits the least anisotropy. In other words, the difference between the shortest and longest distances from the center to the surface of the first BZ is the smallest. This, it was reasoned, increased the likelihood that one-dimensional stop-gaps throughout the full $4\pi$ solid angle would overlap and produce a complete 3D PBG. Subsequently, the photonic band structures of FCC lattices of spheres were studied both theoretically using scalar waves [43], and experimentally at millimeter scales [44]. These initial studies supported the hypothesis that a full 3D PBG could be achieved in the FCC lattice. It was shown, however, that a spherical scatterer within the FCC unit cell (Wigner-Seitz cell) prevents the creation of a PBG between the lowest possible bands due to the polarization degree of freedom of the electromagnetic field [45]. The experimentally observed “gap” in the FCC lattice of spheres was in fact a pseudogap, wherein the gap frequencies are forbidden throughout most, but not all, of the BZ. This leads to a low density of states rather than a total absence of allowed modes. However, an opal lattice\(^3\) of air spheres in a dielectric background (“inverted opal”) does have a small PBG between the higher bands, approximately 4% relative width for a Si structure. The field of opal-based PBG materials was invigorated by the discovery [46] that the size of a silicon inverse opal PBG could be more than doubled through partial rather than complete infiltration of the opal template with silicon. These facts were missed in early theoretical studies due to convergence problems at this gap’s higher normalized center frequency [47].

\(^3\)The opal lattice is a collection of close-packed spheres forming a FCC lattice
Fig. 1.1 shows a computer rendition of the partially infiltrated silicon-inverse opal structure. The concept of fabricating opal structures by colloidal self-assembly has a long, established history [48, 49]. However, materials suitable for the self-assembly process do not have large dielectric constants and low absorption at optical frequencies in tandem, needed for optical PBG formation. Instead, self-assembled silica spheres are used as a template for inversion to a suitable material. Early attempts [50, 51] to infiltrate an opal template with a high refractive index material either failed to achieve sufficient infiltration or led to highly disordered structures. This created widespread belief that suitable inversion of opal templates was either impractical or impossible. The first experimental demonstration of a high quality silicon inverse opal [52] changed this situation dramatically. The opal is first infiltrated by chemical vapor deposition of disilane, followed by selective etching of the silica. This is a process that can be performed on large scales [52–54]. As predicted theoretically [46], the optimal inverted opal structure is achieved when the silica template is only partially infiltrated with silicon, leading to a 9% relative PBG. The small PBG of the inverted opal structure, occurring between the eighth and
ninth photonic bands, is fragile and vulnerable to disorder [54, 55]. Nevertheless, fabrication of high quality inverted opal structures provides a valuable proof of principle for the inversion methods needed for more robust PBG architectures.

The diamond structure, which can be viewed as a FCC lattice with a two “atom” basis with the atoms separated along the (1, 1, 1) crystallographic direction, breaks the spherical symmetry of the FCC lattice of spheres while retaining the FCC BZ and its minimal anisotropy. Consequently, a diamond lattice of overlapping air spheres was theoretically shown to possess a sizeable 3D PBG, approximately 27% of the center frequency when the air spheres sit in a background material with a dielectric constant of 11.9, corresponding to silicon [45]. Fig. 1.2 shows a computer rendition of the diamond lattice of air spheres.

The potential of large PBG formation led to several theoretical blueprints and subsequent fabrication attempts for photonic crystals based on “diamondlike” structures employing non-
spherical bases on a FCC lattice. This began with the fabrication of a FCC lattice of criss-crossing pores exhibiting a 3D PBG in the microwave spectrum [56]. This structure, nick-named Yablonovite, is a special case of a slanted pore (SP) photonic crystal consisting of 3 pores per unit cell. In a more general classification scheme, it is denoted as a “SP-3” PBG material [57, 58]. The SP-3 crystal is conceptually straightforward to implement: a triangular lattice is defined on the \([1, 1, 1]\) plane of the material, and three pores extend from each lattice point, one each in the \((0, 1, 1), (1, 0, 1),\) and \((1, 1, 0)\) directions. When the background material is Si, this structure has a predicted 17% relative PBG. The successful but tedious fabrication of the SP-3 photonic crystal on the centimeter scale spurred many attempts to replicate the structure on the submicron scale. However, this task proved very challenging. Methods involving electron beam lithography followed by reactive ion etching were successful in producing sub-micron pores, but the resulting slabs were only a few periods thick and severe imperfections occurred at the pore crossing points [59, 60]. Experiments with deep x-ray lithography (LIGA) patterning of an x-ray sensitive resist produced several periods of the criss-crossing pores [61], even allowing for the incorporation of controlled defects by multiple exposures [62]. Unfortunately, structures patterned in this fashion, to date, have lattice constants too large for a PBG in the optical regime. Another approach to the fabrication of slanted pore PBG materials is a hybrid scheme involving photo-electrochemical etching to generate one set of pores, followed by focused ion beam etching in macroporous silicon to create the second and third sets of pores [63, 64]. This method was used to synthesize a five-period-thick slab with a PBG centered around 3 \(\mu m\), still larger than the desired 1.5 \(\mu m\) wavelength. Photo-electrochemical etching methods alone have also been used to produce an elongated version of the SP-3 architecture with high aspect ratios [65, 66], nicknamed “Kielovite”. The elongation changes the Bravais lattice symmetry of the structure. The resulting increase in the anisotropy of the first BZ reduces the PBG. In Chapter 2 we discuss the effects of the elongation and demonstrate that its effects on the PBG can be mitigated by modulation of the pore radius. Recently, a variety of slanted pore architectures have been studied and classified. Slanted pore photonic
crystals with only two pores per unit cell (SP-2 structures) have been shown [57, 58] to exhibit gaps larger than that of the more complex SP-3 architectures. Fig. 1.3 shows a computer rendition of the optimized SP-2 structure. The simple geometry of the SP-2 structures also offers greater ease of fabrication and improved structural integrity due to less pore-crossing effects. SP-2 structures have been fabricated [67] using “direct laser writing” (DLW) processes involving two-photon absorption causing polymerization in resins [68–70]. In this process, the desired structure is written point-by-point (“voxel-by-voxel”) into the target material by means of a tightly focused laser spot. Two-photon absorption of the light near the focus alters the chemical properties of the material, allowing for selective chemical etching of the exposed or unexposed regions depending on the particular material. Recently, 2D-3D PBG heterostructure templates have been fabricated using DLW [71].

Another diamondlike structure is the layer-by-layer “woodpile” architecture [72, 73]. This structure consists of four repeating layers, each consisting of parallel rods separated in-plane
by the periodic lattice constant $a$. The first and third layers differ by an in-plane translation of $a/2$ in the direction perpendicular to the rods, and the second and fourth layers differ by a $90^\circ$ rotation from the first and third slices. The optimized woodpile structure, shown in Fig. 1.4, can have a PBG approximately 18% of the gap center frequency when the rods are synthesized with Si. There have been several approaches to address the fabrication of woodpile photonic crystals due to the simplicity of the architecture. The use of established silicon micromachining techniques such as repetitive deposition and etching have produced high-quality structures with relevant feature sizes, but the structures were initially only about one period (between two and five layers) thick [74–76]. Experiments using wafer-fusion and laser-assisted alignment produced two to three periods of the woodpile in the third dimension, and demonstrated the possibility of introducing defects into the structure [77]. An inexpensive method involving nanofabrication of the individual layers followed by microassembly of the separate layers provides a simple way to introduce defects because each layer can be fabricated uniquely [78].
Proper alignment of the layers is achieved by inserting microspheres into fiducial holes in neighbouring plates, but the tedious manner of assembly limits the size of the structure. On the other hand, woodpiles synthesized by laser-induced chemical vapor deposition are limited in the number of layers only by the size of the deposition chamber, but due to the laser spot size, the resulting PBG is centered around 75 μm [79]. Metallic photonic crystals exhibiting enhanced thermal emission near the photonic band edge [80] have been fabricated by the replacement of Si by tungsten in silicon-silica woodpiles, followed by removal of the silica [81]. Woodpiles have also been formed in polymer photoresists through DLW processes [68, 70]. Double inversion of these templates, first from SU-8 to silica, then from silica to silicon, leads to replication of the woodpile structures in silicon [82]. In addition, DLW has been used to fabricate a woodpile in chalcogenide glasses, whose refractive index is sufficient to open a PBG [83].
An alternative diamondlike PBG design is the “square spiral” architecture consisting of interleaved square spiral posts placed on a tetragonal lattice. A computer generated schematic diagram of the square spiral architecture is shown in Fig. 1.5. The optimized square spiral design, in which square spirals of air are created in a Si background, has a relative PBG of 24% [84, 85]. Square spiral photonic crystals, distinguished by the characteristic that each 2D slice of the structure differs only by a continuous translation from its neighbouring slices, are particularly amenable to fabrication by glancing angle deposition methods (GLAD) involving oblique angle physical vapor deposition on a prepatterned substrate coupled with rotational control of the substrate [86, 87]. Optical reflectivity measurements in a weakly disordered version of these silicon square spiral crystals have revealed a 3D PBG of roughly 10% relative to the center frequency [88]. Fabrication of square spirals by DLW has also been demonstrated [89, 90].

Architectures with simple cubic Bravais lattice symmetry can also support the formation of small 3D PBGs [91]. Layer-by-layer type simple cubic structures have been reported. These include silicon sheets with round- and square-shaped holes that were cut with a diamond saw and aligned with a microscope (lattice constant 530 \( \mu \text{m} \)) [92]. Smaller structures have been fabricated by nonselective dry etching and selected wet etching in GaAs (3.5 \( \mu \text{m} \)) [93], and silicon micromachining involving repetitive deposition, etching, and polishing (3.2 \( \mu \text{m} \)) [94]. Alternatively, photo-electrochemical etching of parallel pores with strong pore radius modulation followed by anisotropic widening of the pore structure, producing holes with square cross sections, has been used to produce a simple cubic structure with a lattice constant of 2 \( \mu \text{m} \) [95]. This leads to a doubling of the PBG size from the case of pores with circular cross sections, when the axes of the square holes are rotated by an angle of 45° with respect to the axes of cubic lattice.
1.3 Outline

In this thesis, we present an alternative paradigm for the large-scale micro-fabrication of 3D PBG materials and 3D photonic crystal-based microchips. The photonic crystal architectures we examine are themselves determined in part by particular optical lithographic processes available experimentally. The remainder of the thesis is organized as follows.

In Chapter 2 we discuss the optical properties of a photonic crystal that can be synthesized by oblique angle photo-electrochemical pore etching in silicon. Due to the nature of the etching process, this “Kielovite” pore structure has the Bravais lattice symmetry of an elongated FCC lattice [96]. We show that the resulting increase in the irreducible Brillouin zone of the structure causes a decrease in the PBG size of Kielovite with respect to the ideal SP-3 architectures. We then propose a modulation of the pore diameter that can be achieved by changing the light intensity during the etch process. This results in a doubling of the PBG from the unmodulated case.

In Chapter 3 we provide a detailed analysis of a new paradigm in photonic crystal design and fabrication based on the exposure of a photo-sensitive material by 3D optical interference patterns. The resulting photonic crystal has periodic properties that mimic those of the exposing interference pattern. We consider structures generated by four beam laser interference patterns [97]. By considering point and space group symmetries to produce interference patterns with minimized irreducible Brillouin zones, we obtain laser beam parameters that generate a diamondlike photonic crystal, a novel body-centered cubic architecture, and a simple-cubic structure. We introduce a novel non-inversion symmetric photonic crystal exhibiting two distinct, complete PBGs. We also describe a generalized class of tetragonal photonic crystals that interpolate between the diamondlike and body-centered cubic architectures. A detailed analysis of choices of beam polarizations leading to maximum intensity contrast in the optical interference pattern is presented.

Chapter 4 introduces a novel and simplified approach to produce the diamondlike optical intensity pattern required for photonic band gap synthesis. This is done through the inven-
tion and theoretical characterization of a three-layer optical phase mask [98]. We consider the diffraction-interference pattern resulting from single-beam exposure of the optical phase mask and find a target pattern for producing structures with large PBGs. We then explore the parameter space defined by various three-layer phase mask architectures to generate the target interference pattern. We present examples of photonic crystals that could be synthesized through this method. Finally, we suggest a specific blueprint for an optical phase mask consisting of silicon and silica, placed on a silica substrate, for single-beam illumination (through the substrate) and exposure of a SU-8 photoresist.

In Chapter 5 we demonstrate the possibility of creating broad-band, single-mode 3D optical waveguide networks in the diamondlike structure discussed in the previous chapters. By examining the electromagnetic field distributions in the periodic structure, we obtain design rules to create waveguide channels in all three spatial directions. We then demonstrate high bandwidth, low-loss transmission of light through sharp bends connecting waveguides in different directions. This provides a basis of 3+1 dimensional integrated optics in holographically defined PBG materials. Here, there are three dimensions of geometrical integration and an additional “dimension” of frequency bandwidth.

Finally, in Chapter 6 we make concluding remarks and comment on possible extensions to the work presented here.

Throughout the thesis, we use the plane wave expansion method to calculate the photonic band structure of various photonic crystal architectures. We describe the calculation in Appendix A. Unless otherwise specified, we assume that the high dielectric constant regions of the photonic crystals correspond to silicon and the low dielectric constant regions to air, with dielectric constants of 11.9 and 1, respectively. The diffraction-interference patterns from optical phase masks are calculated using rigorous coupled wave analysis, the details of which are given in Appendix B. We describe the finite-difference time-domain method, used to simulate the propagation of light through waveguide bends, in Appendix C.
Chapter 2

Photonic Band Gap Synthesis by Photo-electrochemical Etching

2.1 Introduction

As mentioned in Sec. 1.2, the FCC lattice of criss-crossing pores, Yablonovite, breaks the spherical symmetry within the FCC unit cell, allowing for the formation of a PBG between the lowest possible bands. This conceptually straightforward diamondlike structure was fabricated in the microwave regime using conventional drill bits [56], but it has proven difficult to produce pores with the sub-micron radii required for a PBG in the optical regime. Electron beam lithography and reactive ion etching methods [59, 60] have been used to produce such pores, but only a few periods of the structure were produced, and there was severe degradation of the structure at the pore crossing points. On the other hand, experiments with x-ray lithography [61] have produced structures with lattice constants in the 10-50 \( \mu m \) range in polymer photoresists. These templates require replication with a high refractive index semiconductor such as silicon, and if this secondary replication step were be performed, the resulting PBG would occur in the 25-125 \( \mu m \) range.

In this chapter, we discuss a new PBG blueprint based on the remarkable discovery [65]
that a stretched FCC lattice can be fabricated using photo-electrochemical etching in single-crystal Si. Photo-electrochemical etching yields pores with high length-to-diameter aspect ratios in the range 100-500 [66]. In the etching process [99, 100], pore tips are formed on the etching surface, for instance by photolithography and alkaline etching. The surface with the pore tips is exposed to a dissolving solution, often HF, while the opposite (back) face is illuminated. The light absorption from the illumination generates electronic holes, which diffuse to the etching surface and are consumed at the pore tips. This promotes dissolution of the material at the pore tips, which in turn grows the pores. The pore radius is controlled only by the amount of illumination. Macropores formed using this technique grow in the $(1, 0, 0)$-direction when the etching surface is normal to $(1, 0, 0)$ and in the $(1, 1, 3)$ family of directions when the etching surface is the $[1, 1, 1]$ crystallography surface. To generate the criss-crossing pore structures discussed here, three pores from the $(1, 1, 3)$ family are grown from points on a triangular lattice defined on the $[1, 1, 1]$-plane of the material, resulting in an FCC lattice that is “stretched” in the $(1, 1, 1)$-direction. We refer to this structure as “Kielovite.” Unfortunately, this deformation results in a crystal with a smaller PBG than that of Yablonovite. However, this etching process allows for modulation of the pore radius along the growth direction. Increasing the illumination increases the overall charge carrier current from the back face to the etching face. Since the number of pore tips remains the same, the pore radius increases in response and thus can be accurately controlled by the amount of illumination. Structures incorporating such modulation have already been demonstrated in 2D photonic crystals [101]. We demonstrate that a suitable pore modulation in Kielovite can yield a PBG of nearly 16% of the gap center frequency.
CHAPTER 2

2.2 Photonic Band Structure of Kielovite and Optimization of the PBG by Pore Modulation

We consider first the naturally occurring Kielovite structure, with no modulation of the pore radius. In this case the only structural parameter to adjust is the overall pore radius, which in turn determines the volume filling fraction of solid material. For simplicity we consider a material with a dielectric constant of 11.9, which corresponds to that of silicon. In contrast, the pores are taken to be filled with air. Band structures are calculated using the plane wave expansion method described in Appendix A with over 720 plane wave directions (over 1440 plane waves in total). The results are practically indistinguishable from those obtained for the same structures using over 1300 plane wave directions. The Fourier coefficients of the dielectric structure are calculated using a discrete Fourier transform with 256 points per direction.

The structure is modeled using a hexagonal lattice, which is defined by primitive lattice vectors $\vec{a}_1 = a \left( \frac{1}{2}, -\frac{\sqrt{3}}{2}, 0 \right)$, $\vec{a}_2 = a \left( \frac{1}{2}, \frac{\sqrt{3}}{2}, 0 \right)$, and $\vec{a}_3 = c \left( 0, 0, 1 \right)$. For our structure, we define...
the etching surface to be the xy-plane, with $a$ being the lattice constant of the triangular lattice. The length of $\vec{a}_3$ is prescribed by the angles between the etching surface normal and the pores. For Kielovite, $c/a = \frac{5}{2}\sqrt{3} = 3.06$. The reciprocal lattice is likewise a hexagonal lattice and the Brillouin zone is shown in Fig. 2.1(a), with the high-symmetry points labelled. It is important to note that Yablonovite has an irreducible Brillouin zone (IBZ) which is the same as that of the FCC Bravais lattice. However, the same is not true for Kielovite. Due to the deformation in the direction perpendicular to the etching surface, the IBZ of Kielovite is considerably larger than the FCC Bravais lattice. Fig. 2.1(b) shows the band structure of Kielovite with no pore radius modulation, at a volume filling fraction of 79% air, which optimizes the band gap. The pores have radius $0.34a$, where $a$ is the lattice constant of the triangular lattice on the etching surface. The resulting PBG, denoted by the hashed area on the figure, is 8%, roughly half the optimized PBG for the FCC lattice with the same dielectric contrast. The origin of the narrowing of the PBG is clearly seen to be the lowering of the fifth and sixth bands at the A-point. Here, the difference in the IBZ between our structure and the FCC lattice of pores is important: if one considers only the IBZ of the FCC lattice, then this A-point is irrelevant.

In order to increase the PBG of the structure, we introduce a modulation in pore radius, symmetrically placed in between pore intersections, as shown in Fig. 2.2(a). Fig. 2.2(b) shows a schematic side view of a pore with such a modulation, in the region between intersections with two other pores. The expanded pore radius occurs over a length $w$. The amplitude of the modulation is denoted as $A$, while the bare pore radius is denoted by $r$. We characterize a structure with a step modulation using these three parameters. The dotted curves show the structure with the same $[r, A, w]$ parameters but with a non-zero healing length, $h$. For a given volume filling fraction, choosing any two of $r$, $A$, or $w$ constrains the third. The modulation amplitude can be either positive (as pictured) or negative, the latter case implying a decrease in the pore radius over the width of the modulation. Fig. 2.3 shows the photonic band structure for a crystal with modulation of the pore radius, characterized by $[r, A, w] = [0.26, 0.11, 0.305]$, implying a volume filling fraction of 79% air. For a background dielectric constant of 11.9
Figure 2.2: (a) Representation of Kielovite with pore modulation, showing the intersection between three pores. (b) Schematic side view of pore with radius modulation of longitudinal extent \( w \) and transverse amplitude \( A \). The bare pore radius is \( r \). The dashed curves represent the modulation with a healing length \( h \).

Figure 2.3: Photonic band structure of Kielovite with positive pore radius modulation, characterized by \( [r, A, w] = [0.26, 0.11, 0.305] \). The volume filling fraction is 79% air, and the resulting PBG is 15.5% relative to the center frequency for a background dielectric constant of 11.9 (silicon). The dependence on the PBG size on the dielectric contrast is shown in the inset.
(silicon), the width of the PBG is 15.5% relative to the center frequency. Clearly the droop in the fifth and sixth bands at the A-point has diminished as a result of pore modulation. This is nearly as wide as the PBG found in Yablonovite with the same contrast in dielectric constants. Fig. 2.3 is representative of the largest PBG we find in the given parameter space. In contrast, we find structures with negative \( A \) have a smaller optimum PBG of 12% of the center frequency. The inset in Fig. 2.3 shows the dependence of the PBG on the background dielectric constant for the optimized structure. One can see that the PBG width initially increases dramatically as the dielectric contrast is increased, and then begins to saturate at large dielectric contrasts.

### 2.3 Robustness of the PBG to Structural Parameter Modifications

We find there is a great deal of flexibility in choosing parameters in order to approach the upper bound for the PBG width. This, in turn, suggests considerable robustness of the optimized PBG to structural parameter variations and random disorder effects. Fig. 2.4 shows the effect on the PBG width of changing \( A \) at various \( r \), with a fixed volume filling fraction of 82% air. The inset
Figure 2.5: Effect of varying the modulation width $w$ on the band gap at various $r$, with corresponding $A$ values shown in the inset. Volume filling fraction is fixed at 79% air. Lengths are given in units of the lattice constant $a$.

Figure 2.6: Effect of varying the bare pore radius $r$ on the band gap at various $w$ and volume filling fractions, with corresponding $A$ values shown in the inset. Lengths are given in units of the lattice constant $a$. 
Figure 2.7: The band edges as functions of changes in the structural parameters, $r$, $A$, and $w$. The relative change is given as a % of the initial value. The initial geometry is characterized by (a) $[r,A,w] = [0.26,0.11,0.305]$, and (b) $[r,A,w] = [0.30,0.07,0.265]$, with the lengths measured in units of the lattice constant $a$.

shows the values of $w$ required for the given $r$, $A$, and filling fractions. Clearly a large band gap can be achieved using several different configurations. Fig. 2.5, on the other hand, shows the effect of varying $w$ at fixed $r$, with volume filling fraction 79% air and $A$ constrained by these parameters. Again, the upper bound on the filling fraction is reached at several $w$. Finally, the effects of varying $r$ are shown in Fig. 2.6. In this case, the volume filling fraction is also changed, and we see that the upper bound is reached at a volume filling fraction of 79%.

It is important to note the effect of disorder in the structural parameters on the PBG. As a result of the fabrication process, small, random variations in the $r$, $A$, and $w$ parameters are likely to appear along the periodic structure. The effect of this can be studied by considering the shift in the band edge frequencies as the structural parameters are varied. The resulting PBG in a structure with weak disorder in these parameters will then be given by the intersection of the PBGs of the perfectly ordered structures whose parameters span the distribution present in the disordered structure [102]. Fig. 2.7 shows the band edges as functions of the structural parameters in perfectly ordered structures, with initial geometries corresponding to $[r, A, w] = [0.26, 0.11, 0.305]$ and $[r, A, w] = [0.30, 0.07, 0.265]$. One can see that the band edges are most sensitive to changes in the bare pore radius, $r$. 
A particularly important issue is the robustness of the PBG to gradual variations (non-zero healing lengths in the step modulation) of the pore radius. Such a gradual change in pore radius is inevitable in the photo-electrochemical etching process. This is modeled by using the hyperbolic tangent function to represent steps. Fig. 2.8 shows the effects of the healing length on the PBG size for $[r, A, w] = [0.26, 0.11, 0.305]$ and $[r, A, w] = [0.30, 0.07, 0.265]$. In both cases, the relative PBG size remains above 15% until the healing length reaches about $0.1a$. Clearly, the PBG remains robust to realistic smoothing effects in the step modulation of the pore radius.

Aside from centered step increases and decreases between pore intersections, we have also explored other modulations to the pore radius, with varying degrees of success with respect to increasing the PBG. For single step increases and decreases, a centralized modulation (symmetrically placed between adjacent pore crossings) produces a larger PBG than asymmetric modulations. Moving the modulation from the center point between pore intersections decreases the gap. Introducing a second step modulation into the pore radius also does not increase the gap to the same level as the single, centered, step increase. For such situations, the gap increases as the parameters tend towards the case of the single step increase. Finally, introducing a small
Chapter 2

Chapter 2

sinusoidal modulation to the pore radius, along the entire length of each pore, increases the relative gap from the 8% to the 11% range. This falls short of the nearly 16% PBG resulting from the more localized step modulations we have described above.

2.4 Discussion

Criss-crossing pore structures created by photoassisted electrochemical etching offer a unique opportunity for low cost, wafer-scale 3D PBG materials in a variety of group IV and III-V semiconductors. These materials consist of semiconductor single crystals and may be suitable for electrical pumping through the solid backbone and various opto-electronic applications.

The photo-electrochemical etching method is unique in that it allows pore depths of several hundred microns on large area wafers. For PBGs centered in the 800 nm to 1.55 μm range, this corresponds to more than $10^4$ unit cells of photonic crystal in each of the transverse directions and more than 100 unit cells in the vertical direction. Using realistic pore modulations, we have demonstrated that a complete 3D PBG spanning up to 16% of the center frequency is attainable in a number of important semiconductor materials, including Si, GaAs, and InP.

The use of optimized, Kielovite, PBG materials for optical micro-circuitry requires the incorporation of planar, line, and point defects into the otherwise 3D periodic lattice. A planar (2D microchip) effect can be introduced by means of larger or smaller modulation of each of the pores at a specified depth into the wafer. Line defects (optical waveguide channels) and point defects (optical micro-cavities) may be introduced by means of focused ion beam exfoliation of the semiconductor backbone at specified locations. It is also of considerable interest to micro-fabricate active regions within the 3D PBG wafer. This might be achieved by means of planar quantum dot layers (for instance InAs dots in InP) buried within the semiconductor wafer, prior to electrochemical etching. Photonic band gap properties may also be tuned through ultra-fast processes such as free carrier injection through optical pulses at frequencies above the PBG and above the electronic semiconductor gap of the PBG backbone [103].
These considerations suggest a broad spectrum of opportunities for “Kielovite” PBG materials. The realization of a 16% complete 3D PBG on wafer scale samples using the prescribed pore modulation during the photo-electrochemical etch would be a major advance relative to the more widely studied 2D macroporous silicon photonic crystals [66]. The realization of this 3D PBG in a single-crystal semiconductor of more than 100 micron depth would also be a unique achievement in the field of photonic crystals.
Chapter 3

PBG Templates Using Optical Interference Lithography

3.1 Introduction

Many previous attempts to synthesize PBG materials have struggled to adapt various fabrication methods to emulate theoretical blueprints ill-suited to fabrication at sub-micron length scales. Others have focused on theoretically adjusting the fabrication parameters of a well-established technique in search of a PBG. The optical interference lithography method, described in this chapter, offers a unique opportunity for efficient large-scale micro-fabrication of 3D PBG structures with large gaps in the optical regime. By employing the 3D interference pattern of four or more laser beams to expose a photopolymerizable material such as a photore sist or polymerizable resin [104–112], nearly perfect long range order (LRO) can be maintained over length scales much larger than the lattice constant of the photonic crystal. At the same time, this technique allows straightforward control over the periodic properties (Fourier coefficients) of the resulting structure through the laser beam parameters. The photoresist material undergoes a chemical alteration when the total light intensity due to the interference pattern, $I(\vec{r})$, at position $\vec{r}$, is maintained over a time interval $\delta \tau$ such that the “exposure” $I(\vec{r})\delta \tau$ ex-
ceeds a specified threshold, $T$. For a negative photoresist, the “underexposed” regions can be selectively removed using a developer substance which leaves the “overexposed” regions intact. (For a positive photoresist, overexposed regions are removed, leaving the underexposed regions intact.) The developed photoresist can then be infiltrated at room temperature with SiO$_2$ [113] and burned away, leaving behind a daughter “inverse” template. Finally, the daughter template is inverted by high temperature infiltration with silicon [52, 114] and selective chemical etching of the SiO$_2$. As a result, a 3D silicon photonic crystal is formed, in which the silicon-air boundary is defined by the original, optical, iso-intensity surface $I(\vec{r})\delta\tau = T$. Alternatively, the photoresist template can be infiltrated with a high refractive index material such as CdSe [115] which results in an inverted photonic crystal after the photoresist is burned or chemically etched away. A third option is to use a photopolymerizable film which is contains titanium [116], producing a direct titania structure after exposure to an intensity pattern and removal of underexposed material. Certain chalcogenide glasses are amenable to direct polymerization could also be used as photoresists to create direct structures in a single step [83].

In this chapter, we discuss the formation of 3D photonic crystals using holographic lithography based on the interference of four laser beams. Other proposed configurations include the use of multiple exposures and phase shifts between exposures [117, 118] and a hybrid five beam configuration with three beams forming a two-dimensional pattern and two other beams forming a one-dimensional pattern [106] in the out of plane direction. However, these configurations require careful manipulation of the relative phases between beams and between exposures. In contrast, in a four beam, single exposure configuration, the relative phases between laser beams does not change the shape of the the interference pattern. In previous theoretical reports, four beam holographic lithography configurations were proposed [118–120] to create structures which emulate particular cases of triply periodic minimal surfaces [121], which have been shown to produce large 3D PBGs [122, 123]. The resulting photonic crystals included a diamond-like structure, a “gyroid” structure with body centered cubic (BCC) Bravais lattice symmetry, and a simple cubic (SC) structure. Using simpler symmetry arguments, holographic
beam configurations for the diamond-like structure and a novel BCC structure have been derived [124]. Here, we describe our approach in detail and find alternative beam configurations for producing the diamond-like, BCC, and SC structures in which the intensity contrast is maximized. We also illustrate a non-inversion symmetric PBG architecture that interpolates between a simple FCC structure and a diamond network structure, and which exhibits two distinct and complete photonic band gaps. We also explore the robustness of the resulting PBGs against perturbations in the beam polarizations and amplitudes. Both the diamond and BCC structures are robust against deviations in the experimental control parameters. In Sec. 3.2 we introduce our framework for describing structures created by holographic lithography. Sec. 3.3 presents our design process for achieving 3D photonic crystals using this method, using the three cubic Bravais lattices. Sec. 3.4 describes a generalized class of tetragonal PBG materials that encompass both the diamond network and BCC structures. Sec. 3.5 describes the properties of our holographic photonic crystals relevant to robust micro-fabrication and error-tolerant PBG formation.

### 3.2 Structure Description

The interference of $N$ monochromatic plane waves of frequency $\omega$, wavevectors $\vec{G}_i$, polarization vectors $\vec{\epsilon}_i$, phases $\theta_i$, and real amplitudes $\mathcal{E}_i$ creates an electric field given by

$$\vec{E}(\vec{r}, t) = e^{-i\omega t} e^{i(\vec{G}_0 \vec{r} + \theta_0)} \left( \mathcal{E}_0 \vec{\epsilon}_0 + \sum_{i=1}^{N-1} \mathcal{E}_i \vec{\epsilon}_i e^{i(\vec{K}_i \vec{r} + \gamma_i)} \right),$$

where

$$\vec{K}_i \equiv \vec{G}_i - \vec{G}_0$$

and $\gamma_i \equiv \theta_i - \theta_0$. The corresponding, stationary intensity pattern is given by:

$$I(\vec{r}) \equiv \vec{E}^*(\vec{r}, t) \cdot \vec{E}(\vec{r}, t)$$
= \sum_{i=0}^{N-1} \mathcal{E}_i^2 + 2 \sum_{i=1}^{N-1} \mathcal{E}_0 \mathcal{E}_1 |\vec{e}_0 \cdot \vec{e}_i| \cos(\vec{K}_i \cdot \vec{r} + \gamma_i + \phi_i) \\
+ 2 \sum_{i>j=1}^{N-1} \mathcal{E}_i \mathcal{E}_j |\vec{e}_i \cdot \vec{e}_j| \cos(\vec{K}_{ij} \cdot \vec{r} + \gamma_i - \gamma_j + \phi_{ij}),

where \vec{K}_{ij} \equiv \vec{K}_i - \vec{K}_j, \phi_i \equiv \arg(\vec{e}_i^* \cdot \vec{e}_i), and \phi_{ij} \equiv \arg(\vec{e}_i^* \cdot \vec{e}_j). The holographic structure is a two phase medium whose phase boundary is defined by the “shape” function

\[ S(\vec{r}, I_{\text{thr}}^{\text{exp}}) = \Theta(I(\vec{r}) - I_{\text{thr}}^{\text{exp}}), \]

where \( I_{\text{thr}}^{\text{exp}} \) is a threshold value and \( \Theta = 1 \) for \( x \geq 0 \) and zero otherwise (Heaviside step function). By convention, we assume the high intensity regions in Eq. (3.2) become the silicon component of the photonic crystal \( (\varepsilon(\vec{r}) = 1) \) where \( I(\vec{r}) < I_{\text{thr}}^{\text{exp}} \) and \( \varepsilon(\vec{r}) = 11.9 \) where \( I(\vec{r}) \geq I_{\text{thr}}^{\text{exp}} \). This corresponds to the case in which a negative photoresist is used to make the photonic crystal template. It will be shown in Sec. 3.5 that for the optimized structures considered here, equivalent structures can be obtained with a positive photoresist by simply adjusting the threshold \( I_{\text{thr}}^{\text{exp}} \).

In the case \( N = 4 \) (which provides the minimum number of non-collinear beams required to produce a nontrivial 3D intensity pattern), Eq. (3.2) becomes \( I(\vec{r}) = I_0 + 2 \Delta I(\vec{r}), \) where \( I_0 \equiv \mathcal{E}_0^2 + \mathcal{E}_1^2 + \mathcal{E}_2^2 + \mathcal{E}_3^2 \) and

\[ \Delta I(\vec{r}) \equiv c_1 \cos(\vec{K}_1 \cdot \vec{r} + \gamma_1 + \phi_1) \]
\[ + c_2 \cos(\vec{K}_2 \cdot \vec{r} + \gamma_2 + \phi_2) \]
\[ + c_3 \cos(\vec{K}_3 \cdot \vec{r} + \gamma_3 + \phi_3) \]
\[ + c_{12} \cos(\vec{K}_{12} \cdot \vec{r} + \gamma_1 - \gamma_2 + \phi_{12}) \]
\[ + c_{13} \cos(\vec{K}_{13} \cdot \vec{r} + \gamma_1 - \gamma_3 + \phi_{13}) \]
\[ + c_{23} \cos(\vec{K}_{23} \cdot \vec{r} + \gamma_2 - \gamma_3 + \phi_{23}), \]
with
\[ c_i = E_0 \bar{E}_i |\bar{e}_i| \quad \text{and} \quad c_{ij} = E_i \bar{E}_j |\bar{e}_i| \cdot |\bar{e}_j|. \] (3.4)

The spatial modulation of the intensity pattern given by Eq. (3.3) is periodic with a lattice whose primitive vectors, \( \bar{a}_i \), satisfy \( \bar{K}_i \cdot \bar{a}_j = 2\pi n \delta_{ij} \), where \( n \) is an integer. As a consequence, the lattice constants are inversely proportional to the frequency of the laser beams.

The phase factors \( \gamma_i \) in Eq. (3.3), which result from the relative phases of the laser beams, can be simultaneously eliminated by a translation of the origin by \( \bar{\rho} = \gamma_1 \bar{\eta}_1 + \gamma_2 \bar{\eta}_2 + \gamma_3 \bar{\eta}_3 \), where \( \bar{\eta}_i \) satisfy \( \bar{K}_i \cdot \bar{\eta}_j = \delta_{ij} \). For configurations with more than four beams, the relative beam phases impart more than a simple translation in the intensity pattern, and cannot be easily ignored. On the other hand, the phase factors \( \phi_i \) and \( \phi_{ij} \), arising from the dot products between beam polarization vectors, cannot in general be simultaneously eliminated. In the case of linearly polarized beams, \( \phi_i \) and \( \phi_{ij} \) are zero for all \( i \) and \( j \) and the intensity pattern is always inversion symmetric relative to position \( \bar{\rho} \). However, in the case of elliptically polarized beams it is possible to obtain an interference pattern that is not inversion symmetric.

By rewriting the “experimental” intensity threshold as \( I_{\text{thr}}^{\exp} = I_0 + 2I_{\text{thr}} \) we arrive at the following simplified shape function:
\[ \Theta(I(\bar{r}) - I_{\text{thr}}^{\exp}) = \Theta(\Delta I(\bar{r}) - I_{\text{thr}}) \] (3.5)

In what follows, we focus our discussion of the resulting shapes on the simplified intensity pattern in Eq. (3.3). (The intensity background \( I_0 \) is nevertheless important, as a large background intensity will overwhelm the variation \( \Delta I(\bar{r}) \).)
3.3 Design of holographic structures which exhibit photonic band gaps

The design problem consists of identifying the set of six polarization and amplitude-dependent coefficients and phases

\[ C = \{ c_i, c_{ij} \}_{i<j=1,3} \]
\[ \Phi = \{ \phi_i, \phi_{ij} \}_{i<j=1,3}, \]

three \( \vec{K}_i \) vectors, and suitable threshold \( I_{\text{thr}} \), that generates a photonic crystal (through the shape function given by Eq. (3.5)) with a complete PBG. Given the parameters of the interference pattern \( C, \Phi, \) and \( \vec{K}_i \), the laser beam directions, amplitudes, and polarizations are then determined by finding the four beam directions, \( \{ \vec{G}_i \}_{i=0,3} \), which satisfy Eq. (3.1), then using these \( \vec{G}_i \) to find the four amplitudes and polarization vectors, \( \{ E_i, \vec{e}_i \}_{i=0,3} \), which satisfy the non-linear set of six equations given by Eq. (3.4).

The identification of \( C \) and \( \Phi \) and the choice of \( \vec{K}_i \) are obtained by two guiding principles: (i) choose a given Bravais lattice, and (ii) identify architectures leading to the smallest possible irreducible Brillouin zones (IBZ), then incrementally relax this condition if the resulting structure is too symmetric for a fundamental gap to open. In order to satisfy criterion (i), it is necessary and sufficient to choose the three \( \vec{K}_i \) vectors to be linear combinations with integral coefficients of vectors from the set \( \{ \vec{b}_i \} \), where we denote by \( \{ \vec{a}_i, \vec{b}_i \}_{i=1,3} \) a set of primitive and reciprocal vectors, respectively, of the desired Bravais lattice. On the other hand, criterion (ii) is far more restrictive. Indeed, only a very limited set of \( \{ C, \Phi, \vec{K}_i \} \) combinations generate intensity pattern with a sufficiently high symmetry.

Suppose that the desired holographic structure has a cubic symmetry (SC, BCC, or FCC). Fig. 3.1 shows several reciprocal lattice vectors of a simple cubic lattice, grouped by length. In order of increasing length, the first 3 sets of lattice vectors in the cubic reciprocal space are:
Figure 3.1: Reciprocal space of a simple cubic lattice. The first (red), second (green), and third (blue) order neighbours are located at the centers of the cube faces, the centers of the cube edges, and the cube corners, respectively. $\vec{b}_1$, $\vec{b}_2$, and $\vec{b}_3$ denote the primitive simple cubic reciprocal lattice vectors.

- (Red in Fig. 3.1) $\mathcal{B}^a = \{\pm \vec{b}_s^i\}$ of length $2\pi/a$, reaching the centers of the cube faces;

- (Green) $\mathcal{B}^b = \{\pm \vec{b}_b^i\} \cup \{\vec{b}_b^i - \vec{b}_b^j\}_{i \neq j}$ of length $2\pi\sqrt{2}/a$, reaching the centers of the cube edges; and

- (Blue) $\mathcal{B}^c = \{\pm \vec{b}_c^i\} \cup \{\pm(\vec{b}_c^i + \vec{b}_c^j + \vec{b}_c^k)\}$ of length $2\pi\sqrt{3}/a$, reaching the cube corners.

Here $i$ and $j$ run from 1 to 3 and $\vec{b}_s^i$, $\vec{b}_b^i$, and $\vec{b}_c^i$ denote the three primitive vectors of the SC, BCC, and FCC reciprocal lattices, respectively.

Choosing $\vec{K}$ vectors from one of these sets generates a holographic structure with a specific cubic symmetry. The first order reciprocal lattice vectors generate an SC spatial lattice, the second order vectors a BCC lattice, and the third order vectors a FCC lattice. The fourth set of vectors (not shown in Fig. 3.1) again generates an SC lattice, with a lattice constant of $|a|/2$ in this case. Similarly, higher order sets generate intensity patterns that can be described as one of the fundamental lattices (SC, FCC, or BCC) with increasingly small lattice constants. We therefore restrict our choice for the set of target vectors to the first 3, illustrated sets. We define
the set $\mathcal{T}$ of “target vectors” as a subset $\mathcal{T} \subset \mathcal{K}$, where $\mathcal{K} \equiv \{ \vec{K}_1, \vec{K}_2, \vec{K}_3, \vec{K}_{12}, \vec{K}_{13}, \vec{K}_{23} \}$ corresponding to nonzero terms in Eq. (3.3) (or, equivalently, nonzero coefficients in $\mathcal{C}$). The requirement of high symmetry can be achieved by choosing $\mathcal{T}$ simply to be a subset of one of the vector sets $\mathcal{B}^*$. Since $\Delta I(\vec{r})$ is insensitive to the sign of the target vectors in $\mathcal{T}$, an upper bound on the size of the sets $\mathcal{T}$ is 3 in the case of $\mathcal{B}^s$, 6 in the case of $\mathcal{B}^b$, and 4 in the case of $\mathcal{B}^f$.

### 3.3.1 Face Centered Cubic

We first illustrate the choice of $\mathcal{C}$ coefficients and $\Phi$ phases using the FCC Bravais lattice. Since there are only four distinct directions in the $\mathcal{B}^f$ set (Blue in Fig. 3.1), the target vector set can be denoted as $\mathcal{T} = \{ \vec{T}_1, \vec{T}_2, \vec{T}_3, \vec{T}_4 \}$. One possible choice for the three $\vec{K}_i$ vectors is the following:

$$
\vec{K}_1 = \frac{2\pi}{a} (1, 1, 1) \\
\vec{K}_2 = \frac{2\pi}{a} (0, 2, 0) \\
\vec{K}_3 = \frac{2\pi}{a} (-1, 1, 1)
$$

This leads to the choice $\mathcal{T} = \{ \vec{K}_1, \vec{K}_3, \vec{K}_{12}, \vec{K}_{23} \}$, and $\mathcal{C} = \{ *, 0, *, 0, * \}$ where $*$ indicates a non-zero real coefficient. We denote the target coefficients as $\mathcal{C} = \{ \tau_1, 0, \tau_2, \tau_3, 0, \tau_4 \}$ and target phases as $\Phi = \{ \xi_1, 0, \xi_2, \xi_3, 0, \xi_4 \}$ so that Eq. (3.3) becomes

$$
\Delta I(\vec{r}) = \sum_{i=1}^{4} \tau_i \cos(\vec{T}_i \cdot \vec{r} + \xi_i).
$$

Noting that the photonic band structure is invariant to the space group of the crystal, we endeavor to find the coefficients $\tau_i$ such that $\Delta I(\vec{r})$ is invariant under changes of the form $\vec{r} \rightarrow \mathcal{S}^d_{j, \delta}(\vec{r}) \equiv \mathcal{O}^d(\vec{r}) + \delta$, where we have defined $\mathcal{O}^d = \{ \mathcal{O}^d_j \}_{j=1, \ldots, 48}$ as the set of FCC point group operations. Such an intensity pattern satisfies the requirement for the smallest possible
IBZ. Operating on $\Delta I(\vec{r})$ with $S^{\delta}_{1,\delta}$ yields

$$
\Delta I(\vec{r})^{S^{\delta}_{1,\delta}} = \frac{4}{4} \sum_{i=1}^{4} \tau_i \cos(T_i \cdot S^{\delta}_{1,\delta}(\vec{r})) = \sum_{i=1}^{4} \tau_i \cos(O_i^j(T_i) \cdot \vec{r} + \xi_i + \zeta_i),
$$

(3.9)

where $O^r = \{O_i^j\}_{j=1,48}$ is the set of point group operations of the FCC reciprocal space, and $
\{\zeta_i = T_i \cdot \vec{\delta}\}_{i=1,4}$ is a set of four phase factors. Since the target vector set $T$ is a subset of $K$, in general the $\zeta_i$ are not independent, and are a subset of $\{\varphi_1, \varphi_2, \varphi_3, \varphi_1 - \varphi_2, \varphi_1 - \varphi_3, \varphi_2 - \varphi_3\}$, where $\varphi_i = \vec{K}_i \cdot \vec{\delta}$. Since the phases $\zeta_i$ depend on only three independent variables, they can be eliminated by a translation of the origin. Also, for our particular choice of target vectors, it can be verified that $O_i^j(T_i) \in \{\pm \vec{T}_1, \pm \vec{T}_2, \pm \vec{T}_3, \pm \vec{T}_4\}$. Since the sign of $\vec{T}_i$ leaves $\Delta I(\vec{r})$ unchanged, it follows that the point group operations $O_i^d$ simply permute the coefficients $\{\tau_i\}$ as they appear in Eq. (3.8), in the form

$$
\Delta I(\vec{r}) = \sum_{i=1}^{4} \tau_i \cos(T_i \cdot \vec{r})^{S^{\delta}_{1,\delta}} \rightarrow \sum_{i=1}^{4} \tau_{\mathcal{P}_j(i)} \cos(T_i \cdot \vec{r}),
$$

where $\mathcal{P}_j$ is a permutation of the indices $\{1, 2, 3, 4\}$ completely determined by $O^d$. Invariance of $\Delta I(\vec{r})$ can therefore be determined by requiring that $|\tau_i| = 1$ for all $i$. Furthermore, three of the four phases $\xi_i$ can be removed by a translation of the origin. The target FCC intensity pattern can then be written as

$$
\Delta I_{\text{fcc}}(\vec{r}) = \cos(\vec{b}_1 \cdot \vec{r}) + \cos(\vec{b}_2 \cdot \vec{r}) + \cos(\vec{b}_3 \cdot \vec{r}) + \cos((\vec{b}_1 + \vec{b}_2 + \vec{b}_3) \cdot \vec{r} + \xi),
$$

(3.10)

where $\xi \equiv \xi_4$ is the single remaining phase and $\{\vec{b}_i\}$ are the primitive vectors of the FCC reciprocal space. The choice $\xi = 0$ leads to an intensity pattern resembling a FCC lattice of spheroid “atoms”, as illustrated in Fig. 3.2(a). This indicates that a fundamental band gap does not open. (It is possible for a higher-order gap to open between bands 5 and 6, characteristic of disconnected $F\bar{4}3m$ structures [125], which are FCC lattices of slightly non-spherical atoms.) On the other hand, the choice $\xi = \pi$ produces an intensity pattern, shown in Fig. 3.2(b), ex-
hibiting a strong resemblance to a diamond network structure and corresponding to the double diamond (D) surface [121]. This is the diamond-like structure studied in previous theoretical reports [118–120]. Accordingly, our calculations, presented in the next section, show that a PBG as large as 25% opens between the 2nd and 3rd bands in a structure whose solid component has a dielectric constant of 11.9 (Si). It is interesting to note that a single phase in the intensity pattern differentiates between the FCC lattice of spheroids and the diamond structure and therefore determines the existence of a fundamental PBG. In the optical interference lithography technique, this phase can be controlled directly though the choice of laser beam amplitude and polarization pairs.

Diamondlike structure

Now that we have obtained the desired intensity pattern, Eq. (3.10) with $\xi = \pi$, it is straightforward to determine holographic beam parameters which produce this pattern. First, it is necessary to determine the wavevectors $\vec{G}_l$ of the incident laser beams, according to Eq. (3.1)
and Eq. (3.7). The following vectors of length $\sqrt{5}\pi/a$ satisfy our requirements:

\[ \vec{G}_0 = \frac{\pi}{a}(0, -2, -1) \]  
\[ \vec{G}_1 = \frac{\pi}{a}(2, 0, 1) \]  
\[ \vec{G}_2 = \frac{\pi}{a}(0, 2, -1) \]  
\[ \vec{G}_3 = \frac{\pi}{a}(-2, 0, 1). \]

It is then necessary to determine the polarization vectors which satisfy

\[ \{c_1, c_2, c_3, c_{12}, c_{13}, c_{23}\} = \{1, 0, 1, 1, 0, -1\} \]  
\[ \{\phi_1, \phi_2, \phi_3, \phi_{12}, \phi_{13}, \phi_{23}\} = \{0, 0, 0, 0, 0, 0\} \]

In order to describe the polarization vector for a given $\vec{G}_i$, it is convenient to introduce two mutually perpendicular unit vectors “up”, $\vec{U}_i$, and “right”, $\vec{R}_i$, to complete an orthogonal triad ($\vec{U}_i, \vec{R}_i, \vec{G}_i$) such that

\[ \vec{R}_i = \vec{G}_i \times \hat{z} / |\vec{G}_i \times \hat{z}| \]  
\[ \vec{U}_i = \vec{R}_i \times \vec{G}_i / |\vec{G}_i| \]  
\[ \vec{U}_i \times \vec{R}_i = \vec{G}_i / |\vec{G}_i|, \]

where ($\hat{x}, \hat{y}, \hat{z}$) define unit vectors in a specific laboratory coordinate frame. (If $\vec{G}_i \parallel \hat{z}$, then by convention we choose $\vec{R}_i = \hat{x}$.) An elliptical polarization vector can then be expressed as the sum of two linear polarization vectors in the up and right directions:

\[ \vec{\epsilon}_i = \cos(\varphi_i)\vec{U}_i + e^{i\beta_i} \sin(\varphi_i)\vec{R}_i, \]
with $\varphi_i$ describing the relative amplitudes and $\beta_i$ the relative phase between the two linear polarization vectors. For linear polarizations, the relative phase is zero and hence a linear polarization vector can be expressed as:

$$\vec{\epsilon}_i = \cos(\varphi_i)\vec{U}_i + \sin(\varphi_i)\vec{R}_i,$$

(3.16)

where in this case $\varphi_i$ can be interpreted as a polarization angle. Beam polarizations and intensities which produce the desired pattern are derived by finding parameters that minimize the intensity background $I_0$, while satisfying the desired values for the $c$ and $\phi$ coefficients. If one applies an overall scale to the $c$ coefficients, then the minimal value of $I_0$, as well as the four beam intensities, will be scaled accordingly. The minimization is performed using a Differential Evolution method (see, e.g., [126]), which finds a global minimum for $I_0$. In this method, one generates a randomly distributed set of $N$-dimensional vectors in the $N$-dimensional parameter space (in which the constraints on $c$ and $\phi$ are satisfied). Each vector is “mated” with a random combination of the other vectors to create a trial vector. If the trial vector improves the value of $I_0$, then it replaces the original vector. The mating step is iterated until the minimum is found. By minimizing $I_0$ while setting $\{c_1, c_2, c_3, c_{12}, c_{13}, c_{23}\} = \{1, 0, 1, 0, -1\}$ and $\{\cos(\phi_1), \cos(\phi_2), \cos(\phi_3), \cos(\phi_{12}), \cos(\phi_{13}), \cos(\phi_{23})\} = \{1, 1, 1, 1, 1, 1\}$, one arrives at the following elliptical polarization parameters:

$$\{\mathcal{E}_0, \mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3\} = \{1.29, 1.52, 1.34, 1.08\}$$

(3.17)

$$\{\varphi_0, \varphi_1, \varphi_2, \varphi_3\} = \{34.8^\circ, 66.6^\circ, 40.8^\circ, 14.6^\circ\}$$

$$\{\beta_0, \beta_1, \beta_2, \beta_3\} = \{90.0^\circ, -90.0^\circ, 90.0^\circ, -90.0^\circ\}.$$

These polarizations achieve a value of 6.93 for the intensity background $I_0$, and the total intensity reaches a maximum of 12.6. It should be noted that this particular numerical solution is not unique [118–120]. The beam configuration represented by this solution is shown in Fig. 3.3(a).
Figure 3.3: Diagram of beam configurations which generate the FCC (diamond) intensity pattern using (a) elliptically polarized and (b) linearly polarized beams. The plane spanned by $\vec{G}_0$ and $\vec{G}_2$ is perpendicular to the plane spanned by $\vec{G}_1$ and $\vec{G}_3$. The ellipses and circles at the end of each wavevector describe the polarization ellipse of the corresponding beam, as one looks down $\vec{G}_i$, with the dashed line (passing through the polarization ellipse or circle) corresponding to the $\vec{G}_0$-$\vec{G}_2$ or $\vec{G}_1$-$\vec{G}_3$ plane. The $\vec{R}$ and $\vec{U}$ pairs for each beam, defined in Eq. (3.14), are shown next to the corresponding polarization ellipse or circle.

The plane spanned by $\vec{G}_0$ and $\vec{G}_2$ ($\vec{G}_0$-$\vec{G}_2$) is perpendicular to the plane spanned by $\vec{G}_1$ and $\vec{G}_3$ ($\vec{G}_1$-$\vec{G}_3$). The angle between $\vec{G}_0$ and $\vec{G}_2$ equals the angle between $\vec{G}_1$ and $\vec{G}_3$ and has the value 126.9°. The polarization ellipses are shown next to the corresponding beams, depicting the path traced by the polarization vector as one looks down the wavevector. The dashed lines passing through the polarization ellipses lie in the respective planes defined above.

The linear polarization parameters:

$$\{\mathcal{E}_0, \mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3\} = \{2.08, 0.93, 1.29, 2.26\}$$

$$\{\varphi_0, \varphi_1, \varphi_2, \varphi_3\} = \{-29.3^\circ, 6.5^\circ, -46.9^\circ, -100.7^\circ\}$$

also satisfy Eq. (3.12) and Eq. (3.13) while minimizing $I_0$. However, as noted in [120], the ratio $I_{\text{max}}/I_0$ in this case is $17.6/11.97$ which is smaller than the one obtained above with elliptical polarizations. This linear polarization beam configuration is shown in Fig. 3.3(b). The polarization angles are shown as one looks down the wavevector, relative to the $\vec{G}_0$-$\vec{G}_2$ or
Figure 3.4: (a) The iso-intensity surface generated by Eq. (3.10), with $\xi = \pi/2$ at a solid volume fraction of $\approx 23\%$, with the field intensity mapped to the color bar. (b) The corresponding photonic band structure with an 11.9:1 dielectric contrast, indicating a 12.5\% PBG between bands 2 and 3, and a nearly 5\% PBG between bands 5 and 6. The positions of the high symmetry points are shown in the inset.

Non-inversion symmetric structure

By extending to non-inversion symmetric structures it is possible to achieve a connected $F43m$ (corresponding to the space group) structure. This structure has a two-atom basis where, unlike the diamond lattice, the two atoms are disproportionate in size. It has been shown that connected $F43m$ structures display PBGs both between the second and third bands, and between the fifth and sixth bands [125]. The relevant intensity pattern corresponds to Eq. (3.10) with $\xi = \pi/2$. Fig. 3.4(a) shows the iso-surface of this intensity pattern which generates a structure with a solid volume fraction of $\approx 23\%$, where high intensity regions correspond to the solid parts of the structure. When silicon is used to synthesize the structure in an air background, a 12.5\% PBG emerges between bands 2 and 3 (characteristic of the diamond structure achieved with $\xi = \pi$), and a nearly 5\% PBG emerges between bands 5 and 6 (characteristic of the FCC lattice of spheroids achieved with $\xi = 0$). The photonic band structure obtained in this case is shown in Fig. 3.4(b).
The desired intensity pattern can be obtained by adjusting the polarization vectors and amplitudes of the laser beams used to generate the diamond structure above, while retaining the wavevectors $\vec{G}_1$. In this case, the laser beam amplitude and polarization pairs must obey

$$\{c_1, c_2, c_3, c_{12}, c_{13}, c_{23}\} = \{1, 0, 1, 1, 0, 1\} \quad (3.19)$$

and

$$\{\phi_1, \phi_2, \phi_3, \phi_{12}, \phi_{13}, \phi_{23}\} = \{0, 0, 0, 0, \pi/2\}. \quad (3.20)$$

Since the structure lacks inversion symmetry, elliptical polarizations must be used. One set of elliptical polarization parameters which minimize $I_0$ with the constraints imposed by Eq. (3.19) and Eq. (3.20) is:

$$\{\mathcal{E}_0, \mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3\} = \{1.36, 1.36, 1.36, 1.36\} \quad (3.21)$$

$$\{\phi_0, \phi_1, \phi_2, \phi_3\} = \{37.7^\circ, 37.7^\circ, 37.8^\circ, 37.8^\circ\}$$
\[ \{ \beta_0, \beta_1, \beta_2, \beta_3 \} = \{28.6^\circ, 208.6^\circ, 28.6^\circ, 208.6^\circ \}. \]

These parameters achieve a value of 7.39 for the intensity background \( I_0 \) and a maximum total intensity of 14.78. Fig. 3.5 shows this beam configuration. The dashed lines passing through the polarization ellipses lie in either the \( \vec{G}_0-\vec{G}_2 \) or \( \vec{G}_1-\vec{G}_3 \) plane. All four ellipses are tilted by an angle of approximately \( 53.2^\circ \) from the corresponding plane. In all cases, the major axis is 4.1 times the length of the minor axis.

### 3.3.2 Body Centered Cubic structure

Next, we consider a holographic structure based on the BCC Bravais lattice. There are six distinct directions in the Green set of vectors in Fig. 3.1, corresponding to the \( \mathcal{B}^b \) set. In order to obtain a non-trivial pattern which possesses the full symmetry of the BCC Bravais lattice, one needs to use all six of these directions. Unfortunately, none of the possible combinations for \( C \) generates an inversion symmetric structure with a full photonic band gap. It is possible to relax the symmetry conditions by removing the inversion symmetry, which results in the gyroid (G) surface described in [121]. Instead, we relax our symmetry conditions by choosing only 4 of the 6 target directions, giving a target vector set \( \mathcal{T} = \{ \vec{T}_1, \vec{T}_2, \vec{T}_3, \vec{T}_4 \} \), which leads to a larger IBZ and an intensity pattern of lower symmetry. One possible choice for the three \( \vec{K}_i \) vectors is:

\[
\begin{align*}
\vec{K}_1 &= \frac{2\pi}{a}(0, 1, 1) \\
\vec{K}_2 &= \frac{2\pi}{a}(1, 1, 0) \\
\vec{K}_3 &= \frac{2\pi}{a}(1, 0, 1).
\end{align*}
\]

This leads to the choice \( \mathcal{T} = \{ \vec{K}_1, \vec{K}_3, \vec{K}_{12}, \vec{K}_{23} \} \), and \( \mathcal{C} = \{ *, 0, *, 0, * \} \). Using a similar derivation to the one presented in the FCC case but replacing the FCC point group operations with those of the BCC point group, one can write the BCC intensity pattern in terms of the
Figure 3.6: The optimized BCC architecture generated by Eq. (3.23) with a solid volume filling fraction of ≈ 22%. When the solid regions (interior of depicted iso-intensity surfaces) consist of silicon and the background is air, a PBG of 21% is obtained.

The choice $\xi = 0$ produces an intensity pattern resembling a BCC lattice of spheres, which produces no fundamental gap. However, the choice $\xi = \pi$ generates a BCC structure whose basis is similar to that of the diamond structure. Fig. 3.6 shows the optimized structure when $\xi = \pi$, which produces a PBG of 21% for a silicon structure in an air background.

Holographic beam parameters which produce this intensity pattern are determined straightforwardly as before. The target vectors in $T$ can be generated by the following $\vec{G}$ vectors of length $\sqrt{3}\pi/a$:

$$\Delta I_{\text{bcc}}(\vec{r}) = \cos(\vec{T}_1 \cdot \vec{r}) + \cos(\vec{T}_2 \cdot \vec{r}) + \cos(\vec{T}_3 \cdot \vec{r}) + \cos(\vec{T}_4 \cdot \vec{r} + \xi). \quad (3.23)$$

The choice $\xi = 0$ produces an intensity pattern resembling a BCC lattice of spheres, which produces no fundamental gap. However, the choice $\xi = \pi$ generates a BCC structure whose basis is similar to that of the diamond structure. Fig. 3.6 shows the optimized structure when $\xi = \pi$, which produces a PBG of 21% for a silicon structure in an air background.

Holographic beam parameters which produce this intensity pattern are determined straightforwardly as before. The target vectors in $T$ can be generated by the following $\vec{G}$ vectors of length $\sqrt{3}\pi/a$:

$$\vec{G}_0 = \frac{\pi}{a}(-1, -1, -1) \quad (3.24)$$
Figure 3.7: Diagram of beam configurations which generate the BCC intensity pattern using (a) elliptically polarized and (b) linearly polarized beams. The plane spanned by \( \vec{G}_0 \) and \( \vec{G}_2 \) is perpendicular to the plane spanned by \( \vec{G}_1 \) and \( \vec{G}_3 \).

\[
\vec{G}_1 = \frac{\pi}{a} (-1, 1, 1) \\
\vec{G}_2 = \frac{\pi}{a} (1, 1, -1) \\
\vec{G}_3 = \frac{\pi}{a} (1, -1, 1).
\]

The beam amplitudes and polarizations obey \( \{c_1, c_2, c_3, c_{12}, c_{13}, c_{23}\} = \{1, 0, 1, 1, 0, -1\} \) and \( \{\phi_1, \phi_2, \phi_3, \phi_{12}, \phi_{13}, \phi_{23}\} = \{0, 0, 0, 0, 0, 0\} \). Elliptically polarized beam parameters which obey these constraints and minimize \( I_0 \) are:

\[
\{\mathcal{E}_0, \mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3\} = \{1.19, 1.19, 1.19, 1.19\} \tag{3.25}
\]

\[
\{\phi_0, \phi_1, \phi_2, \phi_3\} = \{30.0^\circ, 30.0^\circ, 30.0^\circ, 30.0^\circ\}
\]

\[
\{\beta_0, \beta_1, \beta_2, \beta_3\} = \{90.0^\circ, -90.0^\circ, 90.0^\circ, -90.0^\circ\}.
\]

It is interesting to note that, with this configuration, the BCC intensity pattern can be created using four laser beams of equal intensities. With this configuration, the intensity background \( I_0 \) is 5.66, with the total intensity ranging from 0 to \( 2I_0 \). The beam configuration represented by this solution is shown in Fig. 3.7(a). The plane spanned by \( \vec{G}_0 \) and \( \vec{G}_2 \) (\( \vec{G}_0 \cdot \vec{G}_2 \)) is perpendicular
to the plane spanned by $\vec{G}_1$ and $\vec{G}_3$ ($\vec{G}_1\cdot\vec{G}_3$). The angle between $\vec{G}_0$ and $\vec{G}_2$ equals the angle between $\vec{G}_1$ and $\vec{G}_3$ and has the value $109.5^\circ$. The polarization ellipses are shown next to the corresponding beams, depicting the path traced by the polarization vector as one looks down the wavevector. The dashed lines passing through the polarization ellipses lie in the respective planes defined above.

Linearly polarized beams can be used to generate the BCC structure, but as in the case of the diamond structure, the minimum value of $I_0$ is larger than in the case of elliptical polarizations. Here, the value of $I_0$ achieved is 10.17 and the maximum total intensity is 15.83:

$$\{\varepsilon_0, \varepsilon_1, \varepsilon_2, \varepsilon_3\} = \{1.11, 1.98, 1.97, 1.09\}$$

$$\{\varphi_0, \varphi_1, \varphi_2, \varphi_3\} = \{-6.1^\circ, 21.9^\circ, 107.7^\circ, 39.7^\circ\}$$

This linear polarization beam configuration is shown in Fig. 3.7(b). Again, the polarization angles are shown as one looks down the wavevector, relative to the $\vec{G}_0\cdot\vec{G}_2$ or $\vec{G}_1\cdot\vec{G}_3$ plane.

### 3.3.3 Simple Cubic

Finally, we consider a holographic structure based on the SC Bravais lattice, which is the simplest of the cubic structures. There are only three distinct directions in the set $B^s$ (Red set online) of vectors in Fig. 3.1 and consequently only three vectors in the target vector set, i.e. $T = \{\vec{T}_1, \vec{T}_2, \vec{T}_3\}$. In this case, we make the simple choice $\vec{T}_i = \vec{K}_i = \vec{b}_i^1$, so that the $C$ coefficients are given by $C = \{*, *, *, 0, 0, 0\}$, where $*$ denotes a non-zero real coefficient. Again, without loss of generality the first three nonzero coefficients can be chosen to be 1; in this case, this applies to all nonzero coefficients. The intensity pattern is thus given by

$$\Delta I(\vec{r}) = \cos(\vec{T}_1\cdot\vec{r}) + \cos(\vec{T}_2\cdot\vec{r}) + \cos(\vec{T}_3\cdot\vec{r}).$$

(3.27)
Figure 3.8: The optimized SC architecture generated by Eq. (3.27) with a solid volume filling fraction of $\approx 24\%$. When the solid regions (corresponding to regions with a red hue) consist of silicon and the background is air, a PBG of 10.5\% is obtained.

This pattern has a simple cubic Bravais lattice and is invariant to all symmetry operations of the simple cubic point group, thereby satisfying our design requirements. The intensity iso-surface of the optimized Si SC structure is shown in Fig. 3.8. A full photonic band gap of 10.5\% opens between bands 5 and 6 for this optimized structure, which has a solid volume filling fraction of $\approx 24\%$.

The target vectors in $T$ can be generated by the following $\vec{G}$ vectors of length $\sqrt{3}\pi/a$:

\[
\vec{G}_0 = \frac{\pi}{a}(-1, -1, -1) \\
\vec{G}_1 = \frac{\pi}{a}(1, -1, -1) \\
\vec{G}_2 = \frac{\pi}{a}(-1, 1, -1) \\
\vec{G}_3 = \frac{\pi}{a}(-1, -1, 1).
\]
Figure 3.9: Diagram of beam configurations which generate the SC intensity pattern using (a) elliptically polarized and (b) linearly polarized beams. The beams are set up in an “umbrella” configuration, where $\vec{G}_1$, $\vec{G}_2$, and $\vec{G}_3$ each make an angle of 70.5° with $\vec{G}_0$ and are spread evenly around the azimuth. In (a), only beam 0 is elliptically polarized, with a polarization ellipse whose major axis is rotated 15.3° from the projection of $\vec{G}_1$ onto the plane normal to $\vec{G}_0$. In (b), the polarization angle of beam 0 is measured with respect to the projection of $\vec{G}_1$ onto the plane normal to $\vec{G}_0$, whereas the other polarization angles are measured with respect to the $\vec{G}_1-\vec{G}_0$ plane, for $i = 1\ldots3$, with the wavevector pointing into the page.

and beam polarizations which obey \{c_1, c_2, c_3, c_{12}, c_{13}, c_{23}\} = \{1, 1, 1, 0, 0, 0\} and \{\phi_1, \phi_2, \phi_3, \phi_{12}, \phi_{13}, \phi_{23}\} = \{0, 0, 0, 0, 0, 0\} and minimize $I_0$ are:

$$
\begin{align*}
\{\mathcal{E}_0, \mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3\} &= \{1.79, 1.02, 1.02, 0.88\} \\
\{\varphi_0, \varphi_1, \varphi_2, \varphi_3\} &= \{50.1^\circ, -7.8^\circ, -67.8^\circ, 52.2^\circ\} \\
\{\beta_0, \beta_1, \beta_2, \beta_3\} &= \{275.8^\circ, 0^\circ, 0^\circ, 0^\circ\}.
\end{align*}
$$

(3.29)

In this case, a “umbrella” configuration of the beams is used (see Fig. 3.9). Each of the wavevectors $\vec{G}_1$, $\vec{G}_2$, and $\vec{G}_3$ make an angle of 70.5° with $\vec{G}_0$ and are spread evenly around the azimuth. Only beam 0 is elliptically polarized; the major axis of the polarization ellipse (depicted as the dashed line passing through the polarization ellipse) makes an angle of 15.33° with the projection of $\vec{G}_1$ onto the plane normal to $\vec{G}_0$. The other three beams are linearly polarized, with polarization vectors making identical angles of 52.24° with the $\vec{G}_0-\vec{G}_1$ planes. The background intensity $I_0$ is 6.07, and the total intensity ranges from 0.07 to 12.07. If one
CHAPTER 3

constrains all four polarizations to be linear, the parameters

\[
\{E_0, E_1, E_2, E_3\} = \{1.92, 0.64, 1.28, 1.28\} \quad (3.30)
\]

\[
\{\varphi_0, \varphi_1, \varphi_2, \varphi_3\} = \{-15.5^\circ, 67.8^\circ, 7.7^\circ, -52.2^\circ\}
\]

yield a minimum value of 7.35 for \(I_0\), with the maximum total intensity reaching 13.35. The linear beam configuration is shown in Fig. 3.9(b).

3.4 Generalized tetragonal structures

The diamond (FCC) and BCC structures described in the Sec. 3.3 can be considered as special cases of a larger class of photonic crystals. The varying intensity pattern associated with these structures can be written as

\[
\Delta I(\vec{r}) = \cos(\vec{T}_1 \cdot \vec{r}) + \cos(\vec{T}_2 \cdot \vec{r}) + \cos(\vec{T}_3 \cdot \vec{r}) - \cos(\vec{T}_4 \cdot \vec{r}), \quad (3.31)
\]

where the target vectors, \(\vec{T}_i\), are given by:

\[
\vec{T}_1 = \left( -\frac{2\pi}{a}, \frac{2\pi}{a}, \frac{2\pi}{c} \right)
\]

\[
\vec{T}_2 = \left( \frac{2\pi}{a}, -\frac{2\pi}{a}, \frac{2\pi}{c} \right)
\]

\[
\vec{T}_3 = \left( \frac{2\pi}{a}, \frac{2\pi}{a}, -\frac{2\pi}{c} \right)
\]

\[
\vec{T}_4 = \left( \frac{2\pi}{a}, \frac{2\pi}{a}, \frac{2\pi}{c} \right).
\]

The general structure can be modelled in a tetragonal unit cell whose aspect ratio is given by the quantity \(c/a\). By varying the aspect ratio, one can scale the structure along the \(z\)-direction. The aspect ratio can be written in terms of the acute angle between any one of the target vectors and the \(z\)-axis, \(\xi\), by

\[
c/a = |\tan(\xi)|/\sqrt{2}. \quad (3.33)
\]
Figure 3.10: Relative size of the full photonic band gap as a function of the angle, $\xi$, between the target vectors, $\vec{T}_i$, and the z-axis. The structure has a solid volume fraction of 22.1%. The solid has a dielectric constant of 11.9, corresponding to silicon. The BCC structure corresponds to $\xi = 45^\circ$ and the diamond (FCC) structure corresponds to $\xi = 54.74^\circ$.

The diamond structure is achieved when $\xi = \arctan(\sqrt{2}) = 54.7^\circ$ (corresponding to $c/a = 1$) and the BCC structure results when $\xi = 45^\circ$ (corresponding to $c/a = 1/\sqrt{2}$).

The desired target vectors can be obtained by changing the angle between wavevectors, which we denote by $\nu$, in the counter-propagating scheme used for the FCC and BCC structures described in Sec. 3.3 (see, e.g., Fig. 3.3). For target vectors characterized by a given $\xi$, an angle $\nu$ given by

$$\nu = 2 \arccos \left( \frac{\cos(\xi)}{\sqrt{2 - \cos^2(\xi)}} \right)$$

is sufficient. As shown in Fig. 3.3 and Fig. 3.7, angles between wavevectors of $126.9^\circ$ and $109.5^\circ$ satisfy the conditions for FCC and BCC structures, respectively. Beam polarizations which satisfy the constraint

$$\{c_1, c_2, c_3, c_{12}, c_{13}, c_{23}\} = \{1, 0, 1, 1, 0, -1\}$$
$$\{\cos(\phi_1), \cos(\phi_2), \cos(\phi_3), \cos(\phi_{12}), \cos(\phi_{13}), \cos(\phi_{23})\} = \{1, 1, 1, 1, 1, 1\}$$

can then be found using the minimization procedure described previously.

Fig. 3.10 shows the size of the relative photonic band gap as $\xi$ varies, for structures with
Figure 3.11: Photonic band structure of the generalized structure with $\xi = 50^\circ$, at a solid volume fraction of 22.1% and a dielectric contrast of 11.9 to 1, corresponding to silicon. The high symmetry points and the irreducible Brillouin zone are shown in the inset. This exhibits a PBG of 23%.

a dielectric contrast of 11.9 to 1, corresponding to silicon in air. The solid volume fraction in all cases is 22.1%. The maximum PBG occurs at $\xi = 54.74^\circ$, which is the diamond structure.

Fig. 3.11 shows the photonic band structure for a structure with $\xi = 50^\circ$, between the BCC and FCC cases. A full photonic band gap of 23% opens for this structure.

3.5 Robustness of holographic photonic crystals

We now turn our attention to the properties of the inversion symmetric holographic photonic crystals obtained from the intensity patterns derived in the previous section. For a given intensity pattern, it is first necessary to determine the optimal value of the threshold $I_{\text{thr}}$ in the simplified shape function, Eq. (3.5). The choice of $I_{\text{thr}}$ corresponds to choosing a particular iso-intensity surface, and therefore the solid volume filling fraction of the resulting crystal. The one-to-one mapping from the $I_{\text{thr}}$ to the volume fraction is displayed in Fig. 3.12 for the FCC, BCC, and SC structures. The functional dependence of the volume fraction (measured in %)
Figure 3.12: The volume solid versus threshold used in the shape function Eq. (3.5), for FCC, BCC, and SC structures. The FCC and BCC curves overlap each other because both structures are members of the generalized HLPC structures described in Sec. 3.4. The solid material is found in the regions where $\Delta I(\vec{r}) > I_{\text{thr}}$.

on $I_{\text{thr}}$ is not strictly linear, but can be taken to be so for the volume fractions of interest. The linear part of the mapping can be written as:

$$f_f = -21I_{\text{thr}} + 50$$
$$f_b = -21I_{\text{thr}} + 50$$
$$f_s = -29I_{\text{thr}} + 50,$$

where $f_f$, $f_b$, and $f_s$ are the volume fractions of the FCC, BCC, and SC structures, respectively. Since the FCC and BCC structures are both specific examples of the generalized structure described in Sec. 3.4, the mapping is identical for the two structures. One may note that this mapping is symmetric around a volume fraction of 50%. In fact, it can be shown that, for the three cubic structures we have obtained, taking $I_{\text{thr}} \rightarrow -I_{\text{thr}}$ produces an equivalent but inverted structure (solid and air regions are interchanged), to within a translation of the origin. In terms of a physical (experimentally measured) intensity, this corresponds to $I_{\text{thr}}^{\exp} \rightarrow 2I_0 - I_{\text{thr}}^{\exp}$. This implies that the desired structure can be achieved equivalently by both single inversion and double inversion processes simply by adjusting the threshold value accordingly.
Similarly, one can compensate for the distinction between positive and negative photoresist materials by changing the holographic exposure time or overall intensity. Consider the shape functions $S_d$ of the direct structure and $S_i$ of the inverted structure, given respectively by:

$$S_d(\vec{r}, I_{thr}) = \Theta(\Delta I(\vec{r}) - I_{thr}) \tag{3.36}$$

$$S_i(\vec{r}, I_{thr}) = \Theta(I_{thr} - \Delta I(\vec{r})).$$

We endeavour to find $\vec{\rho} = \vec{r}' - \vec{r}$ such that $S_d(\vec{r}, I_{thr}) = S_i(\vec{r}', -I_{thr})$. This implies that $\Delta I(\vec{r}') = -\Delta I(\vec{r})$, a condition which is met provided that

$$\vec{K}_i \cdot \vec{\rho} = (2n_i + 1)\pi \tag{3.37}$$

$$\vec{K}_{ij} \cdot \vec{\rho} = (2n_{ij} + 1)\pi,$$

where $n_i$ and $n_{ij}$ are integers, for all $i$ such that $c_i \neq 0$ and all $i, j$ such that $c_{ij} \neq 0$. Recall that $c_i$ and $c_{ij}$ are the members of the set $C$ defined in Eq. (3.6). Eq. (3.37) can only be satisfied if, when $c_{ij}$ is non-zero, either $c_i$ or $c_j$ is zero. The format of the set $C$ of the three inversion symmetric structures discussed above satisfies this condition. It can be shown that the corresponding translation vectors, $\vec{\rho}$, are $\vec{\rho}_f = \left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2}\right)$ for the FCC structure, $\vec{\rho}_b = \left(\frac{a}{2}, \frac{a}{2}, 0\right)$, for the BCC structure, and $\vec{\rho}_s = \left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2}\right)$, for the SC structure.

Fig. 3.13 displays the relative size of the full photonic band gap as a function of the solid volume fraction for the FCC, BCC, and SC structures composed of a material with a dielectric constant of 11.9 (Si) in an air background. The optimized FCC structure occurs at a solid volume fraction $\approx 21.5\%$ and has a relative fundamental gap (between the 2nd and 3rd bands) of 25%. The optimized BCC structure, which is $\approx 22\%$ solid, also has a fundamental gap, which is 21% of the gap center frequency in this case. Finally, for a solid volume fraction of $\approx 24\%$, a full photonic band gap of 10.5% opens between bands 5 and 6 for the optimized SC structure. The photonic band structure diagrams for the three optimized structures are shown.
Figure 3.13: Relative size of the full photonic band gap as a function of the solid volume fraction, for the FCC, BCC, and SC structures. The solid has a dielectric constant of 11.9, corresponding to silicon. The optimized FCC structure is \( \approx 21.5\% \) solid and generates a relative gap of 25\%. The optimized BCC structure is \( \approx 22\% \) solid and generates a relative gap of 21\%. The optimized SC structure is \( \approx 24\% \) solid and generates a relative gap of 10.5\%.

in Fig. 3.14. Fig. 3.15 shows the dependence of the relative photonic band gap on the index of refraction of the solid material for the three optimized structures. For the FCC structure, a full photonic band gap appears when the refractive index is larger than about 1.97. The relative width increases with the index of refraction until saturation at about 38\%. The refractive index threshold for the BCC structure is approximately 2.24 and the relative PBG saturates at 34\%. The index threshold for the SC structure is 2.77 and the relative PBG saturates at 16.5\%.

The global intensity contrast, defined as \( \max(2\Delta I(\vec{r})|I_0) \), is of important practical concern. The larger the contrast, the more effective the developing process to create the polymer photonic crystal template. An alternative metric for measuring the global intensity contrast can be found in [119]. The intensity contrast depends both on the shape being created and on the particular beam configuration used to create that shape. Table 3.1 shows the global intensity contrast for each of the beam configurations for the inversion symmetric structures discussed in Sec. 3.3. For each structure, the use of elliptically polarized beams improves the contrast over the case when only linearly polarized beams are used. The elliptical beam configuration for the BCC structure achieves a “perfect” contrast ratio of 1, meaning that a value of zero total
Figure 3.14: Photonic band structure diagrams for the optimized (a) FCC, (b) BCC, and (c) SC holographic photonic crystals structures characterized by an 11.9:1 dielectric contrast. The positions of the high symmetry points together with the corresponding irreducible Brillouin zones are shown in the insets.
Figure 3.15: Relative size of the full photonic band gap as a function of the index of refraction of the solid material, for the optimized FCC, BCC, and SC structures. The background is assumed to be air. The threshold index of refraction for the emergence of a photonic band gap is 1.97 for the FCC structure, 2.24 for the BCC structure, and 2.77 for the SC structure. The inset shows a magnified view of the curve, near the threshold indices of refraction for the FCC and BCC structures.

Table 3.1: Global intensity contrast in the interference patterns of the various beam configurations. The global intensity contrast is defined as the ratio of the amplitude of the varying part of the intensity, $\max(|2\Delta I(\vec{r})|)$, and the background intensity $I_0$. The use of elliptical polarizations improves the global intensity contrast for each of the three structures.
intensity is found in the interference pattern.

When comparing the exposure efficiency of different interference patterns, it is not sufficient to consider only the global intensity contrast. Disorder in the PBG template may arise from polymer inhomogeneities that lead to small, random variations in the exposure threshold from point to point in the bulk photoresist. This, in turn, may cause “roughening” of the interface between “exposed” and “unexposed” polymer even though the iso-intensity contours are perfectly smooth. Therefore, it is useful to maximize the gradient of the intensity pattern at precisely the threshold intensity iso-surface. This minimizes the spatial extent of “exposure roughening.” In order to compare the intensity contrasts for the FCC, BCC, and SC structures, we define an average intensity contrast factor for an iso-intensity surface at $I_{\text{thr}}$, $C_{\text{avg}}(I_{\text{thr}})$, as

$$C_{\text{avg}}(I_{\text{thr}}) = \frac{\int_{\partial V} \vec{\nabla} \left[ \Delta I(\vec{r}) \right] \cdot d\vec{A}}{(I_0 + 2I_{\text{thr}}) \int_{\partial V} \vec{n} \cdot d\vec{A}},$$ (3.38)

where $V$ corresponds to the region which becomes the interior of the resulting structure and $\partial V$ its surface (i.e. the iso-intensity surface). In other words, the contrast factor gives the average value of the intensity gradient along the iso-intensity surface, normalized by the iso-intensity value. Normalization by the iso-intensity value means that the contrast factor is not symmetric with respect to a solid volume fraction of 50%. Using the Gauss’ theorem and taking the area of the iso-intensity surface as $A$, the contrast factor can be rewritten as

$$C_{\text{avg}} = \frac{1}{(I_0 + 2I_{\text{thr}})A} \int_V \vec{\nabla}^2 [\Delta I(\vec{r})] dV.$$

(3.39)

Fig. 3.16(a) shows a plot of the average intensity contrast factor, $C_{\text{avg}}$, as a function of the volume fraction of solid for the FCC, BCC, and SC structures. The contrast factor is calculated by discretizing the conventional (cubic) unit cell in $256^3$ boxes and sampling the appropriate intensity pattern. The area of the iso-intensity surface in the cubic cell is calculated by approx-
Figure 3.16: Plot of the (a) average intensity contrast factor, $C_{avg}$, and (b) minimum intensity contrast $C_{min} = \min_{\Delta I(\vec{r})=I_{thr}} |\vec{\nabla}[\Delta I(\vec{r})] \big / (I_0 + 2I_{thr})|$ as functions of the volume fraction of solid for the FCC, BCC, and SC structures, created using elliptically polarized beams which produce minimal background intensities. The solid part of the photonic crystal corresponds to regions where the intensity exceeds the threshold value.

Imitating the surface with a triangular mesh. The volume integral is calculated by taking

$$\int_V \vec{\nabla}^2[\Delta I(\vec{r})] dV \rightarrow \sum_{\Delta I(\vec{r}) \leq I_{thr}} \vec{\nabla}^2[\Delta I(\vec{r})] v,$$

where $v$ is the volume of the small voxels and $\vec{\nabla}^2[\Delta I(\vec{r})]$ is calculated analytically from the corresponding intensity pattern. The solid part of the photonic crystal corresponds to regions where the intensity exceeds the threshold value. This could be achieved using negative photoresists and double inversion. Near the respective optimal solid volume fractions ($\approx 22\%$), the contrast factors for the FCC and BCC structures are approximately equal, and are larger than the SC contrast factor. However, near 78% solid volume fraction (which corresponds to the inverted structure), the BCC contrast factor becomes larger than the FCC contrast factor. This is relevant if a single inversion process is used in conjunction with a negative photoresist, or if double inversion is used with a positive photoresist. In addition to considering average intensity gradient, we examine the minimum intensity gradient for various iso-intensity surfaces.
by finding the figure of merit [104]

\[
C_{\text{min}} = \min_{\Delta I(\vec{r}) = I_{\text{thr}}} |\vec{\nabla} [\Delta I(\vec{r})]/(I_0 + 2I_{\text{thr}})|. 
\] (3.40)

This is calculated analytically for every point on the triangular mesh used to approximate a given iso-intensity surface. The regions where contrast is minimum along the threshold iso-intensity surface represent the weak points of the photonic crystal template. These regions are most susceptible to disorder in the holographic process. Shown in Fig. 3.16(b), \(C_{\text{min}}\) gives a measure of the worst case for each iso-intensity surface. In this case, the FCC interference pattern has the best characteristics near the optimized volume fraction of 22%, whereas the FCC and BCC patterns have similar characteristics near 78% volume fraction. It should be noted that the SC interference pattern appears to achieve the worst case near both the optimized direct and inverted volume fractions.

Finally we consider the sensitivity of the holographic photonic crystals to imprecision in the laser beam parameters. We do this by considering the trajectories of the photonic band edges as beam polarizations and amplitudes are perturbed from the optimal configurations. Fig. 3.17 shows the photonic band edges of the FCC, BCC, and SC structures as a single beam...
amplitude is perturbed from the optimal value. Only the worst (most sensitive) case out of the four possible beam perturbations is shown for each of the structures. The FCC structure shows the most robustness against amplitude perturbations, allowing the single beam amplitude to range from 70% to 250% of the optimal value before the gap closes, with the BCC structure showing similar characteristics. On the other hand, a 10% perturbation in the single beam amplitude closes the gap in the case of the SC structure. Next, we consider perturbations to the polarization vectors in the optimal elliptically polarized beam configurations used to create the structures described in this paper. Recall Eq. (3.15) where we write an elliptical polarization vector as the sum of two linear polarizations such that $\vec{\varepsilon} = \cos(\varphi)\vec{U} + e^{i\beta}\sin(\varphi)\vec{R}$.

Fig. 3.18 shows the photonic band edges of the three structures when the quantity $\tan(\varphi)$, which describes the relative amplitude of the two linear components, is perturbed from the optimal value. The dependence of the photonic band edges on perturbations of $\beta$, the relative phase between the linear polarization components, is shown in Fig. 3.19. For both graphs, only the worst case out of the four possible perturbations for each structure is displayed. For these elliptically polarized beam configurations, it is noted that the photonic band gap of the BCC structure is most robust against beam parameter perturbations, while the SC structure displays the least robustness. Finally, we consider perturbations to a single polarization angle, $\varphi$, for
Figure 3.19: The photonic band edges of the optimized FCC, BCC, and SC structures as functions of perturbations in the angle $\beta$ (see Eq. (3.15)). The structure is assumed to consist of a material of dielectric constant 11.9 in an air background.

Figure 3.20: The photonic band edges of the optimized FCC, BCC, and SC structures as functions of perturbations in single linear polarization angles $\varphi$. The structure is assumed to consist of a material of dielectric constant 11.9 in an air background.
the optimal linearly polarized beam configurations in Fig. 3.20, by changing the polarization angle of a single beam. Fig. 3.20 shows the photonic band edges of the inversion symmetric FCC, BCC, and SC structures as the polarization angle of the most sensitive beam is perturbed. In the worst case, the photonic band gap of the BCC structure remains open after a $8^\circ$ change in a single polarization angle, whereas for the FCC structure, a $6^\circ$ perturbation closes the gap. Again, the SC structure is least robust.

### 3.6 Discussion

In summary, we have derived beam configurations for creating FCC, BCC, and SC photonic crystals using holographic lithography through simple, intuitive symmetry considerations. The guiding principle in this procedure is that a large PBG can be obtained by choosing a structure with the smallest possible irreducible Brillouin zone. The FCC structure, which resembles the diamond network structure, exhibits a full photonic band gap of 25% when made with materials with a dielectric contrast of 11.9:1. Our results also reveal that an optimized geometrical structure within the unit cell enables the BCC lattice to exhibit a PBG comparable to that of the widely studied diamond lattice. Here the photonic band gap is 21% for materials with a dielectric contrast of 11.9:1. Finally, we have found a simple cubic holographic architecture which exhibits a PBG of roughly 11% in the case of Si:air materials. This SC PBG material can be achieved using a simple “umbrella configuration” for the interfering laser beams. In each case, we find that an equivalent but inverted structure can be achieved simply by changing the threshold intensity. This implies that there need be no distinction between direct structures and structures made by inversion techniques. The beam configurations which we describe are optimal with respect to maximizing the intensity contrast in the respective laser interference patterns. The FCC and BCC structures exhibit similar contrast near the optimal filling fractions, while the SC structure displays worse contrast. For all three structures, the use of elliptically polarized beams enables better intensity contrast than can be achieved by the use
of linearly polarized beams alone. We have also studied the sensitivity of our holographic structures to perturbations of the amplitudes and polarization angles of the holographic laser beams. The FCC and BCC structures each continue to exhibit full photonic band gaps even as a single linear polarization angle is adjusted by $6^\circ$ or a single beam amplitude is adjusted between 70 and 240% of the optimal value. These structures also show robustness against perturbations in a single polarization when elliptical polarizations are used. These results suggest that holographic lithography provides a fault-tolerant approach to PBG micro-fabrication.

All three of the structures we describe yield photonic band gaps centered at wavelengths approximately twice the wavelength of the incident interfering laser beams. Therefore, in order to achieve PBGs at the 1.55 $\mu$m wavelength preferred for telecommunications, it is necessary to use a photoresist or other photo-polymerizable material which can be exposed by laser beams of wavelength of about 750 nm. The SU-8 negative photoresist which has been used in several experimental studies [105, 107, 109] is intended for near-ultraviolet rather than near-infrared lithography [127]. In this case, a two-photon absorption process may be necessary to expose the photoresist. Other issues to be considered are the post-processing (infiltration and inversion) limitations imposed on the final, high-index structure. For example, in some architectures, an infiltration process may not be able to produce complete inversions of a template, and pockets of air may persist in thicker regions of the infiltrating material (partial inversion). The presence of such imperfections may have a deleterious effect on the optical properties of the resulting photonic crystal.
Chapter 4

Optical Phase Mask Lithography: A New Paradigm for Photonic Band Gap Synthesis

4.1 Introduction

In Chapter 3 we discussed the holographic lithography method as an approach to large-scale synthesis of 3D photonic crystals with large PBGs in the optical regime. We demonstrated that using single exposure holographic lithography based on the interference pattern of four laser beams, it is possible to produce a diamondlike structure with a PBG approximately 25% of the center frequency when synthesized with Si. Despite this promise, the precise alignment of four laser beams from different directions is experimentally inconvenient. Restricting all four beams to be launched from the same half-space in an umbrella setup reduces the PBG significantly [128, 129]. The diamondlike intensity pattern can be generated by a five-beam umbrella setup, or by multiple exposures of two or three beams [130]. Nevertheless, the beam geometries, polarizations, and amplitudes still must be individually controlled.

In this chapter, we circumvent these complications using an interference pattern generated
by a single beam diffracting through a carefully designed optical phase mask [131]. The use of diffractive interference patterns from phase masks has previously been shown to produce diamondlike photonic crystals provided that two independent optical exposures are performed with two separate positions of the phase mask [132]. However, re-alignment of the second exposure with the first exposure is a daunting experimental challenge. Simple FCC structures that do not lead to a large PBG can be achieved with a single exposure [133]. A prism-based diffractive element has recently been suggested as an alternative approach to realize diamondlike interference patterns [134]. Here, we introduce a novel approach to create a diamondlike structure by OPML based on single exposure of a photoresist by a laser beam leading to a five-beam interference pattern. We present a phase mask design that yields a diamondlike structure with a PBG of 24% of the gap center frequency when synthesized with a material with a dielectric constant of 11.9. In Sec. 4.2 we introduce the target five-beam intensity pattern and its relation to the intensity pattern emerging from the diffraction of a single beam through an OPM. In Sec. 4.3, we describe the proposed OPM architecture. In Sec. 4.4 we show several phase mask geometries that can produce photonic crystals with large PBGs and we study the effects on the resulting PBG when the phase mask parameters are varied and the polarization of the incident beam is varied. In particular, we find that when the photoresist has a refractive index corresponding to 1.67 (undeveloped SU-8 at 355-nm wavelength [107]), the ideal index contrast for the OPM is in the range of 1.7 to 2.3. In Sec. 4.5 we propose a silicon-silica OPM configuration that may be able to leverage established silicon micromachining techniques for the fabrication of the phase mask, and show how this may be used in conjunction with various photoresists to create photonic crystals.

4.2 Diffraction of light by optical phase masks

Consider a single, monochromatic beam with vacuum wavelength $\lambda_0$ and wavevector $\vec{k}_0 = -\frac{2\pi}{\lambda_0} \hat{z}$, normally incident onto an optical phase mask and exposing a region with refractive
index $n^(-)$ below the mask. The phase mask is assumed to have a square Bravais lattice symmetry in the $x$-$y$ plane, with lattice constant $a$, finite thickness in the $z$-direction, and mirror planes normal to $\hat{x}$ and $\hat{y}$. For a uniform incident beam with infinite extent in the $x$- and $y$-directions, the electric field in the exposure region consists of the unscattered beam with wavevector $\vec{G}_{00} = -\frac{2\pi n^(-)}{\lambda_0} \hat{z}$ and diffracted beams with wavevectors $\vec{G}_{mn} = \frac{2\pi}{a} (m, n, -\gamma_{mn})$, where $m$ and $n$ are arbitrary integers. These diffracted beams have wavevector components in the $x$-$y$ plane $\frac{2\pi}{a} (m, n, 0)$ corresponding to the Fourier components of the OPM dielectric profile. The $z$-component of the wavevector of mode $(m, n)$ is determined by the condition of energy conservation $|\vec{k}_0| = |\vec{G}_{mn}|/n^(-)$:

$$\gamma_{mn} = \pm \left[ \alpha^2 - m^2 - n^2 \right]^{1/2}; \quad \alpha \equiv \frac{an^(-)}{\lambda_0}. \quad (4.1)$$

In general, $\gamma_{mn}$ can be a complex number, describing either propagating or evanescent beams in the region of the photoresist ($z < 0$). In order to guarantee periodicity in the intensity pattern, it is desireable to have five and only five propagating beams in the exposure region, namely the $(0, 0), (0, \pm 1),$ and $(\pm 1, 0)$ modes, with corresponding wavevectors

$$\vec{G}_{00} = \frac{2\pi}{a} (0, 0, -q_0) \quad (4.2)$$
$$\vec{G}_{ij} = \frac{2\pi}{a} (i, j, -q_1)$$

where $\bar{i} \equiv -i$ and $\bar{j} \equiv -j$. Here we have defined

$$q_j \equiv \sqrt{\alpha^2 - j}. \quad (4.3)$$

In order for these modes to propagate in the exposure region, we require $\left(\frac{an^(-)}{\lambda_0}\right)^2 > 1$, or $\lambda_0/a < n^(-)$. The next lowest order modes are the $(\pm 1, \pm 1)$ modes, which have wavevectors of the form $\vec{G}_{\pm 1\pm 1} = \frac{2\pi}{a} (\pm 1, \pm 1, -q_2)$. For these (and all higher order) modes to be evanescent in the exposure region, the condition $\left(\frac{an^(-)}{\lambda_0}\right)^2 < 2$, or $\lambda_0/a > n^(-)/\sqrt{2}$, must be
satisfied. Therefore, in order to retain only the desired modes, the incident beam wavelength is
constrained by:

\[
\frac{n(-)}{\sqrt{2}} < \frac{\lambda_0}{a} < n(-).
\]  \hspace{1cm} (4.4)

Provided that the constraint in Eq. (4.4) is satisfied, then an intensity pattern is produced
corresponding to the interference pattern of 5 monochromatic plane waves of frequency \( \omega \),
wavevectors \( \vec{G}_l \) corresponding to Eq. (4.2), polarization vectors \( \vec{E}_l \), and phases \( \theta_l \), where \( l \) is in
the set \( L = \{00, 10, \bar{1}0, 0\bar{1}, \bar{0}1\} \). The electric field associated with this interference pattern is
given by

\[
\vec{E}(\vec{r}, t) = e^{-i\omega t} e^{i(\vec{G}_{00}\cdot\vec{r} + \theta_{00})} \left[ \vec{E}_{00} + \sum_{l \neq 00} \vec{E}_l e^{i(\vec{K}_l\cdot\vec{r} + \varphi_l)} \right],
\]  \hspace{1cm} (4.5)

where \( \vec{K}_l \) and \( \varphi_l \) are defined as

\[
\vec{K}_l \equiv \vec{G}_l - \vec{G}_{00} \hspace{1cm} (4.6)
\]

\[
\varphi_l \equiv \theta_l - \theta_{00}.
\]

The corresponding intensity pattern is given by

\[
I(\vec{r}) = I_0 + 2 \sum_{l \neq 00} \eta_{00,l} \cos[\vec{K}_l \cdot \vec{r} + \tau_{00,l} + \varphi_l]
\]

\[
+ 2 \sum_{l \neq 00} \sum_{l' > l} \eta_{l,l'} \cos[(\vec{K}_l - \vec{K}_{l'}) \cdot \vec{r} + \tau_{l,l'} + \varphi_l - \varphi_{l'}],
\]  \hspace{1cm} (4.7)

where

\[
I_0 \equiv \sum_l |\vec{E}_l|^2
\]  \hspace{1cm} (4.8)

describes the constant intensity background, and

\[
\eta_{l,l'} \equiv |\vec{E}_{l'}^* \cdot \vec{E}_l|
\]  \hspace{1cm} (4.9)

\[
\tau_{l,l'} \equiv \arg(\vec{E}_{l'}^* \cdot \vec{E}_l).
\]
The spatial modulation of this intensity pattern is periodic with a Bravais lattice whose reciprocal lattice vectors can be represented by any three vectors from the set \( \mathcal{K} = \{ \vec{K}_{10}, \vec{K}_{\bar{1}0}, \vec{K}_{01}, \vec{K}_{\bar{0}1} \} \):

\[
\vec{K}_{ij} = \left( \frac{2\pi i}{a}, \frac{2\pi j}{a}, \frac{2\pi}{c} \right)
\]  

(4.10)

where \( \bar{i} \equiv -i \) and \( \bar{j} \equiv -j \). Here we have defined

\[
c \equiv a[q_0 - q_1]^{-1} = a \left[ \alpha - \sqrt{\alpha^2 - 1} \right]^{-1}.
\]

(4.11)

It is easy to verify that the fourth vector from \( \mathcal{K} \) can then be written as a linear combination, with integral coefficients, of the other three vectors in the set. This reveals that the five beam intensity pattern resulting from diffraction of light through the OPM has tetragonal Bravais lattice symmetry, with aspect ratio \( c/a \).

The form of the intensity pattern can be simplified by symmetry arguments. For a normally incident beam and a phase mask with reflection symmetry in both \( x \) and \( y \), as considered here, the electric field components and phases satisfy the following symmetries:

\[
E_{10}^x = E_{\bar{1}0}^x, \quad E_{10}^y = E_{\bar{1}0}^y, \quad E_{10}^z = -E_{\bar{1}0}^z, \quad \phi_{10} = -\phi_{\bar{1}0},
\]

(4.12)

\[
E_{01}^x = E_{0\bar{1}}^x, \quad E_{01}^y = E_{0\bar{1}}^y, \quad E_{01}^z = -E_{0\bar{1}}^z, \quad \phi_{01} = -\phi_{0\bar{1}}.
\]

The relations involving the phases \( \phi \) imply that they can be eliminated by a translation of the origin, \( \vec{r} \rightarrow \vec{r} - \vec{\delta}_1 \), where \( \vec{\delta}_1 = a/2\pi(\phi_{10}, \phi_{01}, 0) \). Using the fact that the unscattered (central) beam is transverse \( (E_{00}^z = 0) \), the relations Eq. (4.12) involving the E-field components imply that

\[
\eta_{00-10} = \eta_{00-\bar{1}0} \equiv c_1; \quad \tau_{00-10} = \tau_{00-\bar{1}0} \equiv \phi_1
\]

(4.13)

\[
\eta_{00-01} = \eta_{00-\bar{0}1} \equiv c_2; \quad \tau_{00-01} = \tau_{00-\bar{0}1} \equiv \phi_2
\]
Here the relations involving $\phi_i$ are modulo $2\pi$. Defining $c_5 \equiv \eta_{10-10}$, $\phi_5 \equiv \tau_{10-10}$, $c_6 \equiv \eta_{01-01}$, and $\phi_6 \equiv \tau_{01-01}$, and noting that $(\vec{K}_{01} - \vec{K}_{10}) = (\vec{K}_{01} - \vec{K}_{10})$ and $(\vec{K}_{01} - \vec{K}_{10}) = (\vec{K}_{01} - \vec{K}_{10})$, we can write the intensity pattern in the photoresist as:

\[
I(\vec{r}) = I_0 + 2\{c_1 \cos[\vec{K}_{10} \cdot \vec{r} + \phi_1] + c_1 \cos[\vec{K}_{10} \cdot \vec{r} + \phi_1]
\]

\[
+ c_2 \cos[\vec{K}_{01} \cdot \vec{r} + \phi_2] + c_2 \cos[\vec{K}_{01} \cdot \vec{r} + \phi_2]
\]

\[
+ 2c_3 \cos \phi_3 \cos[(\vec{K}_{01} - \vec{K}_{10}) \cdot \vec{r}]
\]

\[
+ 2c_4 \cos \phi_4 \cos[(\vec{K}_{01} - \vec{K}_{10}) \cdot \vec{r}]
\]

\[
+ c_5 \cos[(\vec{K}_{10} - \vec{K}_{10}) \cdot \vec{r} + \phi_5]
\]

\[
+ c_6 \cos[(\vec{K}_{01} - \vec{K}_{01}) \cdot \vec{r} + \phi_6].
\]

(4.14)

In Chapter 3 we showed that structures with large PBGs can be created by intensity patterns of the form

\[
I(\vec{r}) = I_0 + C\{\cos(\vec{K}_{10} \cdot \vec{r}) + \cos(\vec{K}_{10} \cdot \vec{r}) + \cos(\vec{K}_{01} \cdot \vec{r}) - \cos(\vec{K}_{01} \cdot \vec{r})\},
\]

(4.15)

where $C$ is a real number\(^1\). In order to write Eq. (4.14) in this form, we make another translation $\vec{r} \rightarrow \vec{r} - \delta_2$, where $\delta_2$ satisfies $\vec{K}_{10} \cdot \delta_2 = \phi_1$, $\vec{K}_{10} \cdot \delta_2 = \phi_1$, and $\vec{K}_{01} \cdot \delta_2 = \phi_2$. It is easy to verify that the translation $\delta_2 = (0, (\phi_2 - \phi_1)a/2\pi, \phi_1 c/2\pi)$ satisfies these conditions. Under this change of coordinates, the intensity pattern becomes

\[
I(\vec{r}) = I_0 + 2\{c_1 \cos[\vec{K}_{10} \cdot \vec{r}] + c_1 \cos[\vec{K}_{10} \cdot \vec{r}]
\]

\[
+ c_2 \cos[\vec{K}_{01} \cdot \vec{r}] + c_2 \cos[\vec{K}_{01} \cdot \vec{r} + 2(\phi_2 - \phi_1)].
\]

(4.16)

\(^1\)In Chapter 3 the vectors are written in terms of a different coordinate system, rotated by $45^\circ$ in the $x$-$y$ plane.
Finally, in order to achieve an intensity pattern corresponding to Eq. (4.15), we desire to find a phase mask which produces modes whose corresponding E-fields satisfy:

\[ c_1 = c_2, \]
\[ \phi_2 - \phi_1 = \pm \frac{\pi}{2}, \text{modulo } 2\pi, \]
\[ 2c_j \cos \phi_j = 0, j = \{3, 4\}, \]
\[ c_5 = c_6 = 0. \]

Eq. (4.17) provides a target pattern against which actual intensity patterns from various phase masks can be evaluated. For a given intensity pattern, we search for the largest achievable PBG, by calculating the photonic bands for structures whose solid-air boundaries are defined by several iso-intensity surfaces of the pattern. The optimal intensity threshold is then defined as one whose iso-intensity surface yields the largest PBG when the developed photoresist is replaced with silicon. However, by comparing the coefficients of intensity patterns to those in Eq. (4.17), one can save computational effort by discarding those intensity patterns which differ greatly from the target intensity pattern.

### 4.3 Optical Phase Mask Architecture

We propose a three-layer phase mask architecture, as shown in Fig. 4.1, to achieve the target intensity pattern described in Sec. 4.2. The phase mask consists of two identical, orthogonally-arranged, one-dimensional binary gratings separated by a homogeneous slab. The motivation
Figure 4.1: Schematic representation of a three-layer phasemask. The top and bottom layers are orthogonally-oriented binary gratings and the middle layer is a homogeneous slab.

for choosing such a design comes from its simplicity and its flexibility through variation of design to deliver the target diffraction pattern. The ideal intensity pattern described by Eq. (4.16) and Eq. (4.17), shown in Fig. 4.2, consists of four repeating intensity slices along the tetragonal direction of the unit cell. This is characteristic of diamond-like structures. The four slices are labelled as A, B, C, and D in Fig. 4.2. Slices A and C differ by an in-plane translation, and slices B and D are a $90^\circ$ rotation from slices A and C. In a very crude picture, the top layer of the proposed phase mask can be thought of as creating a two-dimensional diffraction pattern which generates the A and C slices of the desired shape, while the bottom layer generates a similar diffraction pattern that is rotated by $90^\circ$ and translated in the vertical direction. The homogeneous OPM layer separating the binary gratings is introduced as a mechanism to control the translation between the diffraction patterns created by the two orthogonal, one-dimensional gratings so that the spacing between the slices A, B, C, and D is appropriate. However, this simple picture provides only a rough guide to the overall diffraction pattern. It does not account for the effects of reflections at layer boundaries and interference between the two orthogonal diffraction patterns of the separated grating layers of the OPM. Therefore the true intensity
Figure 4.2: Four unit cells (one unit cell in the vertical direction) of an iso-intensity surface in the target intensity pattern, \( I(\vec{r}) = I_0 + C \{ \cos(\vec{K}_{10} \cdot \vec{r}) + \cos(\vec{K}_{10} \cdot \vec{r}) + \cos(\vec{K}_{01} \cdot \vec{r}) - \cos(\vec{K}_{01} \cdot \vec{r}) \} \). The three planes indicate positions at \( c/4, 2c/4 \) and \( 3c/4 \) along the tetragonal direction.

pattern must be calculated carefully.

Here, the diffraction-interference pattern created by the phase mask is calculated using the rigorous coupled wave analysis method described in Appendix B, with a \( 1024 \times 1024 \) grid and truncation order 441. In each layer of the OPM, and in the homogeneous regions above and below, the electromagnetic field is expanded in terms of modes whose wavevector \( x \)- and \( y \)-components correspond to the Fourier components of the OPM dielectric profile in the \( x-y \) plane. In regions that are homogeneous in \( x \) and \( y \), the \( z \)-component of wavevector of each mode is given by Eq. (4.1). In regions where the dielectric profile is periodic in the \( x-y \) plane, the \( z \)-component of the wavevector is calculated by Fourier expansion of the field in Maxwell’s equations. The resulting diffraction-interference pattern is obtained by matching boundary conditions at the interfaces between the layers. Photonic band structures are calculated with the plane wave expansion method described in Appendix A using over 1440 plane waves, while Fourier coefficients of the dielectric structure are calculated using a discrete Fourier transform with 512 points per direction.
The binary grating layers of the phase mask, each of thickness $d$, consist of alternating regions of refractive index $n_a$ and $n_b$ with periodicity $a$. The $n_a$ regions have width $w$ and the $n_b$ regions have width $(a - w)$. We characterize a given phase mask geometry by the set of adjustable parameters $[w, d, t]$. All lengths are expressed in units of $a$, the lattice constant of the phase mask and of the resulting photonic crystal.

### 4.4 Photonic Band Gap Formation

In this section, we demonstrate the ability of our proposed OPM architecture to generate intensity patterns that can be used to synthesize silicon structures with large predicted PBGs. For concreteness, the refractive indices of the regions above the phase mask (from which the incident beam is launched) and below the phase mask (the region to be exposed) are $n^{(+)} = 1$, corresponding to air, and $n^{(-)} = 1.67$, corresponding to undeveloped SU-8 [107], respectively. We restrict our discussions to configurations that produce an intensity pattern with an aspect ratio $c/a = \sqrt{2}$, corresponding to a FCC Bravais lattice. In Sec. 3.4 we demonstrated that this ratio maximizes the PBG. Accordingly, we take the vacuum wavelength of the incident beam to be

$$\lambda_0 = \frac{2\sqrt{2}n^{(-)}a}{3}. \quad (4.18)$$

The polarization vector of the incident beam is characterized by

$$\vec{E}_{\text{inc}} = \cos(\psi)\hat{x} - e^{ix} \sin(\psi)\hat{y}, \quad (4.19)$$

where $\hat{x}$ and $\hat{y}$ are unit vectors in the $x$- and $y$-directions, respectively, $\psi$ is the linear polarization angle from $\hat{x}$ as measured looking along the incident beam, and $\chi$ is an “ellipticity” angle which indicates the phase delay between the $x$ and $y$ polarization components. In order to simplify the problem, we choose a linearly polarized incident beam ($\chi = 0$). The symmetry of the target diamond structure suggests that we choose $\psi = 45^\circ$, so that the diffracted beams
4.4.1 Direct Structures

We first discuss photonic crystal structures consisting of solid material in the regions of high light intensities (above the threshold of the photoresist) and air in the regions of low light intensity, (below the threshold). Such “direct structures” could be made by silicon double inversion [82] of an SU-8 polymer photoresist exposed by the optical interference pattern or by a single step in certain chalcogenide glasses that are amenable to direct photo-polymerization [83]. For illustration, we consider the case in which the grooves of the phase mask consist of air, so that $n_b = 1$. Fig. 4.3 shows an iso-intensity surface in the interference pattern created by a
phase mask with \([w, d, t] = [0.50a, 0.50a, 0.90a]\) and \(n_a = 2.00\). The diamond-like characteristics of the interference pattern are apparent in the dielectric “nodes” connected to their nearest neighbours by tetrahedral “bonds.” The five beams created in the photoresist by illumination of the phase mask from above have the wavevectors given in Eq. (4.2). The polarization vectors of these beams are determined by rigorous coupled wave analysis and are given by

\[
\vec{E}_{00} = (0.176 + i0.283, -0.145 - i0.303, 0) \quad (4.20)
\]
\[
\vec{E}_{10} = (-0.110 + i0.002, 0.218 - i0.147, -0.310 + i0.004)
\]
\[
\vec{E}_{10} = (-0.110 + i0.002, 0.218 - i0.147, 0.310 - i0.004)
\]
\[
\vec{E}_{01} = (0.129 + i0.202, -0.004 - i0.083, -0.011 - i0.235)
\]
\[
\vec{E}_{01} = (0.129 + i0.202, -0.004 - i0.083, 0.011 + i0.235).
\]

The symmetry of the intensity pattern Eq. (4.20) is comparable to the target symmetry in Eq. (4.17). Quantitatively,

\[
[c_1, c_2, \cos(\phi_1 - \phi_2), 2c_3 \cos \phi_3, 2c_4 \cos \phi_4, c_5, c_6] = (4.21)
\]
\[
[0.119, 0.106, 0.044, 0.000, 0.010, 0.015, 0.009].
\]

High quality materials synthesis requires that the contrast in the optical diffraction pattern, between the highest light intensity regions and the lowest light intensity regions, is maximum. This makes the process less vulnerable to random fluctuations causing unwanted disorder in the developed photoresist. A dynamic range of the intensity pattern which is the largest possible fraction of the background intensity, \(I_0\), leads to the most effective exposure and development of the photoresist. Accordingly, we define the intensity contrast as

\[
C \equiv (I_{\text{max}} - I_{\text{min}})/(2I_0). \quad (4.22)
\]
This is equivalent to the global intensity contrast defined in Sec. 3.5. The intensity pattern in Fig. 4.3 has a background intensity $I_0 = 0.818$, calculated from the polarization vectors according to Eq. (4.8), and reaches a minimum value $I_{\text{min}} = 0.204$ and a maximum value $I_{\text{max}} = 1.500$. The intensity contrast is therefore $C = 0.762$. In comparison, in Sec. 3.5 we saw that the maximum intensity contrast that can be achieved using counter-propagating four-beam interference lithography to generate a diamond-like photonic crystal is 0.816 when elliptical polarizations are allowed, and 0.472 when only linear polarizations are used.

Fig. 4.4 shows the solid volume fraction and the PBG of the silicon replica of the developed photoresist (with a corresponding dielectric constant of 11.9) as functions of the threshold iso-intensity for photo-polymerization, $I_{\text{thr}}$. The mapping of the percentage volume fraction, $f$, to the iso-intensity value can be approximated as $f = -93I_{\text{thr}} + 126$. The optimized structure has a solid volume fraction of 24% and yields a 3D PBG of spectral width $\Delta \omega/\omega_0 = 24\%$. The photonic band structure corresponding to the optimized structure is shown in Fig. 4.5. The 3D PBG opens between bands 4 and 5, and is centered at $a/\lambda_0 = 0.38$. The gap is bounded on the upper edge at the $R$ point and on the lower edge somewhere on the $\Gamma$–$X$ segment.
Chapter 4

Figure 4.5: Photonic band structure diagram for the optimized structure created by the intensity pattern in Fig. 4.3 characterized by 11.9:1 dielectric contrast. The inset shows the positions of the high symmetry points in the reciprocal lattice. A 3D PBG of width \( \Delta \omega/\omega_0 = 24\% \) opens between bands 4 and 5.

It is important to consider the robustness and sensitivity of the PBG to changes in the structural phase mask parameters. The lattice constant of the phase mask grooves is equal to the lattice constant of the photonic crystal in the \( xy \)-plane. It follows that to produce a structure with a PBG in the optical regime, the phase mask must have sub-micron features. Typically, a 3D PBG centered at 1.5 microns made from a silicon photonic crystal requires a lattice constant \( a \approx 600 \text{nm} \). Fig. 4.6 shows the change in the photonic band gap edges of the resulting structure when the phase mask geometry deviates from \( [w, d, t] = [0.50a, 0.50a, 0.90a] \), for a fixed value of the photo-polymerization intensity threshold. For small deviations in \( d \) and in \( t \) the effects are similar, since both cause changes in the path length of light passing through the phase mask. However, changes in \( d \) have the additional effect of changing the strength of the diffraction by the phase mask. Therefore, at larger deviations, the effect of a change in \( d \) differs from that of a change in \( t \).

Fig. 4.7 shows an isosurface plot of the magnitude of the PBG in three-dimensional space of \( [w, d, t] \), for a direct silicon structure created from a phase mask with \( n_a = 2.0 \). The isosurface
Figure 4.6: The photonic band edges as functions of the change in the geometry of the phase mask. The deviation is measured a difference from a phase mask with $[w, d, t] = [0.50a, 0.50a, 0.90a]$. The photo-polymerization intensity threshold is held constant and the structure is characterized by a 11.9:1 dielectric contrast.

Figure 4.7: Iso-surface plot of the magnitude of the PBG in three dimensional $[w, d, t]$-space for a direct silicon OPML photonic crystal created from a phase mask with $n_a = 2.0$. The isosurface corresponds to a gap size of $\Delta \omega/\omega_0 = 20\%$. The relative PBG is larger than 20% inside the volume.
Figure 4.8: (a) The relative PBG size (solid line) and band edge positions (dashed lines) as functions of the linear polarization angle, $\psi$. The PBG magnitude remains above 10% over a change in $\psi$ of $\pm 5^\circ$. (b) PBG size and band edge positions as functions of the “ellipticity” of the incident beam, $\chi$. When $\chi = 0^\circ$, the incident beam is linearly polarized, with linear polarization angle $\psi = 45^\circ$, while at $\chi = \pm 90^\circ$, the incident beam is circularly polarized. The beam passes through a phase mask with geometry $[w, d, t] = [0.50a, 0.50a, 0.90a]$, and the resulting intensity pattern is synthesized with a 11.9:1 dielectric contrast at a photopolymerization intensity threshold of 1.10 times the incident beam intensity.

shown in Fig. 4.7 corresponds to a gap size $\Delta\omega/\omega_0 = 20\%$. Regions inside the depicted surface represent structures with PBGs larger than 20% relative to the gap center frequency. At constant values of the groove width $w$, when each grating thickness $d$ is increased, the grating separation $t$ must be decreased in order for the geometry to remain in the large PBG region. The size of the PBG tends to be more sensitive to changes in $t$ than in $d$ and $w$. The minimum sensitivity to $t$ is reached for values of $w$ between 0.50a and 0.55a.

The variation of the intensity pattern (and PBG of the resulting structure) with changes in the incident beam characteristics is also of importance. Although we do not make use of the incident beam as a design parameter here, it is worthwhile, for practical purposes, to know the robustness of the diffraction-interference pattern (and resulting PBG) against deviations in the incident beam parameters. First, we consider the effect of changing the linear polarization angle, $\psi$, on the relative PBG size and band edge positions. The results are shown in Fig. 4.8(a). The relative PBG magnitude remains above 10% over a change in $\psi$ of $\pm 5^\circ$. Removing the linear polarization restriction on the incident beam provides further design flexibility by al-
Chapter 4

Following the ellipticity angle $\chi$ in Eq. (4.19) to vary. For illustration, we consider a simple path in the two-dimensional polarization parameter space by fixing $\psi = 45^\circ$ and allowing $\chi$ to vary. Fig. 4.8(b) shows the relative PBG size and band edge positions as $\chi$ is varied from $0^\circ$ (corresponding to the linear polarization) to $\pm 90^\circ$ (corresponding to two orthogonal circular polarizations). The PBG does not close at any value of $\chi$, although the relative PBG size drops to just above $10\%$ when the incident beam is circularly polarized. This indicates that the intensity pattern is more dependent on the relative amplitudes of the polarization vector components in the $\hat{x}$ and $\hat{y}$ directions than on the relative phase between the two components.

Another practical concern is the possibility of a slanted profile for the binary grating layers of the OPM as a result, for example, of etching methods that do not generate perfectly normal edges reliably. We consider the case when the profiles of both binary gratings are deflected from the normal by an angle $\alpha$, as depicted in Fig. 4.9. We approximate these slanted binary gratings with ten unslanted binary gratings of equal thickness so that the profile resembles a staircase. Fig. 4.10 shows the dependence of the PBG size and the diffracted beam strengths on $\alpha$. The primary effect of the slanted grating profile is to change the energies of the zeroth-order (undiffracted) transmitted and reflected beams, with a minimal change in the diffracted beams. The upshot is that a shift occurs in the overall intensity in the photoresist, and, thus, the optimal intensity threshold is changed. Since in Fig. 4.10 the threshold intensity is held constant, this
Figure 4.10: The relative PBG size in a silicon replica (left ordinate axis) and diffracted beam strengths (right ordinate axis) as functions of the deflection from normal of the binary grating profiles, at a constant intensity threshold.

means an increasing deviation from the optimal value as the deflection increases, leading to the decrease in predicted PBG size.

The refractive index of the phase mask is a particularly important design consideration. Fig. 4.11 shows the PBG size in $[w, d, t]$-space with groove width $w = 0.50$, using different phase masks with refractive indices of $n_a = 1.95$, $n_a = 2.00$, and $n_a = 2.05$. For each of the refractive indices, we identify regions in the $[d, t]$ parameter space where structures with large PBGs can be generated upon replication with silicon. As one decreases the refractive index of the phase mask from $n_a = 2.00$ to $n_a = 1.95$, a shallower grating depth $d$ and larger separator layer thickness $t$ are required to compensate and produce structures with large PBGs. On the other hand, as the refractive index is increased from $n_a = 2.00$ to $n_a = 2.05$, not only does the large PBG region move to larger groove depth $d$ and smaller grating separation $t$, but the maximum PBG size also drops to about 18%. It is important to note that for high refractive indices, even with small changes in the refractive index of the phase mask, the size of the PBG can vary greatly. For example, a phase mask geometry with $d = 0.50a$, $t = 0.90a$, which and $n_a = 2.0$ produces a structure with a 24% PBG at $I_{\text{thr}} = 1.10$. The same mask structure produces only a 15% PBG for $n_a = 2.05$ and does not even produce a PBG when $n_a = 1.95$. It
Figure 4.11: The relative PBG size of structures created by different phase masks with refractive indices (a) $n_a = 1.95$, (b) $n_a = 2.00$, and (c) $n_a = 2.05$ in $[w, d, t]$-space with groove width $w = 0.50$. The shade in a rectangle corresponds to the PBG size at the value of the grating depth $d$ and separator layer thickness $t$ at the lower left corner of the rectangle, according to the bar on the right. The photo-polymerization intensity threshold is set at a value of 1.10 times the incident beam intensity.
is therefore important to choose phase mask structure according to the particular composition of the mask.

It is of considerable importance to define an ideal range of refractive index contrasts for the optical phase mask. This is governed by a trade-off between high intensity contrast in the interference-diffraction pattern and robustness of the optical interference pattern to random perturbations in the OPM architecture. Both of these factors are important for the development of high quality PBG materials with minimal disorder. Fig. 4.12 shows the relative gap size of structures resulting from phase masks with groove width \( w = 0.50 \) and refractive indices \( n_a = 1.7, n_a = 2.3, \) and \( n_a = 2.5 \), with corresponding threshold intensities \( I_{\text{thr}} = 0.78 \), \( I_{\text{thr}} = 1.37 \), and \( I_{\text{thr}} = 0.93 \). When \( n_a = 1.7 \) and \( n_a = 2.3 \), there are large PBG regions in \([w, d, t]\)-space, comparable in size to the regions shown for \( n_a = 2.0 \) in Fig. 4.11. However, when the refractive index of the phase mask increases to \( n_a = 2.5 \), the large PBG regions in the \([w, d, t]\)-space shrink considerably. This implies that the interference-diffraction pattern is very sensitive to small perturbations in the phase mask structure. For phase masks with \( n_a \) greater than 2.5, this undesirable sensitivity worsens and large PBG regions in \([w, d, t]\)-space are no longer robust to manufacturing error in the OPM. On the other hand, when the refractive index of the phase mask is decreased below \( n_a = 1.7 \), the intensity contrast of the resulting interference pattern is lowered. This in turn makes the photonic crystal architecture more susceptible to disorder arising from inhomogeneities in the photoresist and small random variations in the photo-polymerization threshold.

### 4.4.2 Inverse Structures

In the previous section, we considered photonic band gap architectures that were high refractive index replicas of the optical diffraction-interference pattern where the optical intensity exceeds a prescribed threshold value. On the other hand, the situation may arise wherein the final photonic crystal structure will be defined by high refractive index material in the low intensity regions of OPML and consist of air in the high intensity regions of the OPM.
Figure 4.12: PBG size of structures created by phase masks with refractive indices (a) $n_a = 1.7$, (b) $n_a = 2.3$, and (c) $n_a = 2.5$, with groove width $w = 0.50$, and various values of grating depth $d$ and separator thickness $t$. The corresponding photo-polymerization threshold intensities are (a) $I_{\text{thr}} = 0.78$, (b) $I_{\text{thr}} = 1.37$, and (c) $I_{\text{thr}} = 0.93$. The shade of a rectangle in the figure corresponds to the PBG size resulting from a phase mask with values of $d$ and $t$ at the lower left corner of the rectangle.
diffraction-interference pattern. We refer to these as “inverse structures.” For example, use of a negative photoresist and a single inversion process, or a positive photoresist and a double inversion process will yield such results. For the target intensity pattern described in Eq. (4.16) with the coefficients given in Eq. (4.17), the equivalent but inverted structure (solid and air regions interchanged) is defined by the iso-intensity value $I_{\text{thr}}$ obtained by the “transformation” $I_{\text{thr}} \rightarrow -I_{\text{thr}} + 2I_0$ (to within a translation of $(a/2, a/2, c)$), as we have shown in Sec. 3.5. For the specific, idealized intensity pattern, the PBG structure can be achieved using either fabrication algorithm, yielding solid material in high intensity regions (direct structure) or yielding solid material in the “transformed” low intensity regions (inverse structure). However, this equivalence is specific to the idealized, target intensity. When the coefficients in the intensity pattern do not match the targets in Eq. (4.17), then there is no simple “transformation” to equivalent but inverted structures at different intensity thresholds. Since OPML intensity patterns in this paper differ slightly from the idealized, target pattern (see Eq. (4.21)), it is necessary to consider separately the case of “inverse structures.”

With the understanding that the actual OPML intensity pattern differs slightly from the target pattern, we revisit the phase mask with $[w, d, t] = [0.50a, 0.50a, 0.90a]$ and $n_a = 2.0$. Application of the algorithm $I_{\text{thr}} \rightarrow -I_{\text{thr}} + 2I_0$ with initial threshold $I_{\text{thr}} = 1.10$ and $I_0$ calculated from Eq. (4.20) yields a transformed threshold intensity $I_{\text{thr}} = 0.54$. When the regions illuminated by intensities lower than the threshold value are infiltrated by a solid with dielectric constant 11.9, the resulting structure displays an 18% PBG, at a solid volume fraction of $\approx 24\%$. Adjusting the intensity threshold to $I_{\text{thr}} = 0.58$ produces an optimized structure with a 19% PBG, several percent smaller than the case where the over-exposed regions consist of the same solid material.

While the phase mask with geometry $[w, d, t] = [0.50a, 0.50a, 0.90a]$ is better suited to “direct” PBG architectures, other phase mask geometries exist for which the opposite is true. For example, a phase mask with geometry $[w, d, t] = [0.50a, 0.10a, 0.50a]$ generates the diffraction-interference pattern shown in Fig. 4.13, with an intensity contrast $C' = 0.53$. This leads
Figure 4.13: The iso-intensity surface at photo-polymerization intensity threshold $I_{thr} = 0.43$ in the intensity pattern generated by a phase mask with $[w, d, t] = [0.50a, 0.10a, 0.50a]$, $n_a = 2.0$, and $n_b = 1.0$. The volume fraction of the region inside the surface is $\approx 22\%$. When the low intensity regions (regions inside the surface) are replicated with a material with dielectric constant 11.9 in an air background, the resulting structure displays a 24\% 3D PBG.
Figure 4.14: PBG size of structures created by phase masks with groove width $w = 0.50a$, and grating depth $d$ and grating separation $t$ varying. The refractive index of the phase mask is $n_a = 2.0$ and the photo-polymerization intensity threshold is set at $I_{\text{thr}} = 0.43$. Regions exposed to intensities below $I_{\text{thr}}$ are replicated with a material with dielectric constant 11.9. The shade of a rectangle displays, according to the colorbar to the right, the PBG resulting from a phase mask with $d$ and $t$ corresponding to the values at the lower left corner of the rectangle.

Regions exposed to intensities below $I_{\text{thr}}$ are replicated with a material with dielectric constant 11.9. The shade of a rectangle displays, according to the colorbar to the right, the PBG resulting from a phase mask with $d$ and $t$ corresponding to the values at the lower left corner of the rectangle.

to a structure with a 24% PBG after Si infiltration of the regions with light intensity below $I_{\text{thr}} = 0.43$ in the template. On the other hand, the “direct” silicon structure (filling high-intensity regions) yields, at best, only a 21% PBG when the threshold intensity is optimized to $I_{\text{thr}} = 0.70$. Fig. 4.14 shows the PBG map of “inverse structures” created by phase masks with $w = 0.50a$ and various values of $d$ and $t$. Here, the phase mask index of refraction is $n_a = 2.00$ and the photo-polymerization intensity threshold is $I_{\text{thr}} = 0.43$. There are several geometries in the region surrounding $[w, d, t] = [0.50a, 0.10a, 0.50a]$ which yield “inverse structures” exhibiting a large PBG. The other large PBG regions in the figure point to the possibility of generating large PBG structures with other phase mask geometries. For each particular region, the actual PBG can be made larger than those shown in Fig. 4.14 when $I_{\text{thr}}$ is further optimized. This underscores the importance of considering the intended exposure and inversion processes.
4.5 Proposed OPML Configurations

In this section we describe configurations for OPM lithography using silicon-silica phase masks. The binary gratings of the proposed OPM consist of alternating silicon and silica regions. The homogeneous central layer, separating the gratings above and below, consists of silicon. This suggests that the OPM could be fabricated by established semiconductor microlithography techniques similar to those used for the fabrication of silicon woodpile photonic crystals [74–76]. Fig. 4.15 shows a schematic diagram of our blueprint. The silicon-silica phase mask is mounted on a silica substrate, shown at the top of Fig. 4.15. We restrict the filling ratio of the binary grating layers to be 50%. In other words, the silica and silicon regions both have width \( w = 0.5a \). A sacrificial acrylic (PMMA) layer is introduced between the OPM and the photoresist. This layer can be destroyed after exposure so that the photoresist can be removed without causing damage. We assume that the incident beam illuminates the OPM setup through the silica substrate, at a vacuum wavelength \( \lambda_0 = 800 \text{ nm} \). Crystalline silicon absorbs light weakly at this wavelength. Accordingly, we introduce an imaginary part to its refractive index: \( n_{\text{Si}} = 3.679 + i0.004 \). This corresponds to an absorption coefficient \( \alpha \simeq 630 \text{ cm}^{-1} \). The refractive indices for silica and PMMA, on the other hand, are purely real: \( n_{\text{SiO}_2} = 1.45 \) and \( n_{\text{PMMA}} = 1.50 \). The choice of photoresist is left as a design parameter which we explore in the ensuing sections.

For a given wavelength of the illuminating light, \( \lambda_0 \), and a fixed refractive index of the photoresist, \( n^{(-)} \), it is worthwhile to revisit the condition given in Eq. (4.18) for obtaining an interference pattern with a FCC Bravais lattice. This yields a constraint on the lattice constant of the OPM (equal the lattice constant of the interference pattern):

\[
\alpha = \frac{3\lambda_0}{2\sqrt{2}n^{(-)}}, \tag{4.23}
\]
Figure 4.15: Proposed configuration for OPM lithography using silicon-silica phase masks. The binary grating layers consist of alternating silicon and silica regions, and the separator slab is silicon. A PMMA layer is introduced between the OPM and the photoresist. The incident beam illuminates the OPM through the silica substrate.
Figure 4.16: PBG map of silicon-synthesized structures created by Si-SiO₂ OPM architectures with an SU-8 photoresist, with groove width \( w = 0.50a \). The shade in a rectangle corresponds to the PBG width at the value of the grating depth \( d \) and separator thickness \( t \), according to the colorbar on the right. Here, \( a \) is the OPM grating periodicity, \( \Delta \omega \) is the frequency range of the PBG, and \( \omega_0 \) is the PBG center frequency. The threshold intensity for photo-polymerization is set at a value of 1.2 times the incident beam intensity.

This scale of grating periodicity, in turn dictates the center frequency of the resulting PBG. It implies that the OPM must be tailor made for a given choice of photoresist when a target PBG material is determined.

### 4.5.1 SU-8 photoresist

We first consider exposure of an SU-8 photoresist with \( n^{(-)} = 1.67 \). According to Eq. (4.23), an OPM grating period \( a = 508 \text{ nm} \) is required for a FCC optical interference pattern. If this interference pattern is eventually used to synthesize a silicon photonic crystal, the PBG will be centered at around \( 1.3 \mu \text{m} \). Fig. 4.16 shows the relative gap sizes of silicon-synthesized structures resulting from Si-SiO₂ OPMs with a SU-8 photoresist. The OPM has groove width \( w = 0.50a \), and the photo-polymerization intensity threshold is set at 1.2 times the incident beam intensity. A region of large PBG formation exists around \( d = 0.10a \) and \( t = 1.25a \).

In order to study the effect of the sacrificial PMMA layer, we focus on an OPM with
Figure 4.17: Effect of the PMMA layer on the resulting PBG widths of silicon-synthesized structures created by a Si-SiO$_2$ OPM with a SU-8 photoresist. The OPM has geometry $[w, d, t] = [0.50a, 0.12a, 1.23a]$. The shade in a rectangle corresponds to the PBG size at the PMMA layer thickness and photo-polymerization intensity threshold (in units of the incident beam intensity) at the lower left corner of the rectangle, according to the colorbar on the right.

geometry $[w, d, t] = [0.50a, 0.12a, 1.23a]$. Fig. 4.17 shows the PBG size as a function of the PMMA layer thickness and the photo-polymerization intensity threshold. The first-order diffracted modes are evanescent in the PMMA layer due to the lower refractive index of PMMA as compared to that of SU-8. Consequently, the strength of these diffracted modes is lower when the PMMA layer is introduced. As a result, when the PMMA thickness increases, the optimal intensity threshold value decreases. However, since the refractive index of PMMA is close to that of SU-8, the shift is fairly small.

4.5.2 As$_2$S$_3$ photoresist

An alternative photosensitive material is the chalcogenide glass As$_2$S$_3$. We now consider the exposure of an As$_2$S$_3$ photoresist with $n(\nu) = 2.39$ [135]. In this case, a FCC interference pattern is obtained when the OPM has a lattice constant $a = 355$ nm. A silicon replica of the developed photoresist (optimized to have the largest PBG) will then have a PBG centered at
Figure 4.18: PBG map of silicon-synthesized structures created by Si-SiO$_2$ OPMs with an As$_2$S$_3$ photoresist. The binary gratings of the OPM have groove width $w = 0.50a$, and the photo-polymerization intensity threshold is set at a value of 1.3 times the incident beam intensity.

around 940 nm. If the As$_2$S$_3$ structure is used as a photonic crystal directly, the PBG is centered around 790 nm, with smaller gap owing to the lower refractive index of the chalcogenide glass. Fig. 4.18 shows a map of PBG widths for silicon-synthesized structures created by a Si-SiO$_2$ OPM with As$_2$S$_3$ photoresist. The binary gratings of the OPM have groove width $w = 0.50a$ and the photo-polymerization intensity threshold is set at a value of 1.3 times the incident beam intensity. Again, a region of large PBG formation is found. The effect of the PMMA layer thickness on the PBG size is shown in Fig. 4.19. The dependence on the PMMA thickness is much stronger than with the SU-8 photoresist, due to the larger refractive index mismatch between PMMA and As$_2$S$_3$.

4.6 Discussion

We have shown that single-exposure, optical phase mask lithography (OPML) based on diffraction-interference patterns from a single beam normally incident on suitably designed phase masks can be used to create diamondlike photonic crystals with large PBGs. The phase mask design
was facilitated by introducing a target five-beam interference pattern in an umbrella configuration, identical to the four-beam counter-propagating interference pattern proposed in Chapter 3 for generating a diamondlike photonic crystal. Using the OPM to generate five interfering beams from a single incident beam places the role of controlling the relative phases, polarizations, amplitudes, and wavevectors of the interfering beams on the phase mask itself. Unlike multi-beam holographic lithography, in OPML only the parameters of the single incident beam need to be precisely controlled. The relative PBG sizes of final silicon-based “direct” structures remain over 10% even when the linear polarization angle changes by $\pm 5^\circ$. Since the OPML intensity pattern is determined by the design of the phase mask, it is only possible to realize a close approximation to the target intensity pattern of more general five-beam interference. The resulting reduction of symmetry in the OPML pattern, however, leads only to a slight decrease in the PBG size (from 25% to 24% in the cases discussed here). The reduction in symmetry also leads to a distinction between “direct” and “inverse” photonic crystal architectures. The intensity contrast in OPML is comparable to that which can be achieved using counter-propagating four-beam holography. The optimal phase mask geometry is sensitive to the refractive indices
of the phase mask and the photoresist. Therefore, the phase mask structure must be tailored specifically to the chosen constituent materials. Moreover, there may be several regions in the parameter space of phase mask geometries that can produce a suitable intensity pattern. We provided an illustration of a robust geometry, suitable to fabricate a “direct” silicon PBG material. The PBG in this “direct” silicon structure persists despite 8% variations in the thickness of the homogeneous middle layer of the phase mask, and despite more than a 10% variation in either the width or thickness of the phase mask grooves. By expanding the parameter space of the phase mask design, other blueprints for fabricating photonic crystals by single-exposure phase mask lithography may be found. For instance, the depth of the upper and lower gratings can be allowed to vary independently.

The fabrication of the phase mask, itself, requires high precision semiconductor microlithography. The lattice constant of the phase mask grating equals the lattice constant of the resulting photonic crystal itself, with corresponding sub-micron feature sizes. However, after the phase mask is fabricated, it can be used repeatedly to expose many photoresists, offering the possibility of efficient mass production of 3D PBG materials.
Chapter 5

Circuits for Light in Holographically Defined Photonic Band Gap Materials

5.1 Introduction

In previous chapters we demonstrated that diamondlike 3D architectures leading to large photonic band gaps can be imprinted in a photoresist holographically using multiple laser beam interference or from a single beam diffracting through an optical phase mask. Replication of this diamondlike hologram with a high index material results in a photonic crystal with a large 3D PBG. An important question is whether the PBG architecture, defined by holographic lithography, can serve as a backbone for high-bandwidth, single-mode, optical waveguides and ultradense optical integrated circuitry. In this chapter, we introduce design rules for creating 3D waveguide circuits with sharp, low-loss bends in this photonic crystal.

Waveguide networks in 3D photonic crystals offer robust, PBG-based light confinement in all spatial dimensions. Designs for single-mode, air waveguide networks have been proposed for the woodpile structure [8, 9, 136]. Here, the layer-by-layer architecture allows for the natural inclusion of defects during the fabrication process [77]. A photonic band gap heterostructure, consisting of parallel 2D PC micro-chip layers separated by 3D PBG cladding
layers [38, 39] is predicted to allow for the incorporation of parallel 2D waveguide networks linked by vertical waveguides in the cladding layers [10, 11]. Templates for these heterostructures have been fabricated using direct laser writing (DLW). In DLW two-photon absorption causes exposure of a photoresist [71]. The DLW process, in which discrete volume elements of the photoresist are exposed sequentially, is amenable to the inclusion of defects in the otherwise periodic structure. However, sequential fabrication inherent to DLW is inefficient in the construction of the background PBG material. On the other hand, holographic lithography techniques offer the ability to create large 3D PBG materials with long range order, efficiently and at low cost, but do not provide an obvious route to the inclusion of predetermined defects in the periodic lattice. The 3D optical interference pattern used to create a diamondlike structure consists of only four sinusoidal terms comprising the intensity pattern. In contrast, a well defined, localized defect in the periodic lattice requires a large number of Fourier terms. This would require a correspondingly large number of beams to create the desired interference pattern. Instead, it has been suggested that an undeveloped photoresist, already patterned with holographic lithography, could subsequently be exposed using DLW to create defects [137]. This requires alignment of the DLW and optical phase mask setups. Here, we present designs for single mode, air waveguide channels in the diamondlike structure, that can be achieved by suitable alignment of the two optical writing methods. We also introduce design rules for sharp waveguide bends, enabling the creation of a full 3D waveguide network, exhibiting greater than 98% transmission over a 90 nm bandwidth for in-plane bends, and a 75 nm bandwidth for bends into the vertical dimension. In Sec. 5.2, we briefly review the periodic backbone structure and describe the computational techniques and parameters used. In Sec. 5.3 we consider the design of waveguides in the diamond background structure in various crystallographic directions. In Sec. 5.4, we develop design rules for nearly lossless waveguide bends obtained by forming junctions between waveguides in different directions.
5.2 Design Parameters

In this section, we use the tetragonal Bravais lattice form of the diamondlike structure from Chapter 4, defined by

\[ I(\mathbf{r}) = I_0 + C \Delta I, \]  

(5.1)

where \( I_0 \) and \( C \) are constants depending on the particular phase mask or multi-beam configuration used, and

\[
\Delta I = \cos \left[ \frac{2\pi}{a} \left( x + z/\sqrt{2} \right) \right] + \cos \left[ \frac{2\pi}{a} \left( x - z/\sqrt{2} \right) \right] \\
+ \cos \left[ \frac{2\pi}{a} \left( y + z/\sqrt{2} \right) \right] - \cos \left[ \frac{2\pi}{a} \left( y - z/\sqrt{2} \right) \right].
\]  

(5.2)

This intensity pattern has tetragonal Bravais lattice symmetry with aspect ratio \( c/a = \sqrt{2} \), where \( c \) is the lattice constant in the vertical direction. This optimizes the PBG of the generalized tetragonal structure in Sec. 3.4. We focus on the varying part of the intensity pattern, Eq. (5.2). After replication of the developed photoresist with a high index material, the resulting photonic crystal consists of solid material in the regions where \( \Delta I \) either exceeds or falls below some threshold, \( I_{\text{thr}} \). For concreteness, we consider the latter scenario, corresponding to the situation where the regions exposed by DLW become air defects in the final silicon photonic crystal. This could be achieved in practice by a modification of the recently established double inversion technique for SU-8 photoresist templates. In the original fabrication protocol [82], the SU-8 template is fully infiltrated by room temperature chemical vapor deposition (CVD) of SiO\(_2\) and the SU-8 removed by plasma etching or calcination in air. The inverted SiO\(_2\) template is then infiltrated by Si CVD and the SiO\(_2\) removed by chemical etching, producing a silicon replica of the over-exposed regions of the photoresist. A modified fabrication protocol can be employed to produce a silicon replica of the underexposed regions. In this new protocol [138], the first infiltration step is modified to produce only a thin shell of SiO\(_2\) surrounding the SU-8 template. Subsequent Si infiltration then creates an inverse of the original polymer template.
We choose \( I_{\text{thr}} = -1.4 \) so that the solid regions of the final PBG material are characterized by \( \Delta I < -1.4 \) and the air regions by \( \Delta I > -1.4 \). The equivalent but inverted structure (air and solid regions interchanged) can be obtained by setting \( I_{\text{thr}} = +1.4 \) and translating the origin by \( (a/2, a/2, 0) \). This structure has a solid volume fraction of approximately 21% and exhibits a 25% relative 3D PBG when the solid regions consist of silicon, with dielectric constant 11.9.

### 5.2.1 Computational Methods

Photonic band structures are calculated using the PWEM (Appendix A). For the bulk PC with no defects, over 2600 plane waves are used. Fourier coefficients are obtained using a discrete Fourier transform with 512 points per direction. The band frequencies obtained differ by less than 0.3% from those obtained using over 4300 plane waves. Waveguide modes are calculated using a supercell technique, with 1 unit cell in the waveguide direction and 6 unit cells in the other two directions, using 9000 plane waves in the PWEM. This creates, in effect, a periodic structure with parallel waveguide channels repeating in intervals of 6 unit cells. Convergence is realized when the waveguide dispersion relations become independent of the size of the supercell. Fourier coefficients of the dielectric structure in the supercell are obtained using 128 points per unit cell (768 points in the supercell directions). The calculated band frequencies differ by less than 1% from those obtained using over 24000 plane waves. In addition, increasing the supercell size to 7 unit cells in the non-waveguide directions produces less than a 0.1% change in the waveguide dispersion relations, indicating the adequacy of the chosen supercell size for isolating the effects of the parallel waveguide channels. Light propagation through the waveguide channels is modelled using the FDTD method (Appendix C) with 12 mesh points per \( a \) (unit cell in the \( x \)- and \( y \)-directions) and 16 mesh points per \( c \) (unit cell in the \( z \)-direction). The grid spacing in the \( z \)-direction is adjusted to maintain the desired aspect ratio \( c/a = \sqrt{2} \). Transmission and reflection spectra are obtained by calculating the Poynting vector fluxes through planar surfaces perpendicular to the waveguide channels. We use planar surfaces extending over three unit cells in each direction away from the waveguide.
5.3 Waveguide Design

Waveguide channels can be formed by introducing a series of defects in the photonic crystal structure. In general, the removal of material from a photonic crystal creates air modes originating from the bands on the lower edge of the PBG, whereas the addition of material creates dielectric modes originating from the upper band edge [5]. Following the procedure introduced in Ref. [11], we examine the electromagnetic field distributions in the originating bands of the perfect structure in order to determine the desired defect locations. Removing dielectric material in those locations where field energy is concentrated near the lower band edge mode facilitates the creation of broad bandwidth, single-mode, air waveguides. Removal of dielectric from other regions tends to produce multimode or narrow band waveguides that are much more susceptible to backscattering losses in the presence of small amounts of random disorder. A similar procedure was later used to design waveguides in a body-centered cubic holographic PC [139].

We first consider the design of air waveguides in the $x$- and $y$-directions. Air waveguide modes originate from those bands of the bulk PC at the lower edge of the band gap. Fig. 5.1
Figure 5.2: Electric displacement field for the diamondlike PC, for Bloch vectors along the $x$- and $y$-directions with length 0.25 $[2\pi/a]$, at an arbitrary instant in time, for the (a) third and (b) fourth bands. The field vectors are shown as green arrows superimposed onto the dielectric surface of the photonic crystal in a unit cell, shown in yellow. High intensity regions of the field are shown in shaded red.

shows the photonic band structure of the bulk PC in the $x$- and $y$- directions, which are equivalent due to the symmetry of the structure. Fig. 5.2(a) and (b) show the electric displacement field distributions for the third and fourth bands, respectively, at a Bloch vector of length 0.25 $[2\pi/a]$ and some arbitrary instant in time. The shaded red regions correspond to regions of high field intensity. These high intensity regions are centered at the tetrahedral “bonds” characteristic to the diamond architecture. Fig. 5.3 shows the mode frequency of a localized state of light as a function of the sphere radius for a spherical air defect centered at $(0, 0, 0)$. This is equivalent to introducing an air defect centered at any of the intensity maxima in Fig. 5.2(a) or Fig. 5.2(b), due to the symmetry of the structure.

We now focus on the distribution in Fig. 5.2(a). The fields are clearly concentrated along lines in the $x$-direction, with intensity maxima centered at $(a/4, a/4, c/4)$, $(3a/4, a/4, c/4)$, $(a/4, 3a/4, 3c/4)$, and $(3a/4, 3a/4, 3c/4)$, and field vectors pointing in the $x$-$z$ plane. Both our current structure and the woodpile PBG structure [72, 73], as diamondlike architectures,
are characterized by “nodes” of material joined by tetrahedral “bonds”. In the woodpile architecture, the dielectric nodes are centered at the meeting points between perpendicular rods. As a result, a correspondence can be made between the field vector lines in our holographically defined PBG material and the dielectric rods running in the $x$-direction in the woodpile PBG structure. This suggests that waveguide channels in the $x$-direction, with electric fields polarized in the $x$-$z$ plane, can be obtained by removing material around each point $((2m + 1)a/4, a/4, c/4)$ or around each point $((2m + 1)a/4, 3a/4, 3c/4)$, where $m$ is the sequence of integers chosen to span the desired waveguide length. We denote these waveguides as $X_{xz}^{a/4}$ and $X_{xz}^{3a/4}$, respectively, where the superscript indicates the plane of polarization and the subscript indicates the $y$- and $z$-coordinates of the defect centers. These waveguides correspond to removing a single rod to create a waveguide channel in the woodpile structure. We refer to these waveguides that follow the field vector lines as type I waveguides. Fig. 5.4 shows a type I waveguide in the woodpile PBG material. Similarly, the field patterns in Fig. 5.2(b) suggest that waveguides in the $y$-direction, with field vectors in the $y$-$z$ plane, can be obtained by removing material around $(a/2, ma/2, 0)$ or $(0, ma/2, c/2)$. In our naming scheme, these
Figure 5.4: Type I waveguide in the woodpile structure. The waveguide is characterized by a missing rod in the top layer shown.

waveguides are denoted as \( Y_{\frac{a}{4}}^{yz} \) and \( Y_{\frac{c}{4}}^{yz} \), respectively.

As a detailed illustration of a type I waveguide, we investigate the case where material is removed around the points \( ((2m + 1)a/4, a/4, c/4) \), creating a waveguide in the \( x \)-direction, \( X_{\frac{a}{4}}^{xz} \). The other cases, for both the \( x \)- and \( y \)-directions, are analogous due to the symmetry of the structure. For simplicity, we assume that material is removed from spheres centered at the intensity maxima. Further optimization of the waveguide single-mode bandwidth may be possible using defects better tailored to the ellipsoidal shape of the high intensity regions. Fig. 5.5(a) shows the waveguide with removed regions of the periodic backbone indicated by red. The radius of the air spheres is 0.25\( a \). We find that this choice of radius maximizes the bandwidth of the waveguide mode without introducing undesired modes. Due to the linear nature of the waveguide, these spherical defects could be replaced by a cylindrical air hole with matching radius, passing through the centers of the spheres. The additional material removed would not disturb any additional high field intensity regions in Fig. 5.2, so the waveguide mode
Figure 5.5: (a) Waveguide in the $x$-direction, $X_{xz}^{yz}$, with material removed at spheres of radius $0.25a$ centered at $((2m+1)a/4, a/4, c/4)$. The removed regions are indicated by red. (b) Corresponding dispersion relation. The single-mode region of the waveguide mode spans the normalized frequency range $a/\lambda \sim 0.354 - 0.401$.

would not be altered significantly. The corresponding waveguide band structure is shown in Fig. 5.5(b). The removal of material from the periodic structure creates air modes originating from the lower edge of the PBG. In this case, the waveguide mode is created by disturbing two high field intensity regions per unit cell in the waveguide direction. As a result, the waveguide mode consists of two bands, originating from the first and third bands in the periodic structure. These are the bands in the periodic structure whose electromagnetic mode field patterns are polarized in the $x$-$z$ plane, as is the waveguide mode. The single-mode region of the waveguide mode spans the normalized frequency range $a/\lambda \sim 0.354 - 0.401$, corresponding to a bandwidth of 199 nm if the waveguide mode is centered at $1.5 \mu m$ ($a \sim 600$ nm). The group velocity of light in the waveguide with Bloch vector near 0.4 $[2\pi/a]$ reaches approximately 0.15 times the speed of light in vacuum. This group velocity is somewhat lower than the group velocity attained in the corresponding waveguide of a 2D-3D PBG heterostructure [38].

In addition to waveguide channels that follow the lines of concentrated field intensity, it is also possible to create waveguides that cut across these lines. We refer to these channels as type II waveguides. This involves the creation of one defect per unit cell along the direction orthogonal to the field vector lines. For a type II waveguide in the $y$-direction, the defect can be
centered at any of the high field intensity regions in Fig. 5.2(a), provided the defect is repeated along the $y$-direction. Creating air defects at any of the high intensity regions in Fig. 5.2(b), with the appropriate periodicity, leads to a waveguide in the $x$-direction. Fig. 5.6(a) shows a two unit cells of a waveguide channel in the $y$-direction created by spherical defects of radius 0.30$a$ centered at $(a/4, (4m + 1)a/4, c/4)$, with the removed regions of the periodic structure in red. In our classification scheme, this waveguide is denoted $Y_{2,4}^{XZ}$, as the electric fields for this waveguide mode are polarized in the $x$-$z$ plane. Fig. 5.6(b) shows the corresponding waveguide band structure, consisting of a single, monotonic band spanning the normalized frequency range $a/\lambda \sim 0.370 - 0.436$. This waveguide is analogous to the “Type II $Y$” waveguide in woodpile photonic crystals studied by Li and Ho [136], except that the bandwidth in our case is wider due to the larger PBG of the holographic diamond structure\(^1\). Fig. 5.7 shows a type II waveguide in the woodpile PBG material. The group velocity of light in the waveguide

\(^1\)Li and Ho also studied a so-called “Type I $Y$” waveguide, whose central axis is shifted by $a/4$ in the $x$-direction relative to the waveguide presented here. This alternate waveguide channel studied by Li and Ho exhibits double-mode operation throughout most of the frequency range. In the field distribution picture we use here, this double-mode behaviour can be explained by noting that such a waveguide channel will disturb two of the high-intensity regions in each unit cell.
with Bloch vector near 0.3 \([2\pi/a]\) reaches approximately 0.22 times the speed of light in vacuum. This is nearly the group velocity attained in the in-plane waveguides of 2D-3D PBG heterostructures [38].

Waveguides in the vertical \((z)\) direction can also be designed by examining the band structure and field distributions for waves propagating in the \(z\)-direction near the lower edge of the complete PBG. Fig. 5.8 shows the band structure for the unaltered PC along the \(z\)-direction. There are two doubly degenerate pairs of bands below the PBG. The field intensity distributions closely resemble the distributions for Bloch vectors in the \(x\)- and \(y\)-directions, with intensity maxima occurring at the same locations as in the previous case. However, there is no high-bandwidth waveguide obtained by removing material in a straight line in the vertical direction. In analogy with 2D-3D heterostructures [10, 11], a zig-zag pattern of dielectric removal must be used. For concreteness, we consider removing material at the intensity maxima shown in the Fig. 5.2(a). In this case, the intensity maxima are found at \((a/4, a/4, c/4), (3a/4, a/4, c/4),\)
(a/4, 3a/4, 3c/4). A vertical waveguide can be formed by: (1) removing regions centered at a constant $x$ coordinate, such as at $(a/4, a/4, c/4)$, $(a/4, 3a/4, 3c/4)$, and so on (shown in Fig. 5.9(a)); (2) removing regions centered at a constant $y$ coordinate, such as at $(a/4, a/4, c/4)$, $(a/4, a/4, 5c/4)$, and so on (Fig. 5.9(b)); or (3) removing regions without keeping $x$ or $y$ constant, such as at $(a/4, a/4, c/4)$, $(3a/4, 3a/4, 3c/4)$, and so on (Fig. 5.9(c)). We find that removing rods centered at constant $x$ (case 1) maximizes the single-mode waveguiding bandwidth. For cases 2 and 3, the resulting defect modes span a narrow bandwidth. In case 2, the dispersion relation strongly resembles one obtained using a tight binding model describing the waveguide as a series of weakly coupled optical resonators with mode frequencies as shown in Fig. 5.3 [140]. The weak coupling is unable to produce a mode with a wide bandwidth. In order to increase the bandwidth, additional defects must be included, increasing the number of waveguide bands [139]. In cases 1 and 3, one additional defect is created per unit cell in the waveguide direction, causing the formation of a second waveguide band. In case 3, the placement of the defects creates an inversion symmetry. As a result, there is a mode gap between the two waveguide bands, which limits the bandwidth [141]. Similarly, if an ad-
Figure 5.9: Possible schemes for creating vertical waveguides with electric fields polarized in the $x$-$z$ plane, with corresponding band structures shown below: (a) Removing regions centered at a constant $x$-coordinate; (b) Removing regions centered at a constant $y$-coordinate; and (c) Removing regions without keeping $x$ or $y$ constant.
Figure 5.10: (a) Waveguide in the $z$-direction, $Z_{x=a/4}^{XZ}$, with material removed at spheres of radius $0.25a$ centered at $(a/4, a/4, c/4)$ and $(a/4, 3a/4, 3c/4)$ in unit cells along the $z$-direction. The removed regions are indicated in red. (b) Corresponding dispersion relation. The single-mode region of the waveguide mode spans the normalized frequency range $a/\lambda \sim 0.374 - 0.420$.

A secondary defect is created in the locations indicated by the dotted line in Fig. 5.9(b), a mirror reflection plane exists at $x = 0.5a$, and mode gap is formed between the two waveguide bands. On the other hand, the waveguide channel in case 1 lacks both inversion symmetry and a mirror reflection plane, and the resultant lack of a mode gap between the two waveguide modes allows for a large bandwidth.

The air waveguide for case 1 is shown in Fig. 5.10(a) with removed parts indicated in red. We denote this as the $Z_{x=a/4}^{XZ}$ waveguide in our naming scheme. An equivalent waveguide could be created by removing material at the $x = 3a/4$ regions ($Z_{x=3a/4}^{XZ}$). The dispersion relation for this waveguide is shown in Fig. 5.10(b). Again, the waveguide mode consists of two bands, the single-mode portions of which span a normalized frequency range of $a/\lambda \sim 0.374 - 0.420$, corresponding to a bandwidth of 175 nm if the 3D PBG is centered at 1.5 $\mu$m ($a \sim 600$ nm).

The group velocity of light in this waveguide reaches approximately 0.14 times the speed of light in vacuum. The waveguide mode created by this defect has its electric field polarized in the $x$-$z$ plane. An analogous waveguide can be created by removing regions centered at a constant $y$ coordinate from Fig. 5.2(b) ($Z_{y=0}^{YZ}$). In this case, which is the same as case 1 above
rotated by $90^\circ$ about the $z$-axis and translated one quarter of a lattice constant in the vertical direction, the electric field is polarized in the $y$-$z$ plane.

### 5.4 Waveguide Bends

The existence of high-bandwidth, single-mode, linear waveguide channels in three orthogonal directions, within the holographically defined PBG backbone, offers the opportunity for circuits of light within a truly 3D optical microchip. Unlike earlier 2D-3D PBG heterostructures [38, 39], which require alignment and embedding of 2D microchip layers in a 3D PBG material, the holographically defined architectures do not require an intermediate 2D photonic crystal synthesis step. However, careful alignment of the optical fields provided by the optical phase mask for creating the PBG backbone material and the optical voxels for direct laser writing of waveguides is needed. From a design point of view, it is also important to establish that sharp waveguide bends providing nearly perfect transmission of light over a large bandwidth can be engineered within the holographic diamond architecture. In this section, we establish the required design rules.

#### 5.4.1 Horizontal Type I Waveguide Bends

We first investigate bending of light between identical waveguides in the $x$- and $y$-directions. We begin by studying bends between type I waveguide channels along lines of concentrated field intensity, as shown in Fig. 5.5. In this case, the waveguides in the $x$- and $y$-directions are denoted by $X_{xz}^{a/\lambda}$ and $Y_{yz}^{b/\lambda}$, respectively. The shape of the waveguide elbow can be modified by adjusting the termination points of each waveguide, altering the amount of overshoot between the two channels. We use a FDTD simulation to model the transmission of light through the bend using a pulse spanning the frequency range $a/\lambda \sim 0.365 - 0.405$, avoiding the flat parts of the waveguide dispersion curve (slow group velocity) and minimizing the spread of the pulse over the length of the waveguide channels. Fig. 5.11 shows transmission and reflection spec-
Figure 5.11: Transmission (black) and reflection (red) spectra for bends between waveguides in the $x$- and $y$-directions for various bend geometries. The light grey circles in the schematic bend diagrams represent air spheres centered in the $z = c/2$ plane, while the dark grey circles represent air spheres centered in the $z = c/4$ plane.
tra for various bend geometries. The configuration in which both waveguides overshoot each other by a single defect (see third panel of Fig. 5.11) enables over 90% transmission through the bend over the frequency range $a/\lambda \sim 0.372 - 0.405$. This corresponds to a bandwidth of about 130 nm when the PBG is centered at 1.5 $\mu$m. Over 95% transmission is obtained throughout the frequency range $a/\lambda \sim 0.384 - 0.405$ (approximately 80 nm bandwidth), and more than 98% transmission over $a/\lambda \sim 0.398 - 0.405$ ($\sim 25$ nm). In addition, the configuration with no overshoot between the two waveguides (top panel of Fig. 5.11) allows for over 98% transmission over the frequency range $a/\lambda \sim 0.389 - 0.405$ (approximately 60 nm bandwidth), at the cost of low transmission at lower frequencies.

Other bend geometries permit no transmission through the bend at certain frequencies (panels two and four in Fig. 5.11). Due to the bend geometries and the envelope amplitudes of the electromagnetic field at specific wavevectors, the longitudinal profiles of the waveguide mode have nodes at the position where the two channels overlap and strong reflection occurs at specific frequencies. The field in the incoming waveguide channel is unable to excite modes in the outgoing channel and light is not transmitted through the bend. The configuration in the fourth panel of Fig. 5.11, with a single defect overshoot in one channel, and a double defect overshoot in the second channel, can be thought of as a modification of the configuration in the third panel, with an additional side-coupled defect. Indeed, the transmission spectrum for this case corresponds closely to the transmission spectrum obtained for a straight waveguide with a single, side-coupled air cavity. By analogy, the transmission characteristics of the configuration with double defect overshoot for both waveguide channels (bottom panel of Fig. 5.11) are suggestive of a broadened reflection peak resulting from the existence of two cavities.

The transmission characteristics of the bend can be altered by further structural modification. Fig. 5.12 shows the effect of varying the radii of the terminating air spheres (at the endpoint of each linear waveguide segment) on the transmission spectrum of the configuration with single sphere overshoot. A slight decrease of the radii of these terminating defects to $0.20a$ from $0.25a$ increases the transmission by $\sim 2\%$ over a large range of frequency. Fur-
Figure 5.12: Transmission spectra for bends with a single air sphere overlap between the $x$ and $y$ waveguide channels. The radius of the overlapping air spheres, shaded red in the inset, is varied. The other spheres in the body of the waveguide have radius $0.25a$.

Further decreasing the radius to $0.15a$ produces over 95% transmission in the frequency range $a/\lambda \sim 0.365 \sim 0.387$, at the cost of low transmission at higher frequencies. On the other hand, increasing the radii of the terminating spheres decreases the transmission over the entire spectrum.

### 5.4.2 Horizontal Type II Waveguide Bends

We now consider bending between type II waveguides in the $x$- and $y$-directions formed by cutting across lines of concentrated field intensity, as in the waveguide channel depicted in Fig. 5.6. Fig. 5.13 shows the transmission and reflection spectra for light propagating from a $y$ waveguide channel, denoted by $Y_{x^a z^c}$, into various waveguide channels in the $x$-direction, for a pulse spanning the frequency range $a/\lambda \sim 0.380 \sim 0.435$. When light from the $Y_{x^a z^c}$ waveguide is coupled to a $X_{y^b z^d}$ waveguide, as shown in the top panel of Fig. 5.13, over 90% of the light is transmitted over the frequency range $a/\lambda \sim 0.380 \sim 0.409$, corresponding to a bandwidth of about 110 nm for a PBG centered at 1.5 $\mu$m. Transmission above 95% and 98% is obtained over frequency ranges $a/\lambda \sim 0.381 \sim 0.401$ (~80 nm bandwidth for a PBG at 1.5 —micron)
Figure 5.13: Transmission (black) and reflection (red) spectra for bends between alternative waveguides in the $x$- and $y$-directions for various bend geometries. The white, black, and cross-hatched circles in the schematic bend diagrams represent air spheres centered in the $z = c/4$, $z = c/2$, and $z = 0$ planes, respectively.
Figure 5.14: The transmission spectra for bends between $Y_{xz}^{XZ}$ and $X_{yz}^{YZ}$ waveguides in the $x$- and $y$-directions, as the radii of the red-shaded defects are adjusted. The reflection peak is red-shifted as the defect radius is decreased. The unaltered defects have radius $0.30a$.

and $a/\lambda \sim 0.382 - 0.391$ (~35 nm), respectively.

If the light is instead coupled to a parallel $x$-waveguide channel ($X_{yz}^{YZ}$) that is $a/2$ farther away from the termination of the $y$-waveguide, as shown in the middle panel of Fig. 5.13, the 90% transmission frequency range increases to $a/\lambda \sim 0.386 - 0.435$ (~175 nm bandwidth). The frequency ranges for transmission above 95% and 98% improve to $a/\lambda \sim 0.395 - 0.435$ (~140 nm) and $a/\lambda \sim 0.411 - 0.435$ (~80 nm), respectively.

The configuration shown in the bottom panel of Fig. 5.13, with bending between a $Y_{xz}^{XZ}$ waveguide and a $X_{yz}^{YZ}$ waveguide, produces over 98% transmission over almost the entire frequency range studied, except around a strong reflection peak near $a/\lambda = 0.392$. Due to this peak, the transmission drops below 98% in the frequency range $a/\lambda \sim 0.389 - 0.399$. By adjusting the size of the terminating defects for each waveguide, it is possible to change the center frequency of this reflection peak, as shown in Fig. 5.14.
5.4.3 Horizontal Hybrid Waveguide Bends

Due to the existence of two types of waveguides in the $x$- and $y$-directions it is possible to create bends between waveguides that lie in the same $x$-$y$ plane. This corresponds to a link between a type I waveguide and a type II waveguide. Fig. 5.15 shows the transmission and reflection spectrum for a bending configuration with no overshoot for either waveguide channel. About 90% of the light is transmitted over the frequency range $a/\lambda \sim 0.382 - 0.405$, representing about a 90 nm bandwidth when the 3D PBG is centered at 1.5 $\mu$m. Other bend geometries we considered displayed inferior transmission. In addition, the bending bandwidth is inherently limited by the relatively small frequency overlap between the different waveguide modes.

5.4.4 Vertical Bends from Type I Waveguides

We finally consider the bending of light from a waveguide channel in the $x$-$y$ plane into a waveguide channel in the vertical direction. We first investigate coupling from a type I waveguide in the $x$-direction comprised of defects located along the lines of concentrated field intensity of the periodic structure, as illustrated in Fig. 5.5. The mode associated to this waveguide channel, denoted as $X_{\text{xz}}^{xy}$, has its electric field polarized in the $x$-$z$ plane and magnetic field in the $y$-direction. This waveguide can either be coupled to the vertical waveguide denoted by
$Z_{yz}$ or the one denoted by $Z_{xz}$. In the first case, the vertical waveguide mode has electric field polarized in the $y$-$z$ plane and magnetic field polarized in the $x$-direction. When considering the field components perpendicular to the waveguide direction, neither the electric ($\hat{z} \rightarrow \hat{y}$) nor magnetic field ($\hat{y} \rightarrow \hat{x}$) is conserved across the bend. As a result, a bend between these waveguides results in virtually no transmission, because the field from the first waveguide is unable to excite the mode of the second waveguide [11]. The vertical waveguide denoted by $Z_{xz}$, on the other hand, has electric field polarized in the $x$-$z$ plane and magnetic field in the $y$-direction. Here, the perpendicular components of the electric field ($\hat{z} \rightarrow \hat{x}$) are still not conserved across the bend, but the magnetic field component ($\hat{y} \rightarrow \hat{y}$) is conserved. Fig. 5.16 shows the transmission and reflection spectra for various bend geometries between the $X_{xz}$ and $Z_{xz}$ waveguides. As in the case of $x$-$y$ bends, the best case occurs when there is a single defect overshoot for both waveguide channels (see panel 2 of Fig. 5.16). For this geometry, we predict over 95% transmission over the frequency range $a/\lambda \sim 0.387 - 0.405$, corresponding to a bandwidth of approximately 70 nm when the 3D PBG is centered at 1.5 $\mu m$. Other bend geometries either permit relatively low transmission throughout the frequency range (top panel of Fig. 5.16) or exhibit reflection peaks (bottom three panels of Fig. 5.16).

### 5.4.5 Vertical Bends from Type II Waveguides

The bandwidth of bends between vertical waveguides and type I waveguides shown in Fig. 5.5 is limited in part by the relatively small frequency overlap between the two waveguide modes. In contrast, type II waveguides illustrated in Fig. 5.6 are better matched in frequency with the vertical waveguides we have defined. We consider bends into the vertical direction from a type II waveguide in the $x$-direction denoted by $X_{yz}$. The electric field of this waveguide mode is polarized roughly along a diagonal in the $y$-$z$ plane. The magnetic field likewise has non-zero components in both the $y$- and $z$-directions. As a result, it is possible to couple between this waveguide and either orientation of the zig-zag vertical waveguide. Fig. 5.17 shows the transmission and reflection spectra for bends into vertical waveguides where the zig-zag pattern...
Figure 5.16: Transmission (black) and reflection (red) spectra for bends between waveguides in the $x$- (horizontal) and $z$- (vertical) directions for various bend geometries. The light grey circles in the schematic bend diagrams represent air spheres centered in the $y = a/4$ plane, while the dark grey circles represent air spheres centered in the $y = 3a/4$ plane.
Figure 5.17: Transmission (black) and reflection (red) spectra for bends between waveguides in the $x$- (horizontal) and $z$- (vertical) directions for various bend geometries. The waveguide in the $x$-direction is denoted by $X_{yz}$ and the vertical waveguide by $Z_{xz}^{x_3}$ in the top panel and $Z_{xz}^{x_4}$ in the other panels. The white, grey, and black circles in the schematic bend diagrams represent spherical air defects centered in the $y = a/4$, $y = a/2$, and $y = 3a/4$ planes, respectively.
Figure 5.18: Transmission (black) and reflection (red) spectra for bends between waveguides in the $x$- (horizontal) and $z$- (vertical) directions for various bend geometries. The waveguide in the $x$-direction is denoted by $X^{yz}_{2\pi}$ and the vertical waveguide by $Z^{yz}_{y=a/2}$. The spherical air defects are centered in the $y = a/2$ plane.

is formed at a constant $x$-coordinate. In this case, the vertical waveguide mode has its electric field polarized in the $x$-$z$ plane. The top two panels in Fig. 5.17 show configurations where the transmission is relatively low at all frequencies. In contrast, while the bending geometries depicted in the bottom two panels exhibit reflection peaks near $a/\lambda \sim 0.388$, they permit high transmission at higher frequencies. In particular, for the geometry shown in the third panel of Fig. 5.17, we predict over 98% transmission over the frequency range $a/\lambda \sim 0.403 - 0.424$, a bandwidth of approximately 75 nm for a PBG centered at 1.5 $\mu$m. Fig. 5.18 shows results for bends into vertical waveguides formed by zig-zag patterns at a constant $y$-coordinate, denoted by $Z^{yz}_{y=a/2}$. Again, high transmission through the bend is predicted at higher frequencies. For the geometry shown in the bottom panel of Fig. 5.18, over 98% transmission is predicted over the frequency range $a/\lambda \sim 0.409 - 0.418$, a bandwidth of approximately 30 nm for a PBG centered at 1.5 $\mu$m.
5.5 Discussion

We have demonstrated preliminary design rules for creating 3D air waveguide networks in diamondlike photonic crystals suitable for fabrication by optical phase mask or optical interference lithography. High bandwidth linear waveguides are created by removing dielectric material from the periodic PBG backbone along a path that overlaps the high light intensity regions of the lower 3D photonic band. This suggests the possibility of combining efficient optical interference lithography techniques with highly configurable direct laser writing to produce optical microchip circuits with high density. Silicon replicas of the PBG-based circuit, exhibiting air defects in regions exposed by DLW, may be created by modifying the double-inversion technique for polymer photoresists [82]. Instead of fully infiltrating the developed photoresist with SiO$_2$ in the first inversion step, a partial infiltration could be performed. This would result in a thin silica shell coating the SU-8 template [138]. The second inversion step, involving full infiltration by silicon CVD, would then produce an inverse of the original template.

We have designed two types of waveguide channels in the in-plane ($x$ and $y$) directions. Type I waveguides emulate the waveguide created in the familiar woodpile structure when a single rod is removed. Transmission exceeding 95% is predicted over a bandwidth of approximately 80 nm through $x$-$y$ bends between waveguides of this type, when the PBG is centered around 1.5 $\mu$m. Bends between in-plane type II waveguides, formed by creating defects in the direction perpendicular to the first type of waveguide, are predicted to allow greater than 95% transmission over a bandwidth of about 140 nm, and better than 98% transmission over a 90 nm bandwidth. We have studied bends from the in-plane waveguides into the vertical ($z$) direction. For bends from type II waveguides into the vertical direction, we predict greater than 98% transmission over a bandwidth of approximately 75 nm. In comparison to optical circuits in earlier 2D-3D PBG heterostructures, the best waveguide network architecture in the holographically defined diamond PBG material, with type II waveguides in the $x$- and $y$-directions and a zig-zag waveguide in the vertical direction, does not exhibit planar 2D mi-
crochip layers. Instead, the identical $x$- and $y$-direction waveguide channels in the holographic architecture are offset by a quarter of a lattice constant in the third dimension. Truly planar bends between non-identical $x$- and $y$-direction waveguides can be formed, but these exhibit mediocre transmission characteristics. As a result, it may be more complicated to adapt defects and circuit elements from 2D PC microchips to the holographic architecture than to a 2D-3D heterostructure. On the other hand, the overall synthesis of 3D circuits of light in holographically defined PBG materials may involve fewer fabrication steps than required in previously considered 2D-3D PBG heterostructures.
Chapter 6

Discussion and Conclusions

In this thesis, we have developed a theoretical roadmap for the design and synthesis of 3D photonic band gap materials using various optical lithography methods. The most remarkable of these approaches is the technique of optical phase mask lithography, invented during the course of this thesis. We believe that these results provide a significant contribution toward the eventual low cost, high quality, and large-scale synthesis of materials with 3D PBGs in the visible and near-infrared regions. Combined with direct laser writing methods, the optical lithography method offers one of the simplest, yet most versatile approaches to 3D integrated optics and circuits of light in 3D optical microchips.

All of the theoretical designs we have presented here have been developed with actual fabrication processes firmly in mind. However, as various experimental groups begin to tackle the challenge of implementing these blueprints, it becomes necessary to adjust the theoretical designs to account for complexities arising from fabrication. One example of this is in the choice of photoresist for holographic lithography. The polymer photoresist SU-8 is commonly used in experiments involving holographic lithography and direct laser writing. However, SU-8 is subject to shrinkage during the development process, necessitating the creation of a massive wall surrounding the photonic crystal to avoid lattice distortions [70]. Moreover, its low refractive index precludes the possibility of opening a PBG without inversion to a high-index material.
As a result, the use of other photoresists in these processes is a topic of current interest. We have already, for instance, considered the use of the chalcogenide glass $\text{As}_2\text{S}_3$ as a photoresist in Sec. 4.5.

The use of optical phase masks to generate the interference pattern for holographic lithography represents a significant shift in the required experimental effort as compared to multi-beam holographic lithography. In the case of multi-beam interference, the central effort in the exposure of the photoresist is focused on the proper alignment and configuration of the beams. In optical phase mask lithography, this task is replaced by the fabrication of a suitable phase mask, followed by the single beam exposure of the mask at normal incidence. An important advantage to this paradigm is that these two tasks can be performed at separate times and even in separate locations. This division of labor offers the possibility of a workflow in which high quality optical phase masks would be produced in a site equipped for high precision semiconductor microlithography, then sent to various locations to be used in the exposure of multiple photoresists. Replication of the exposed photoresists with high index materials could occur in yet another site specializing in the inversion process.

The holographic lithography methods offer the ability to control the periodic properties of the target photonic crystal. Direct laser writing provides a straightforward route to the inclusion of defects at the templating stage. The creation of 3D PBG materials with these methods requires replication of the photoresist template with a high index material. In contrast, photo-electrochemical pore etching can produce a silicon photonic crystal without the need for inversion. An intriguing possibility is the use of the holographic interference pattern to guide photo-electrochemical pore etching. Electronic holes could be created in the high intensity regions of the interference pattern, promoting dissolution of the silicon in these regions. This would produce a structure replicating the low intensity regions of the holographic interference pattern. A main obstacle is that the illuminating light is scattered at the etch front, muddying the interference pattern. Moreover, this scattering depends on the current state of the etch. In a preliminary study, we calculated the effects on the interference pattern of the
presence of a partially-etched silicon layer filled with a strong absorber. The partially-etched region was assumed to resemble the target diamondlike photonic crystal, and the etching process was assumed to be slow relative to an optical cycle, so that the problem could be treated in a time-independent manner. Fig. 6.1 shows the resulting interference patterns for two different etch states, corresponding to two slices along the target diamondlike structure. Even though the incident exposure is unchanged, the reflections from the partially-etched region cause the interference patterns to differ strongly. However, if the issue of reflections from the etched regions can be overcome, the combination of photo-electrochemistry and holographic lithography could result in the direct synthesis of diamond photonic crystals in silicon.

As we move ever closer to the goal of producing 3D PBG architectures efficiently and at large scales, the design of fabricable defects in photonic crystals becomes increasingly relevant. One possible course of study is to apply the principles of waveguide design used in Chapter 5 to the Kielovite structure. This might result in the creation of a 3D waveguide network directly in a silicon structure. Such a study would involve examining the electromagnetic field distributions of the periodic structure to identify regions of high field intensity, then considering the creation of waveguides by removing material from these regions. In contrast to the case con-
considered in Chapter 5, the waveguide design would need to take into account the geometry of the periodic structure. In particular, the defects would need to be accessible by the lithographic method used to remove those regions (possibly focused ion beam etching [63, 64]). The development of planar defects could also be considered; such defects might be implemented by further modulation of the pore sizes during the etching process.

Another avenue for further research is to extend the waveguide network presented in Chapter 5 to include waveguide channels in diagonal directions, more complicated bending geometries such as U-turns, and other defects such as microcavities. This would provide a more complete blueprint for a PBG-based optical micro-circuit. As well, it would be beneficial to take into account the shape of the DLW voxel in fine-tuning the waveguide network design. The oblong voxel introduces an anisotropy into the system that should be considered.

The use of more complex optical phase mask geometries is another area of interest. In particular, it may be possible to use aperiodic phase masks with defects in the mask to produce structures that also exhibit defects. This would require a balancing act between creating usable defects and maintaining the PBG in the unaltered regions. Optical phase masks with simple point and line defects in the periodic pattern have been suggested [131]. An example of a phase mask with a simple defect is shown in Fig. 6.2. A more far-reaching possibility is to alter the diffraction grating layers of the OPM to produce diffracted beams with optical vortices [142]. If engineered correctly, the interference between plane waves and beams with optical vortices might produce a diamondlike pattern with localized defects [143]. Calculation

![Figure 6.2: Optical phase masks with (a) a simple point defect and (b) lattice dislocation](image)
of the diffraction-interference pattern emanating from a complex phase mask may prove a challenging task. A supercell technique would needed in order to adapt the RCWA method for this scenario, but this would be computationally intensive. Alternatively, the FDTD method could be used, but information about individual modes would be lost. This would be a necessary consideration when studying complex phase mask geometries.
Appendix A

Calculating Photonic Band Structures by Plane Wave Expansion

A.1 Introduction

The photonic band structure is an important and fundamental property used in the design and characterization of photonic crystals. This is the optical analogue to electronic band structures used in condensed matter physics, describing the allowed energy levels (frequencies) of photons at a given crystal momentum (Bloch vector) in an infinite periodic structure. A full PBG in a photonic crystal manifests itself as a frequency range in the photonic band structure in which no allowed levels exist. The plane-wave expansion method (PWEM) [45] is the most versatile method for calculating the photonic band structure of periodic dielectric media. The method relies on the expansion of Maxwell’s equations in a plane-wave basis to produce an eigenvalue equation, depending on the crystal momentum, whose eigenvectors and eigenvalues are the allowed electromagnetic fields and frequencies.
A.2 Derivation of the eigenvalue equation

We consider Maxwell’s equations in macrosopic media:

\[ \nabla \cdot \vec{D} = \rho \]  \hspace{1cm} (A.1) \\
\[ \nabla \cdot \vec{B} = 0 \]  \hspace{1cm} (A.2) \\
\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \]  \hspace{1cm} (A.3) \\
\[ \nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \]  \hspace{1cm} (A.4)

Here, \( \vec{E} \) is the electric field, \( \vec{B} \) is the magnetic induction field, \( \vec{D} \) is the electric displacement field, and \( \vec{H} \) is the magnetic field. \( \rho \) and \( \vec{J} \) are the free charge and free current, respectively, which we take to be zero. In linear, isotropic, non-permeable media we can write

\[ \vec{D} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon \varepsilon_0 \vec{E} \]  \hspace{1cm} (A.5) \\
\[ \vec{H} = \frac{1}{\mu_0} \vec{B} - \vec{M} = \frac{1}{\mu_0} \vec{B} \]  \hspace{1cm} (A.6)

where \( \vec{P} \) is the polarization density, \( \vec{M} \) is the magnetization density, and \( \varepsilon = \varepsilon(\vec{r}) \) is the position-dependent dielectric constant. Maxwell’s equations then reduce to

\[ \nabla \cdot \vec{D} = 0 \]  \hspace{1cm} (A.7) \\
\[ \nabla \cdot \vec{H} = 0 \]  \hspace{1cm} (A.8) \\
\[ \nabla \times \vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t} \]  \hspace{1cm} (A.9) \\
\[ \frac{1}{\varepsilon} \nabla \times \vec{H} = \varepsilon_0 \frac{\partial \vec{E}}{\partial t} \]  \hspace{1cm} (A.10)
The coupled equations for $\vec{E}$ and $\vec{H}$, Eq. (A.9) and Eq. (A.10), can be uncoupled by taking the curl:

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = -\mu_0 \vec{\nabla} \times \frac{\partial \vec{H}}{\partial t} = -\mu_0 \frac{\partial}{\partial t} \vec{\nabla} \times \vec{H} = -\varepsilon_0 \mu_0 \varepsilon \frac{\partial^2 \vec{E}}{\partial t^2}$$

$\Rightarrow \quad \vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = -\varepsilon \frac{\partial^2 \vec{E}}{c^2 \partial t^2}$ \hspace{1cm} (A.11)

$$\vec{\nabla} \times \left( \frac{1}{\varepsilon} \vec{\nabla} \times \vec{H} \right) = \varepsilon_0 \vec{\nabla} \times \frac{\partial \vec{E}}{\partial t} = \varepsilon_0 \frac{\partial}{\partial t} \vec{\nabla} \times \vec{E} = -\varepsilon_0 \mu_0 \frac{\partial^2 \vec{H}}{\partial t^2}$$

$\Rightarrow \quad \vec{\nabla} \times \left( \frac{1}{\varepsilon} \vec{\nabla} \times \vec{H} \right) = -\frac{1}{c^2} \frac{\partial^2 \vec{H}}{\partial t^2}.$ \hspace{1cm} (A.12)

We can assume solutions to these uncoupled wave equations of the form $\vec{E}(\vec{r}, t) = \vec{E}(\vec{r}) e^{i\omega t}$ and $\vec{H}(\vec{r}, t) = \vec{H}(\vec{r}) e^{i\omega t}$, so that we get

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{E}(\vec{r})) = \left( \frac{\omega}{c} \right)^2 \varepsilon(\vec{r}) \vec{E}(\vec{r})$$ \hspace{1cm} (A.13)

$$\vec{\nabla} \times \left( \frac{1}{\varepsilon(\vec{r})} \vec{\nabla} \times \vec{H}(\vec{r}) \right) = \left( \frac{\omega}{c} \right)^2 \vec{H}(\vec{r}).$$ \hspace{1cm} (A.14)

We will focus on Eq. (A.14). In the photonic crystal, $\varepsilon(\vec{r})$ has Bravais lattice symmetry such that

$$\varepsilon(\vec{r} + \vec{R}) = \varepsilon(\vec{r})$$ \hspace{1cm} (A.15)

for any $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$, where $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_2$ are the primitive lattice vectors of the Bravais lattice, and $n_1$, $n_2$ and $n_3$ are integers. The Bloch-Floquet theorem then implies that the solutions to Eq. (A.14) can be written in the form

$$\vec{H}_{nk}(\vec{r}) = e^{i \vec{k} \cdot \vec{r}} \vec{h}_{nk}(\vec{r}),$$ \hspace{1cm} (A.16)

where $\vec{h}_{nk}(\vec{r})$ share the same Bravais lattice symmetry as $\varepsilon(\vec{r})$, i.e. $\vec{h}_{nk}(\vec{r} + \vec{R}) = \vec{h}_{nk}(\vec{r})$. These eigenstates are indexed by the Bloch wave vector, $\vec{k}$, and the band index, $n$, which serves to distinguish the various eigenstates associated with each $\vec{k}$. 
We now expand $\vec{H}_{nk}(\vec{r})$ in terms of orthogonal plane-wave basis functions,

$$\vec{H}_{nk}(\vec{r}) = \sum_{\vec{G}} \sum_{\lambda=1,2} h_{\vec{G}\lambda} \hat{e}_{\vec{G}\lambda} e^{i(\vec{k}+\vec{G}) \cdot \vec{r}}, \quad (A.17)$$

where $\vec{G}$ are reciprocal lattice vectors of the form $\vec{G} = n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3$. Here, $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_2$ are the primitive vectors of the reciprocal lattice of the photonic crystal, and the sum runs through all integers $n_1$, $n_2$ and $n_3$ so that the set $\{\vec{G}\}$ spans all reciprocal space. We choose the unit vectors $\hat{e}_{\vec{G}_1}$ and $\hat{e}_{\vec{G}_2}$ so that $\{\vec{k} + \vec{G}, \hat{e}_{\vec{G}_1}, \hat{e}_{\vec{G}_2}\}$ form an orthogonal set. This automatically satisfies the divergence condition in Eq. (A.8), thereby reducing the number of plane waves per $\vec{G}$ from three (the general case for plane waves in 3d space) to two and consequently reducing the size of the eigenvalue problem by one-third. We can also expand $\vec{e}_{\vec{G}_1}$ in terms of $\{\vec{G}\}$ as

$$\frac{1}{\varepsilon(\vec{r})} = \sum_{\vec{G}} \eta_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}, \quad (A.18)$$

where $\eta_{\vec{G}}$ are simply the Fourier coefficients of $\vec{e}_{\vec{G}_1}$.

Substituting Eq. (A.17) and Eq. (A.18) into Eq. (A.14) and using the product rule for the curl\(^1\) gives

$$\sum_{\vec{G}', \vec{G}''} \sum_{\lambda=1,2} i \left\{ \nabla \times [\eta_{\vec{G}_\lambda} h_{\vec{G}'\lambda} e^{i(\vec{k}+\vec{G}'+\vec{G}'') \cdot \vec{r}}(\vec{k} + \vec{G}') \times \hat{e}_{\vec{G}'\lambda}] \right\} = \left( \frac{\omega_{\vec{k}}}{c} \right)^2 \sum_{\vec{G}} \sum_{\lambda=1,2} h_{\vec{G}\lambda} \hat{e}_{\vec{G}\lambda} e^{i(\vec{k}+\vec{G}) \cdot \vec{r}}. \quad (A.19)$$

Note that we have introduced the notation $\omega_{\vec{k}}$ to emphasize that the solutions to this eigenvalue problem are dependent on $\vec{k}$. Defining $\vec{G} = \vec{G}'+\vec{G}''$ on the left hand side allows us to consider each $\vec{G}$ separately, giving

$$\sum_{\vec{G}'} \sum_{\lambda=1,2} i \left\{ \nabla \times [\eta_{\vec{G}-\vec{G}_\lambda} h_{\vec{G}'\lambda} e^{i(\vec{k}+\vec{G}') \cdot \vec{r}}(\vec{k} + \vec{G}') \times \hat{e}_{\vec{G}'\lambda}] \right\}$$

\(^1\nabla \times (f \vec{V}) = \vec{V} f - \vec{V} \times f \vec{V} \times \vec{V}\)
which can be written, after dividing out the complex exponential and again using the product rule for the curl, as

\[
- \sum_{\vec{G}'} \left\{ \eta_{\vec{G}-\vec{G}'} \sum_{\lambda'=1,2} \left[ \left( \vec{k} + \vec{G} \right) \times \left( \vec{k} + \vec{G}' \right) \times \hat{e}_{\vec{G}'\lambda} \right] \right\} = \sum_{\lambda=1,2} \left( \frac{\omega_{\vec{k}}}{c} \right)^2 h_{\vec{G}\lambda} \hat{e}_{\vec{G}\lambda}.
\]  

(A.21)

Let us consider only the sum over \( \lambda' \) on the left side of Eq. (A.21). This sum can be written explicitly as

\[
\sum_{\lambda'} \left[ \left( \vec{k} + \vec{G} \right) \times \left( \vec{k} + \vec{G}' \right) \times \hat{e}_{\vec{G}'\lambda} \right] \\
= \left( \vec{k} + \vec{G} \right) \times \left( \vec{k} + \vec{G}' \right) \times \left( h_{\vec{G}'1} \hat{e}_{\vec{G}'1} + h_{\vec{G}'2} \hat{e}_{\vec{G}'2} \right) \\
= - \chi_{\vec{k}} \chi_{\vec{G}} \left( \begin{array}{cc} \hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} & -\hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} \\
-\hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} & \hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} \end{array} \right) \left( \begin{array}{c} h_{\vec{G}'1} \\
0 \end{array} \right).
\]

Here we have used the fact that \( \{(\vec{k} + \vec{G}), \hat{e}_{\vec{G}'1}, \hat{e}_{\vec{G}'2}\} \) form an orthogonal set and hence \( \hat{e}_{\vec{G}'1} \times \hat{e}_{\vec{G}'2} = (\vec{k} + \vec{G}') \). By writing the sum over \( \lambda \) on the right hand side of Eq. (A.21) explicitly, we get the infinite-dimensional, generalized eigenvalue equation

\[
\sum_{\vec{G}'} \eta_{\vec{G}-\vec{G}'} \chi_{\vec{k}} \chi_{\vec{G}} \left( \begin{array}{cc} \hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} & -\hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} \\
-\hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} & \hat{e}_{\vec{G}'1} \cdot \hat{e}_{\vec{G}'2} \end{array} \right) \left( \begin{array}{c} h_{\vec{G}'1} \\
0 \end{array} \right) \\
= \left( \frac{\omega_{\vec{k}}}{c} \right)^2 \left( \begin{array}{c} h_{\vec{G}'1} \\\n0 \end{array} \right).
\]  

(A.22)

This is the master equation: diagonalizing the matrix implied by the left hand side gives the allowed frequencies \( \omega_{\vec{k}} \) for a given \( \vec{k} \). The magnetic fields can be reconstructed via Eq. (A.17) and the corresponding electric fields by Eq. (A.10).
A.3 Solving the eigenvalue equation in practice

The eigenvalue equation Eq. (A.22) is infinite-dimensional since the set \( \{ \vec{G} \} \) runs over all reciprocal space. In a realistic situation, the sums over \( \vec{G} \) must be truncated by choosing a finite set of plane waves over which the expansion occurs. The use of a truncated set of plane waves affects the calculation of the Fourier coefficients \( \eta_{\vec{G} - \vec{G}'} \) in Eq. (A.22). One may obtain \( \eta_{\vec{G} - \vec{G}'} \) directly by calculating the Fourier coefficients of the inverse dielectric tensor \( \varepsilon(\vec{r}) \). This is known as the \( \frac{1}{\varepsilon} \) method. Alternatively, one can first calculate the Fourier transform of the dielectric tensor \( \varepsilon(\vec{r}) \) to obtain \( \varepsilon_{\vec{G} - \vec{G}'} \), then invert this to get the \( \eta_{\vec{G} - \vec{G}'} \), making use of the fact that \( \sum_{\vec{G}''} \eta_{\vec{G} - \vec{G}''} \varepsilon_{\vec{G}'' - \vec{G}'} = \delta_{\vec{G}, \vec{G}'} \). This is known as the \( \varepsilon \)-inverse method. These operations are equivalent when performed on the complete \( \{ \vec{G} \} \) basis, but on the truncated basis, the answers vary. It has been noted that the \( \varepsilon \)-inverse method converges more quickly for several geometries [144].

Additionally, the calculation of the Fourier transform of \( \varepsilon(\vec{r}) \) in the \( \varepsilon \)-inverse method (or, alternatively, the Fourier transform of \( \varepsilon(\vec{r}) \) in the \( \frac{1}{\varepsilon} \) method) cannot in general be found analytically. Rather, one must use the discrete Fourier transform to approximate these values. This involves discretization of \( \varepsilon(\vec{r}) \) in the primitive unit cell, which can introduce further inaccuracy into the calculation. In virtually all physical cases, there is an abrupt transition between regions of high dielectric constant and low dielectric constant. Fortunately, the magnitudes of Fourier components arising from a step function decrease as the wavenumber increases, so this inaccuracy can be reduced by increasing the number of points used to sample the primitive unit cell.

A.4 Application of the photonic band structure

Solution of the eigenvalue equation Eq. (A.22) yields the allowed frequencies for photons with a given Bloch wave vector \( \vec{k} \). The existence and location of a full PBG can be verified by calculating the intersection of the stop gaps at all wave vectors in the first Brillouin zone of
the Bravais lattice of the photonic crystal. Depending on the space group symmetry of the structure, the first Brillouin zone may be sub-divided into a number of equivalent so-called “irreducible Brillouin zones;” this reduces the number of wave vectors at which the photonic band structure must be calculated. Furthermore, in practice the boundaries of the full photonic band gap occur along the edges of the irreducible Brillouin zone. We therefore make use of photonic band structure diagrams, drawn along a path of wave vectors on the edges of the irreducible Brillouin zone, to characterize the PBG of a given structure.
Appendix B

Rigorous Coupled Wave Analysis of Holographic Diffraction Patterns

B.1 Introduction

Rigorous coupled wave analysis (RCWA) can be used to describe the diffraction of electromagnetic waves by periodic grating structures [145]. This is achieved by Fourier expanding the electromagnetic fields to solve Maxwell’s equations in individual regions, and solving the boundary conditions between the regions [146]. In this appendix, we give a formulation of the RCWA for calculating the diffraction from an arbitrary, two-dimensional (“crossed”), possibly multiple-layer phase mask. This relies heavily on Li’s work [147, 148] and references therein.

B.2 Problem Definition

Let us consider the diffraction of a single, monochromatic plane wave by a crossed, multi-layer phase mask with arbitrary 2-d Bravais lattice symmetry. The mask is assumed to be composed only of non-magnetic, isotropic materials. The incident beam, with vacuum wavelength \( \lambda_0 \), is shown in Fig. B.1. The wavevector, \( \vec{k} \), is described by the polar angle \( \theta \) between \( \vec{k} \) and the \( z \)-
Figure B.1: Parameters of the incident beam. The wavevector, $\vec{k}$, is described by the polar angle $\theta$ and the azimuthal angle $\phi$, and $\psi$ describes the angle between the (real) polarization vector $\vec{E}$ and the plane of incidence. The vacuum wavelength of the beam is $\lambda_0$.

axis, and the azimuthal angle $\phi$ between the plane of incidence and the $x$-axis. The polarization vector $\vec{E}$ makes an angle $\psi$ with the plane of incidence. For simplicity, we limit our analysis to a linearly polarized incident beam; the extension to elliptical polarizations is straightforward. We can then write the wavevector and polarization unit vectors of the incident beam as:

$$\vec{k} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \phi) \quad (B.1)$$

$$\vec{E} = (\cos \theta \cos \phi \cos \psi + \sin \phi \sin \psi, \cos \theta \sin \phi \cos \psi - \cos \phi \sin \psi, \cos \psi \sin \theta) \quad (B.2)$$

respectively. Here, we rename the usual coordinate system $Oxyz$ as $O\bar{x}^1\bar{x}^2\bar{x}^3$, so that the phase mask is oriented in the $\bar{x}^1\bar{x}^2$-plane. Fig. B.2 gives a side view of the phase mask. The mask is composed of $n$ regions, each of which is non-varying in the $\bar{x}^3$ direction, with the thickness of a particular region $(i)$ given by $d_i$. A mask layer that varies in the $\bar{x}^3$ direction can be approximated by several non-varying slices. The incident beam is sent from the homogeneous region $(n + 1)$ above the grating and the transmitted orders propagate in region $(0)$ (possibly infinitessimally thin). The modes $u^{(i)}$ and $d^{(i)}$ describe the upwards and downwards propagating modes in region $(i)$. In particular, $d^{(n+1)}$ and $u^{(n+1)}$ are the incident beam and reflected
Figure B.2: Side view of the diffraction problem. The phase mask is composed of \( n \) regions, each of which is homogeneous in the \( \vec{x}_3 \) direction; the thickness of region \( (i) \) is given by \( d_i \). Two homogeneous regions, region \( (0) \) and region \( (n + 1) \), flank the mask. The modes \( u^{(i)} \) and \( d^{(i)} \) describe the upwards and downwards propagating modes in region \( (i) \), respectively.
Figure B.3: Top view of the phase mask and the coordinate systems used to describe it. Here, the phase mask is schematically depicted by high symmetry points on the Bravais lattice. The $x^1$- and $x^2$-axes are parallel to a set of primitive lattice vectors of the mask.

modes, respectively, while $d^{(-1)}$ are the modes transmitted through the mask.

In order to tackle masks with arbitrary 2-d Bravais lattice symmetry, we introduce a non-rectangular Cartesian coordinate system $Ox^1x^2x^3$, depicted in Fig. B.3. The phase mask is represented here by lattice points of the Bravais lattice of the region. The $x^1$- and $x^2$-axes, separated by angle $\alpha$, are parallel to the periodic directions of the mask, with respective periodicities $a_1$ and $a_2$. The $x^2$-axis is deflected from the $\bar{x}^2$-axis ($y$-axis) by an angle $\zeta$, related to $\alpha$ by

$$\zeta = \frac{\pi}{2} - \alpha. \quad (B.3)$$

Transformations between $Ox^1x^2x^3$ and $O\bar{x}^1\bar{x}^2\bar{x}^3$ ($Oxyz$) are then given by:

$$\bar{x}^1 = x^1 + x^2 \sin \zeta \quad (B.4)$$

$$\bar{x}^2 = x^2 \cos \zeta$$

$$\bar{x}^3 = x^3$$
and

\[ x^1 = \hat{x}^1 - \hat{x}^2 \tan \zeta \]  
\[ x^2 = \hat{x}^2 \sec \zeta \]  
\[ x^3 = \hat{x}^3. \]  

The covariant and contravariant basis vectors for \( O\hat{x}^1\hat{x}^2\hat{x}^3 \) can be written as:

\[ \vec{b}_1 = \hat{x} \]  
\[ \vec{b}_2 = \hat{x} \sin \zeta + \hat{y} \cos \zeta \]  
\[ \vec{b}_3 = \hat{z} \]  

and

\[ \vec{b}^1 = \hat{x} - \hat{y} \tan \zeta \]  
\[ \vec{b}^2 = \hat{y} \sec \zeta \]  
\[ \vec{b}^3 = \hat{z}, \]  

respectively. Note that these sets of covariant and contravariant basis vectors obey the rule \( \vec{b}_\rho \cdot \vec{b}^{\sigma} = \delta_{\rho\sigma} \), where \( \delta_{\rho\sigma} \) represents the Kronecker delta.

Since we consider only isotropic media, the permittivity and permeability tensors can be written in the \( O\hat{x}^1\hat{x}^2\hat{x}^3 \) coordinate system as \( \bar{\epsilon}^{\tau\chi} = \epsilon \delta^{\tau\chi} \) and \( \bar{\mu}^{\tau\chi} = \mu \delta^{\tau\chi} \). In the \( O\hat{x}^1\hat{x}^2\hat{x}^3 \) representation, then, these tensors are:

\[ \epsilon^{\rho\sigma} = \epsilon g^{\rho\sigma} \]  
\[ \mu^{\rho\sigma} = \mu g^{\rho\sigma}, \]
where \( g^{\rho\sigma} = \sum_{\tau=1}^{3} \frac{\partial x^\rho}{\partial x^\tau} \frac{\partial x^\sigma}{\partial x^\tau} \) is the covariant metric tensor of \( Ox^1.x^2.x^3 \):

\[
\{ g^{\rho\sigma} \} = \begin{pmatrix}
    \sec^2 \zeta & - \sec \zeta \tan \zeta & 0 \\
    - \sec \zeta \tan \zeta & \sec^2 \zeta & 0 \\
    0 & 0 & 1
\end{pmatrix}.
\]

(B.10)

Finally, we define

\[
g \equiv \frac{1}{\det \{ g^{\rho\sigma} \}} = \cos^2 \zeta
\]

(B.11)

for convenience.

### B.3 Maxwell’s Equations in Covariant Form

In order to make use of the non-rectangular Cartesian coordinate system \( Ox^1.x^2.x^3 \) defined in the previous section, we must write Maxwell’s curl equations in covariant form:

\[
\varepsilon_{\rho\sigma\tau} \partial_\sigma E_\tau = ik_0 \sqrt{g} \mu^{\rho\sigma} H_\sigma
\]

(B.12)

\[
\varepsilon_{\rho\sigma\tau} \partial_\sigma H_\tau = -ik_0 \sqrt{g} \epsilon^{\rho\sigma} E_\sigma,
\]

where \( \varepsilon_{\rho\sigma\tau} \) is the Levi-Civita tensor. Here, we make use of the Einstein summation over repeated indices and note that a separate equation is represented for each of the three values of \( \rho \). Writing out the summations and separate equations explicitly yields:

\[
\partial_2 E_3 - \partial_3 E_2 = ik_0 \mu \sec \zeta (H_1 - \sin \zeta H_2)
\]

(B.13)

\[
\partial_3 E_1 - \partial_1 E_3 = ik_0 \mu \sec \zeta (H_2 - \sin \zeta H_1)
\]

(B.14)

\[
\partial_1 E_2 - \partial_2 E_1 = ik_0 \mu \cos \zeta H_3
\]

(B.15)

\[
\partial_2 H_3 - \partial_3 H_2 = -ik_0 \sec \zeta \epsilon (E_1 - \sin \zeta E_2)
\]

(B.16)

\[
\partial_3 H_1 - \partial_1 H_3 = -ik_0 \sec \zeta \epsilon (E_2 - \sin \zeta E_1)
\]

(B.17)
The RCWA method involves finding solutions of Eq. (B.13)–Eq. (B.18) in each region \((i)\) and relating these solutions by the boundary conditions at the region interfaces.

### B.4 Non-homogeneous Regions

We first consider the modes in the non-homogeneous regions by Fourier expanding the covariant Maxwell’s equations (Fourier factorization). We write the electromagnetic field components in a particular region \((s)\) as

\[
E^{(s)}_\sigma(x^1, x^2, x^3) = \sum_{m,n} E^{(s)}_{\sigma mn}(x^3)e^{i(\alpha_m x^1 + \beta_n x^2)} \tag{B.19}
\]

\[
H^{(s)}_\sigma(x^1, x^2, x^3) = \sum_{m,n} H^{(s)}_{\sigma mn}(x^3)e^{i(\alpha_m x^1 + \beta_n x^2)},
\]

where

\[
\alpha_m = k^{(+1)} \sin \theta \cos \phi + m \left( \frac{2\pi}{a_1} \right) \tag{B.20}
\]

\[
\equiv \alpha_0 + m \left( \frac{2\pi}{a_1} \right)
\]

\[
\beta_n = k^{(+1)} \sin \theta \sin(\phi + \zeta) + n \left( \frac{2\pi}{a_2} \right) \tag{B.21}
\]

\[
\equiv \beta_0 + n \left( \frac{2\pi}{a_2} \right).
\]

Here, \(k^{(+1)} = \frac{2m^{(+1)} \lambda_0}{\lambda_n}\) is the length of the wavevector in the \((+1)\) region, which has index of refraction \(n^{(+1)}\). For ease of notation we drop the superscript \((s)\) for the remainder of this section, as the discussion involves a single grating region.
Rules for Fourier factorization

When implemented in practice, the Fourier expansions in the following sections must be truncated. As a result, quantities that in an infinite Fourier expansion are equivalent may not be in practice. In particular, one must take care when performing Fourier factorization of products of discontinuous functions [149]. In the current analysis, we define the following procedure for the Fourier factorization of the product $h(x) = f(x)g(x)$: (1) If $f$ and $g$ have no concurrent jump discontinuities, we use Laurent’s rule: $h_m = \sum_{n=-N}^{N} [f_m - n] g_n$. (2) If $f$ and $g$ have pairwise discontinuities but $h$ is continuous, we use the “Inverse” rule: $h_m = \sum_{n=-N}^{N} [(1) f_m^n - 1 g_n]$. As $N \to \infty$, these rules become equivalent.

Fourier factorization of Maxwell’s Equations

We begin by taking the Fourier transform of Eq. (B.18) with respect to $x^1$, writing the field components in the form of Eq. (B.19), to obtain:

$$
\partial_1 \left[ \sum_m H_{2m}(x^2, x^3) e^{i\alpha_m x^1} \right] - \partial_2 \left[ \sum_m H_{1m}(x^2, x^3) e^{i\alpha_m x^1} \right] = -ik_0 \cos \zeta \sum_m \sum_p \epsilon_{m-p}(x^2, x^3) E_{3p}(x^2, x^3) e^{i\alpha_m x^1}.
$$

Laurent’s rule has been used in performing the Fourier transform of $\epsilon E_3$, since $E_3$ is continuous in the $x^1 x^2$-plane. Performing the Fourier transform with respect to $x^2$ subsequently yields

$$
\partial_1 \left[ \sum_{m,n} H_{2mn}(x^3) e^{i(\alpha_m x^1 + \beta_n x^2)} \right] - \partial_2 \left[ \sum_{m,n} H + 1mn(x^3) e^{i(\alpha_m x^1 + \beta_n x^2)} \right] = -ik_0 \cos \zeta \sum_{m,n} \sum_{p,q} \epsilon_{m-p,n-q} E_{3pq}(x^3) e^{i(\alpha_m x^1 + \beta_n x^2)}.
$$

Finally, we take the derivatives with respect to $x^1$ and $x^2$ to get:

$$
\sum_{m,n} \alpha_m H_{2mn}(x^3) e^{i(\alpha_m x^1 + \beta_n x^2)} - \sum_{m,n} \beta_n H_{1mn}(x^3) e^{i(\alpha_m x^1 + \beta_n x^2)}
$$
\[
- k_0 \cos \zeta \sum_{m,n} \left[ \sum_{p,q} \epsilon_{m-p,n-q} E_{3pq}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} \right].
\] (B.22)

Following the same procedure on Eq. (B.13) and Eq. (B.14) gives:

\[
\sum_{m,n} \beta_n E_{3mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} - \frac{1}{i} \sum_{m,n} \partial_3 E_{2mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} = k_0 \sec \zeta \left[ \sum_{m,n} H_{1mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} - \sin \zeta \sum_{m,n} H_{2mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} \right]
\] (B.23)

and

\[
\frac{1}{i} \sum_{m,n} \partial_3 E_{1mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} - \sum_{m,n} \alpha_m E_{3mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} = k_0 \sec \zeta \left[ \sum_{m,n} H_{2mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} - \sin \zeta \sum_{m,n} H_{1mn}(x^3) e^{i(\alpha_m x_1 + \beta_n x_2)} \right],
\] (B.24)

respectively. Note that we cannot immediately perform the derivative with respect to \(x^3\).

For ease of notation, we can now write Eq. (B.22)–Eq. (B.24) in matrix form, dropping the \(e^{i(\alpha_m x_1 + \beta_n x_2)}\) by orthogonality:

\[
\{\alpha_{mn,pq}\} [H_2] - \{\beta_{mn,pq}\} [H_1] = - k_0 \cos \zeta \{\epsilon_{mn,pq}\} [E_3] \quad \text{(B.25)}
\]

\[
\{\beta_{mn,pq}\} [E_3] - \frac{1}{i} \partial_3 [E_2] = \mu k_0 \sec \zeta ([H_1] - \sin \zeta [H_2]) \quad \text{(B.26)}
\]

\[
\frac{1}{i} \partial_3 [E_1] - \{\alpha_{mn,pq}\} [E_3] = \mu k_0 \sec \zeta ([H_2] - \sin \zeta [H_1]). \quad \text{(B.27)}
\]

Here, \(\{\alpha_{mn,pq}\}\) and \(\{\beta_{mn,pq}\}\) are diagonal matrices defined by

\[
\{\alpha_{mn,pq}\} = \alpha_m \delta_{m,p} \delta_{n,q},
\]

\[
\{\beta_{mn,pq}\} = \beta_n \delta_{m,p} \delta_{n,q}.
\]
where $\delta_{m,n}$ is the Kronecker delta, and $\{\epsilon_{mn,pq}\}$ is the Toeplitz matrix given by

$$\{\epsilon_{mn,pq}\} \equiv \{\epsilon_{m-p,n-q}\}.$$ 

The field component matrices $[F_\sigma]$, where $F \in \{E, H\}$ and $\sigma \in \{1, 2, 3\}$, are column vectors of the form

$$[F_\sigma] \equiv \begin{pmatrix} : \\ F_{\sigma mn} \\ : \end{pmatrix}.$$

From Eq. (B.25) we can solve for $[E_3]$,

$$[E_3] = -\frac{1}{k_0 \cos \zeta} \left( \{\epsilon_{mn,pq}\}^{-1}\{\alpha_{mn,pq}\} [H_2] - \{\epsilon_{mn,pq}\}^{-1}\{\beta_{mn,pq}\} [H_1] \right),$$

and substitute the result into Eq. (B.26) and Eq. (B.27) to get:

$$\frac{k_0 \cos \zeta}{i} \partial_3 [E_1] = \mu k_0^2 ([H_2] - \sin \zeta [H_1])$$

$$- \{\alpha_{mn,pq}\} \left( \{\epsilon_{mn,pq}\}^{-1}\{\alpha_{mn,pq}\} [H_2] - \{\epsilon_{mn,pq}\}^{-1}\{\beta_{mn,pq}\} [H_1] \right)$$

$$\frac{k_0 \cos \zeta}{i} \partial_3 [E_2] = \mu k_0^2 ([H_1] - \sin \zeta [H_2])$$

$$- \{\beta_{mn,pq}\} \left( \{\epsilon_{mn,pq}\}^{-1}\{\alpha_{mn,pq}\} [H_2] - \{\epsilon_{mn,pq}\}^{-1}\{\beta_{mn,pq}\} [H_1] \right).$$

Finally, we can write:

$$\frac{k_0 \cos \zeta}{i} \partial_3 \begin{pmatrix} [E_1] \\ [E_2] \end{pmatrix} =$$

$$\begin{pmatrix} \{\alpha_{mn,pq}\} \{\epsilon_{mn,pq}\}^{-1}\{\beta_{mn,pq}\} - \mu k_0^2 \sin \zeta I & -\{\alpha_{mn,pq}\} \{\epsilon_{mn,pq}\}^{-1}\{\alpha_{mn,pq}\} + \mu k_0^2 I \\ \{\beta_{mn,pq}\} \{\epsilon_{mn,pq}\}^{-1}\{\beta_{mn,pq}\} - \mu k_0^2 I & -\{\beta_{mn,pq}\} \{\epsilon_{mn,pq}\}^{-1}\{\alpha_{mn,pq}\} + \mu k_0^2 \sin \zeta I \end{pmatrix}$$

$$\times \begin{pmatrix} [H_1] \\ [H_2] \end{pmatrix}, \quad (B.28)$$
We now continue Fourier factorization of the remaining Maxwell’s equations. Eq. (B.15) can be treated in the same manner as the previous equations to yield

\[
\sum_{m,n} \alpha_E e^{i(\alpha_m x^1 + \beta_n x^2)} - \sum_{m,n} \beta_H e^{i(\alpha_m x^1 + \beta_n x^2)} = \mu k_0 \cos \zeta \sum_{m,n} H_{3mn} e^{i(\alpha_m x^1 + \beta_n x^2)}. \tag{B.29}
\]

On the other hand, the Fourier factorization of Eq. (B.16) and Eq. (B.17) is more difficult because of the \(\epsilon(E_1 - \sin \zeta E_2)\) and \(\epsilon(E_1 - \sin \zeta E_2)\) terms. In order to proceed, we note that the contravariant components of \(\vec{E}\) can be written in terms of its covariant components by applying the transformation \(E^\rho = g^{\rho\sigma} E_\sigma\), so that \(E^1 = \sec^2 \zeta (E_1 - \sin \zeta E_2)\) and \(E^2 = \sec^2 \zeta (-\sin \zeta E_1 + E_2)\). Eq. (B.16) then becomes

\[\partial_2 H_3 - \partial_3 H_2 = -ik_0 \cos \zeta \epsilon E^1.\]

It is important to note that the \(\epsilon E^1\) is continuous with respect to \(x^1\), so that we can make use of the Fourier factorization rules defined previously. Taking the Fourier transform with respect to \(x^1\) gives

\[
\partial_2 \left[ \sum_m H_{3m}(x^2, x^3) e^{i\alpha_m x^1} \right] - \partial_3 \left[ \sum_m H_{2m}(x^2, x^3) e^{i\alpha_m x^1} \right] = -ik_0 \cos \zeta \sum_m \left[ \sum_p \left[ \frac{1}{\epsilon} \right]_{m-p}^{-1} E_p(x^2, x^3) e^{i\alpha_m x^1} \right],
\]

where \(\left[\frac{1}{\epsilon}\right]_m\) denotes the \(m^{th}\) Fourier coefficient of \(\frac{1}{\epsilon}\) with respect to \(x^1\), as a function of \(x^2\).

We have applied the “Inverse” rule here. By linearity of the Fourier transform, we can write

\[\epsilon_{mn,pq}\] may be calculated using an optimized algorithm such as Trench’s algorithm [150].

\[\text{The inverse of the Toeplitz matrix } \{\epsilon_{mn,pq}\} \text{ may be calculated using an optimized algorithm such as Trench’s algorithm [150].}\]
this as

\[
\partial_2 \left[ \sum_m H_{3m}(x^2, x^3)e^{i\alpha_{m} x^1} \right] - \partial_3 \left[ \sum_m H_{2m}(x^2, x^3)e^{i\alpha_{m} x^1} \right] \\
+ ik_0 \cos \zeta \sum_m \left[ \sum_p (\lceil 1/\epsilon \rceil )^{-1}_{m-p} E_{1p}(x^2, x^3)e^{i\alpha_{m} x^1} \right] \\
= ik_0 \cos \zeta \sin \zeta \sum_m \left[ \sum_p (\lceil 1/\epsilon \rceil )^{-1}_{m-p} E_{2p}^2(x^2, x^3)e^{i\alpha_{m} x^1} \right],
\]

where we have made use of the fact that

\[
\cos^2 \zeta (E_1 - E_2 \sin \zeta) = \cos^2 \zeta E_1 + \sin \zeta (\sin \zeta E_1 - E_2) \\
\quad = E_1 - \sin \zeta E_2 = \cos^2 \zeta E_1.
\]

Due to the orthogonality of the \(e^{i\alpha_{m} x^1}\) terms, we can separate the equations for each \(m\):

\[
\left\{ \partial_2 H_{3m}(x^2, x^3) - \partial_3 H_{2m}(x^2, x^3) + ik_0 \cos \zeta \sum_p (\lceil 1/\epsilon \rceil )^{-1}_{m-p} E_{1p}(x^2, x^3) \right\} \\
= ik_0 \cos \zeta \sin \zeta \sum_m \left[ \sum_p (\lceil 1/\epsilon \rceil )^{-1}_{m-p} E_{2p}^2(x^2, x^3) \right].
\]

Assuming (without proof) that \(\sum_p ([1/\epsilon])^{-1}_{m-p} E_{2p}^2(x^2, x^3)\) is continuous in \(x^2\) and first multiplying both sides by \(\{[1/\epsilon]\}/ik_0 \cos \zeta\), we take the Fourier transform with respect to \(x^2\) and perform derivatives with respect to \(x^1\) and \(x^2\) to obtain:

\[
\sum_{p,q} \frac{1}{\epsilon} \left( \frac{1}{\epsilon} \right)_{m-p,n-q} \left\{ \frac{1}{k_0 \cos \zeta} \right[ \beta_n H_{3mn}(x^3) - \frac{1}{i} \partial_3 H_{2mn}(x^3) \right] \right\} + \sum_{j,l} \sum_{q} ([1/\epsilon]^{-1}_{p-j}) q-l E_{1jl}(x^3) \]

\[
= \sin \zeta E_{2m}^2(x^3), \quad (B.30)
\]

again dropping the exponent by orthogonality. Here, \(\lfloor f \rfloor_q\) denotes the \(q^{th}\) Fourier coefficient of \(f\) with respect to \(x^2\).

For the last remaining Maxwell equation, Eq. (B.17), we again replace the covariant com-
ponents of $\vec{E}$ on the right hand side with the contravariant equivalent,

$$\partial_3 H_1 - \partial_1 H_3 = -i k_0 \cos \zeta \epsilon E_2.$$ 

The $\epsilon E_2$ term is continuous with respect to $x^2$, so we begin by taking the Fourier transform with respect to $x^2$ to obtain

$$\partial_3 \left[ \sum_n H_{1n}(x^1, x^3)e^{i\beta_n x^2} \right] - \partial_1 \left[ \sum_n H_{3n}(x^1, x^3)e^{i\beta_n x^2} \right] = -ik_0 \cos \zeta \sum_n \left[ (1/\epsilon)_{n-1-q} E^2_q(x^1, x^3)e^{i\beta_n x^2} \right],$$

where $[1/\epsilon]_n$ denotes the $n^{th}$ Fourier coefficient of $1/\epsilon$ with respect to $x^2$, as a function of $x^1$.

Following a procedure analogous to the one we used for Eq. (B.16), we finally end up with

$$\sum_{p,q} \frac{1}{\epsilon} mn,pn,q \left\{ \frac{1}{k_0 \cos \zeta} \left[ \frac{1}{i} \partial_3 H_{1mn}(x^3) - \alpha_m H_{3mn}(x^3) \right] + \sum_j \left[ (1/\epsilon)_{j-1} E_{2jl}(x^3) \right] \right\} = \sin \zeta E^1_{mn}(x^3).$$

We can now write Eq. (B.29)–Eq. (B.31) in matrix form:

$$\{\alpha_{mn,pq}\} [E_2] - \{\beta_{mn,pq}\} [E_1] = \mu k_0 \cos \zeta [H_3] \quad (B.32)$$

$$\{(1/\epsilon)_{mn,pq}\} \left( \frac{1}{k_0 \cos \zeta} \{\beta_{mn,pq}\} [H_3] - \frac{1}{ik_0 \cos \zeta} \partial_3 [H_2] + \left\{ \left[ (1/\epsilon)_{p-j} \right]_{q-l} \right\} [E_1] \right\} = \sin \zeta [E^2] \quad (B.33)$$

$$\{(1/\epsilon)_{mn,pq}\} \left( \frac{1}{ik_0 \cos \zeta} \partial_3 [H_1] - \frac{1}{k_0 \cos \zeta} \{\alpha_{mn,pq}\} [H_3] + \left\{ \left[ (1/\epsilon)_{q-j} \right]_{p-l} \right\} [E_2] \right\} = \sin \zeta [E^1]. \quad (B.34)$$

Using Eq. (B.32) to eliminate $[H_3]$, Eq. (B.33) becomes

$$\{(1/\epsilon)_{mn,pq}\} \left( \frac{1}{\mu k_0^2 \cos^2 \zeta} \{\beta_{mn,pq}\} \{\alpha_{mn,pq}\} [E_2] - \frac{1}{\mu k_0^2 \cos^2 \zeta} \{\beta_{mn,pq}\}^2 [E_1] \right)$$
\[
- \frac{1}{i k_0 \cos \zeta} \partial_3 [H_2] + \{ [1/\epsilon]^{-1} [\partial_{j}\partial_{q} l] [E_1] \}
\]

\[
= \sin \zeta \left[ E^2 \right],
\]

which, after multiplying both sides by \(\mu k_0^2 \cos^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1}\) and rearranging terms, gives

\[
- i \mu k_0 \cos \zeta \partial_3 [H_2]
\]

\[
= - \{\beta_{mn,pq}\}^2 [E_1] + \mu k_0^2 \left( \cos^2 \zeta \{ [1/\epsilon]^{-1} [\partial_{j}\partial_{q} l] \} + \sin^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1} \right) [E_1]
\]

\[
+ \{\beta_{mn,pq}\} \{\alpha_{mn,pq}\} [E_2] - \mu k_0^2 \sin^2 \zeta \{(1/\epsilon)_{mn,pq}\} [E_2].
\]  

(B.35)

Under similar treatment, Eq. (B.34) yields:

\[
- i \mu k_0 \cos \zeta \partial_3 [H_2]
\]

\[
= - \{\alpha_{mn,pq}\} \{\beta_{mn,pq}\} [E_1] + \mu k_0^2 \sin \zeta \{(1/\epsilon)_{mn,pq}\} [E_1]
\]

\[
+ \{\alpha_{mn,pq}\}^2 [E_2] - \mu k_0^2 \left( \cos^2 \zeta \{ [1/\epsilon]_{q-j}^{-1} [\partial_{j}\partial_{q} l] \} + \sin^2 \zeta \{(1/\epsilon)_{mn,pq}\} \right) [E_2].
\]  

(B.36)

Finally, we can write Eq. (B.35) and Eq. (B.36) as:

\[
\frac{\mu k_0 \cos \zeta}{i} \partial_3 \left( \begin{array}{c} [H_1] \\ [H_2] \end{array} \right) =
\]

\[
\left( - \{\alpha_{mn,pq}\} \{\beta_{mn,pq}\} + \mu k_0^2 \sin \zeta \{(1/\epsilon)_{mn,pq}\}^{-1} \right) \ldots
\]

\[
\left( - \{\beta_{mn,pq}\}^2 + \mu k_0^2 \left( \cos^2 \zeta \{ [1/\epsilon]^{-1} [\partial_{j}\partial_{q} l] \} + \sin^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1} \right) \right) \ldots
\]

\[
\left( \{\alpha_{mn,pq}\}^2 - \mu k_0^2 \left( \cos^2 \zeta \{ [1/\epsilon]_{q-j}^{-1} [\partial_{j}\partial_{q} l] \} + \sin^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1} \right) \right)
\]

\[
\times \left( \begin{array}{c} [E_1] \\ [E_2] \end{array} \right). 
\]

(B.37)

If we assume that the \(x^3\)-dependence of the field components is simply \(E_{\sigma mn}(x^3) = \ldots \)
\(E_{\sigma mn}e^{i\lambda x^3}\) and \(H_{\sigma mn}(x^3) = H_{\sigma mn}e^{i\lambda x^3}\), then the partial derivative with respect to \(x^3\) is easily obtained and we have
\[
k_0 \cos \zeta \lambda \begin{pmatrix} [E_1] \\ [E_2] \end{pmatrix} = F \begin{pmatrix} [H_1] \\ [H_2] \end{pmatrix}
\]
and
\[
\mu k_0 \cos \zeta \lambda \begin{pmatrix} [H_1] \\ [H_2] \end{pmatrix} = G \begin{pmatrix} [E_1] \\ [E_2] \end{pmatrix},
\]
where we have defined the matrices

\[
F = \begin{pmatrix}
\{\alpha_{mn,pq}\}\{\epsilon_{mn,pq}\}^{-1}\{\beta_{mn,pq}\} - \mu k_0^2 \sin \zeta I & -\{\alpha_{mn,pq}\}\{\epsilon_{mn,pq}\}^{-1}\{\alpha_{mn,pq}\} + \mu k_0^2 I \\
\{\beta_{mn,pq}\}\{\epsilon_{mn,pq}\}^{-1}\{\beta_{mn,pq}\} - \mu k_0^2 I & -\{\beta_{mn,pq}\}\{\epsilon_{mn,pq}\}^{-1}\{\alpha_{mn,pq}\} + \mu k_0^2 \sin \zeta I
\end{pmatrix},
\]
\[
G = \begin{pmatrix}
-\{\alpha_{mn,pq}\}\{\beta_{mn,pq}\} + \mu k_0^2 \sin \zeta \{(1/\epsilon)_{mn,pq}\}^{-1} & \\
-\{\beta_{mn,pq}\}^2 + \mu k_0^2 (\cos^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1}) + \sin^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1} & \\
\{\alpha_{mn,pq}\}^2 - \mu k_0^2 (\cos^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1}) + \sin^2 \zeta \{(1/\epsilon)_{mn,pq}\}^{-1} & \\
\{\beta_{mn,pq}\}\{\alpha_{mn,pq}\} - \mu k_0^2 \sin \zeta \{(1/\epsilon)_{mn,pq}\}^{-1}
\end{pmatrix}.
\]

Now we can write the eigenvalue equation
\[
FG \begin{pmatrix} [E_1] \\ [E_2] \end{pmatrix} = \mu k_0^2 \cos^2 \zeta \lambda^2 \begin{pmatrix} [E_1] \\ [E_2] \end{pmatrix} \equiv \Lambda \begin{pmatrix} [E_1] \\ [E_2] \end{pmatrix},
\]
which we solve to get \(\Lambda\) and \([(E_1), (E_2)]^T\) pairs. The \(x^3\)-component of the wavevector for the \(q^{th}\) mode is then \(\lambda_q = \pm \sqrt{\frac{\pi}{\mu k_0}} \sec \zeta\), where we choose the sign such that the imaginary part of \(\lambda_q\) is non-negative. The magnetic field vectors are easily obtained from
\[
\begin{pmatrix} [H_1]_q \\ [H_2]_q \end{pmatrix} = \frac{\sec \zeta}{\pm k_0 \lambda_q} G \begin{pmatrix} [E_1]_q \\ [E_2]_q \end{pmatrix}.
\]
Here, the sign is chosen depending on whether the upwards-propagating/decaying field (+ sign) or downwards-propagating/decaying field (− sign) is desired. The field expansions in Eq. (B.19) can finally be written as

\[
E_\sigma(x^1, x^2, x^3) = \sum_{m,n,q} E_{\sigma mnq}[u_q e^{i\lambda_q x^3} + d_q e^{-i\lambda_q x^3}] e^{i(\alpha_m x^1 + \beta_n x^2)} \tag{B.42}
\]

\[
H_\sigma(x^1, x^2, x^3) = \sum_{m,n,q} H_{\sigma mnq}[u_q e^{i\lambda_q x^3} - d_q e^{-i\lambda_q x^3}] e^{i(\alpha_m x^1 + \beta_n x^2)},
\]

where \(u_q \) and \(d_q \) denote the unknown amplitudes of the upwards-propagating/decaying and downwards-propagating/decaying fields, respectively. Thus, for a given grating layer \((s)\), we can write

\[
\begin{bmatrix}
E^{(s)}_{1mn}(x^3) \\
E^{(s)}_{2mn}(x^3) \\
H^{(s)}_{1mn}(x^3) \\
H^{(s)}_{2mn}(x^3)
\end{bmatrix} =
\begin{bmatrix}
E_{1mnq} & E_{1mnq} \\
E_{2mnq} & E_{2mnq} \\
H_{1mnq} & H_{1mnq} \\
H_{2mnq} & H_{2mnq}
\end{bmatrix}
\begin{bmatrix}
e^{i\gamma^{(s)}_{mn} x^3} & 0 \\
0 & e^{-i\gamma^{(s)}_{mn} x^3}
\end{bmatrix}
\begin{bmatrix}
u_q^{(s)} \\
d_q^{(s)}
\end{bmatrix}. \tag{B.43}
\]

**B.5 Homogeneous Regions**

In the homogeneous regions, we write the electric field components as Rayleigh expansions,

\[
E_\sigma(x^1, x^2, x^3) = \sum_{m,n} (u_{\sigma mn} e^{i\gamma_{mn} x^3} + d_{\sigma mn} e^{-i\gamma_{mn} x^3}) e^{i(\alpha_m x^1 + \beta_n x^2)} \tag{B.44}
\]

\[
= \sum_{m,n} E_{\sigma mn}(x^3) e^{i(\alpha_m x^1 + \beta_n x^2)}.
\]

The \(x^3\)-component of the wavevector is simply

\[
\gamma_{mn} = \pm[k^2 - \sec^2 \zeta(\alpha_m^2 + \beta_n^2 - 2\alpha_m\beta_n \sin \zeta)]^{1/2}, \tag{B.45}
\]

where \(k\) is the length of the wavevector in the medium, and the sign is chosen such that the imaginary part of \(\gamma_{mn}\) is non-negative. We write the magnetic field components in a more
general form,

\[ H_\sigma(x^1, x^2, x^3) = \sum_{m,n} H_{\sigma mn}(x^3) e^{i(\alpha_m x^1 + \beta_n x^2)}, \tag{B.46} \]

and use Maxwell’s equations to write \( H_{\sigma mn}(x^3) \) in terms of the quantities in Eq. (B.44).

Substituting the above relations for the \( E \)- and \( H \)-components into Eq. (B.13) and Eq. (B.14) yields

\[
\begin{align*}
\beta_n \left( u_{3mn} e^{i\gamma_{mn} x^3} + d_{3mn} e^{-i\gamma_{mn} x^3} \right) - \gamma_{mn} \left( u_{2mn} e^{i\gamma_{mn} x^3} - d_{2mn} e^{-i\gamma_{mn} x^3} \right) \\
= \mu k_0 \sec \zeta \left[ H_{1mn}(x^3) - \sin \zeta H_{2mn}(x^3) \right] \\
\gamma_{mn} \left( u_{1mn} e^{i\gamma_{mn} x^3} - d_{1mn} e^{-i\gamma_{mn} x^3} \right) - \alpha_m \left( u_{3mn} e^{i\gamma_{mn} x^3} + d_{3mn} e^{i\gamma_{mn} x^3} \right) \\
= \mu k_0 \sec \zeta \left[ H_{2mn}(x^3) - \sin \zeta H_{1mn}(x^3) \right],
\end{align*}
\tag{B.47}
\]

for all \( m, n \). We make use of the divergence relation \( \vec{\nabla} \cdot \vec{E} = 0 \), which in our covariant basis can be written as \( k^\sigma E_\sigma = 0 \), keeping in mind the Einstein summation over repeated indices. Note that a given contravariant component of \( \vec{k} \) can be obtained from the covariant components via the sum \( k^\rho = g^{\rho\sigma} k_\sigma \), where \( g^{\rho\sigma} \) is the covariant metric tensor from Eq. (B.8). From Eq. (B.44), the covariant components of \( \vec{k} \) for the upwards and downwards propagating modes of order \( m, n \) are

\[
\begin{align*}
k_{1umn} &= k_{1dmn} = \alpha_m \\
k_{2umn} &= k_{2dmn} = \beta_n \\
k_{3umn} &= -k_{3dmn} = \gamma_{mn},
\end{align*}
\]

applying the covariant metric tensor then yields the contravariant components of \( \vec{k} \):

\[
\begin{align*}
k^1_{umn} &= k^1_{dmn} = \sec^2 \zeta (\alpha_m - \sin \zeta \beta_n) \\
k^2_{umn} &= k^2_{dmn} = \sec^2 \zeta (\beta_n - \sin \zeta \alpha_m) \\
k^3_{umn} &= -k^3_{dmn} = \gamma_{mn}.
\end{align*}
\]
The divergence relation must hold separately for the upwards and downwards propagating modes of order $m, n$:

$$\sec^2 \zeta (\alpha_m - \sin \zeta \beta_n) u_{1mn} + \sec^2 \zeta (\beta_n - \sin \zeta \alpha_m) u_{2mn} + \gamma_{mn} u_{3mn} = 0$$

$$\sec^2 \zeta (\alpha_m - \sin \zeta \beta_n) d_{1mn} + \sec^2 \zeta (\beta_n - \sin \zeta \alpha_m) d_{2mn} - \gamma_{mn} d_{3mn} = 0.$$

Using this result to eliminate $u_{3mn}$ and $d_{3mn}$, and substituting the value of $\gamma_{mn}$ from Eq. (B.45), we can write Eq. (B.47) as

$$\left[ (\beta_n^2 \sin \zeta - \alpha_m \beta_n^2) u_{1mn} + (-k^2 \cos^2 \zeta + \alpha_m^2 - \alpha_m \beta_n \sin \zeta) u_{2mn} \right] e^{i \gamma_{mn} x^3}$$

$$+ \left[ (\alpha_m \beta_n - \beta_n^2 \sin \zeta) d_{1mn} + (k^2 \cos^2 \zeta - \alpha_m^2 + \alpha_m \beta_n \sin \zeta) d_{2mn} \right] e^{-i \gamma_{mn} x^3}$$

$$= \mu k_0 \cos \zeta \gamma_{mn} \left[ H_{1mn}(x^3) - \sin \zeta H_{2mn}(x^3) \right]$$

Writing this in matrix form yields

$$\begin{bmatrix} H_{1mn}(x^3) \\ H_{2mn}(x^3) \end{bmatrix} = \frac{1}{\mu k_0 \cos \zeta \gamma_{mn}} \begin{bmatrix} k^2 \sin \zeta - \alpha_m \beta_n & -k^2 + \alpha_m^2 & -k^2 \sin \zeta + \alpha_m \beta_n & k^2 - \alpha_m^2 \\ k^2 - \beta_n^2 & -k^2 \sin \zeta + \alpha_m \beta_n & -k^2 + \beta_n^2 & k^2 \sin \zeta - \alpha_m \beta_n \end{bmatrix}$$

$$\begin{bmatrix} e^{i \gamma_{mn} x^3} & 0 & 0 & 0 \\ 0 & e^{i \gamma_{mn} x^3} & 0 & 0 \\ 0 & 0 & e^{-i \gamma_{mn} x^3} & 0 \\ 0 & 0 & 0 & e^{-i \gamma_{mn} x^3} \end{bmatrix} \begin{bmatrix} u_{1mn} \\ u_{2mn} \\ d_{1mn} \\ d_{2mn} \end{bmatrix}.$$
From Eq. (B.44), we can also write

\[
\begin{bmatrix}
E_{1mn}(x^3) \\
E_{2mn}(x^3)
\end{bmatrix}
= \begin{bmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
e^{i\gamma_{mn}x^3} & 0 & 0 & 0 \\
0 & e^{i\gamma_{mn}x^3} & 0 & 0 \\
0 & 0 & e^{-i\gamma_{mn}x^3} & 0 \\
0 & 0 & 0 & e^{-i\gamma_{mn}x^3}
\end{bmatrix}
\begin{bmatrix}
u_{1mn} \\
u_{2mn} \\
d_{1mn} \\
d_{2mn}
\end{bmatrix}.
\]

Finally, we can write, for a homogeneous layer \((s)\),

\[
\begin{bmatrix}
E^{(s)}_{1mn}(x^3) \\
E^{(s)}_{2mn}(x^3) \\
H^{(s)}_{1mn}(x^3) \\
H^{(s)}_{2mn}(x^3)
\end{bmatrix}
= \begin{bmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
-C^{(s)}_{mn} & -A^{(s)}_{mn} & C^{(s)}_{mn} & A^{(s)}_{mn} \\
B^{(s)}_{mn} & C^{(s)}_{mn} & -B^{(s)}_{mn} & -C^{(s)}_{mn}
\end{bmatrix}
\begin{bmatrix}
e^{i\gamma^{(s)}_{mn}x^3} & 0 & 0 & 0 \\
0 & e^{i\gamma^{(s)}_{mn}x^3} & 0 & 0 \\
0 & 0 & e^{-i\gamma^{(s)}_{mn}x^3} & 0 \\
0 & 0 & 0 & e^{-i\gamma^{(s)}_{mn}x^3}
\end{bmatrix}
\begin{bmatrix}
u_{1mn} \\
u_{2mn} \\
d_{1mn} \\
d_{2mn}
\end{bmatrix},
\]

where

\[
A^{(s)}_{mn} \equiv \frac{(k^{(s)})^2 - \alpha_m^2}{\mu k_0 \cos \zeta \gamma^{(s)}_{mn}}
\]

\[
B^{(s)}_{mn} \equiv \frac{(k^{(s)})^2 - \beta_n^2}{\mu k_0 \cos \zeta \gamma^{(s)}_{mn}}
\]

\[
C^{(s)}_{mn} \equiv \frac{\alpha_m \beta_n - (k^{(s)})^2 \sin \zeta}{\mu k_0 \cos \zeta \gamma^{(s)}_{mn}},
\]

and \(k^{(s)}\) and \(\gamma^{(s)}_{mn}\) are the length and \(x^3\)-component of \(\vec{k}\) in region \((s)\), respectively. In the region \((n + 1)\) above the phase mask, the downwards propagating mode amplitudes have the values
\[ d_{\sigma mn}^{(n+1)} = I_{\sigma} \delta_{m0} \delta_{n0}, \] where \( I_{\sigma} \) are the components of the incident electric field. Similarly, in the region \((-1)\) below the phase mask, the upwards propagating modes have zero amplitude, i.e. \( u_{\sigma mn}^{(-1)} = 0 \).

### B.6 Solving Boundary Conditions

In Eq. (B.43) and Eq. (B.48) we have expressions for any layer \((s)\) in the phase mask, as well as for the homogeneous regions \((n+1)\) and \((-1)\) above and below the phase mask, of the form

\[
\begin{bmatrix}
E_{1mn}^{(s)}(x^3) \\
E_{2mn}^{(s)}(x^3) \\
H_{1mn}^{(s)}(x^3) \\
H_{2mn}^{(s)}(x^3)
\end{bmatrix} = W^{(s)} \begin{bmatrix}
e^{i\lambda_q x^3} & 0 \\
0 & e^{-i\lambda_q x^3}
\end{bmatrix} \begin{bmatrix}
u_q^{(s)} \\
d_q^{(s)}
\end{bmatrix}
\]

\[ \equiv W^{(s)} \begin{bmatrix}
u_q^{(s)}(x^3) \\
d_q^{(s)}(x^3)
\end{bmatrix}
\]

Since at each layer boundary, \( E_{\parallel} \) and \( H_{\parallel} \) are continuous, at the interface between layers \((s)\) and \((s+1)\), we have

\[
W^{(s+1)} \begin{bmatrix}
u_q^{(s+1)}(x^3) \\
d_q^{(s+1)}(x^3)
\end{bmatrix} = W^{(s)} \begin{bmatrix}
u_q^{(s)}(x^3) \\
d_q^{(s)}(x^3)
\end{bmatrix}
\]

where \( x^3 = \sum_{i=0}^{s} d_i \). The two boundaries of a given layer are related simply by

\[
\begin{bmatrix}
u_q^{(s)}(x^3) \\
d_q^{(s)}(x^3)
\end{bmatrix} = \phi^{(s)} \begin{bmatrix}
u_q^{(s)(s-1)} \\
d_q^{(s)(s-1)}
\end{bmatrix}
\]

(B.50)
These two relations combine to give an expression linking the field amplitudes from layer to layer:

\[
\begin{bmatrix}
    u_q^{(s+1)}(x^{3(s)}) \\
    d_q^{(s+1)}(x^{3(s)})
\end{bmatrix}
= \begin{bmatrix}
    W^{(s+1)} W^{(s)} \phi^{(s)} \\
    \end{bmatrix}
\begin{bmatrix}
    u_q^{(s)}(x^{3(s-1)}) \\
    d_q^{(s)}(x^{3(s-1)})
\end{bmatrix}
= t^{(s)}
\begin{bmatrix}
    u_q^{(s)}(x^{3(s-1)}) \\
    d_q^{(s)}(x^{3(s-1)})
\end{bmatrix}
\]  

(B.51)

The boundary condition problem could be solved in principle by applying this expression recursively to link the field amplitudes from the extreme layers \((n+1)\) and \((0)\). However, this method suffers from numerical instability as the thickness of the problem becomes large. This is due to the presence of the exponential term \(e^{-i\lambda^{(s)}_q ds}\) in the \(\phi^{(s)}\) matrix, which grows exponentially as the layer thickness increases, and accumulates as Eq. (B.51) is applied repeatedly.

In order to avoid the growth of this exponential term, we recast the problem in terms of a stack matrix, \(S^{(n)}\), defined such that the fields in regions \((0)\) and \((n+1)\) are related by

\[
\begin{bmatrix}
    u_q^{(n+1)} \\
    d_q^{(0)}
\end{bmatrix}
= S^{(n)}
\begin{bmatrix}
    u_q^{(0)} \\
    d_q^{(n+1)}
\end{bmatrix}
\equiv
\begin{bmatrix}
    T^{(n)}_{uu} & R^{(n)}_{ud} \\
    R^{(n)}_{du} & T^{(n)}_{dd}
\end{bmatrix}
\begin{bmatrix}
    u_q^{(0)} \\
    d_q^{(n+1)}
\end{bmatrix}.
\]  

(B.52)

The submatrices \(T^{(n)}_{uu}\) and \(T^{(n)}_{dd}\) are transmission matrices for upwards- and downwards-propagating modes, respectively, transmitted between regions \((0)\) and \((n+1)\), and submatrices \(R^{(n)}_{ud}\) and \(R^{(n)}_{du}\) are reflection matrices for reflected modes in regions \((n+1)\) and \((0)\), respectively. In order to build a recursive relation to obtain the \(S^{(n)}\) matrix, we define an \(s^{(s)}\) matrix relating adjacent regions \((s)\) and \((s+1)\) in a similar manner as above,

\[
\begin{bmatrix}
    u_q^{(s+1)} \\
    d_q^{(s)}
\end{bmatrix}
= s^{(s)}
\begin{bmatrix}
    u_q^{(s)} \\
    d_q^{(s+1)}
\end{bmatrix}
\equiv
\begin{bmatrix}
    t^{(s)}_{uu} & r^{(s)}_{ud} \\
    r^{(s)}_{du} & t^{(s)}_{dd}
\end{bmatrix}
\begin{bmatrix}
    u_q^{(s)} \\
    d_q^{(s+1)}
\end{bmatrix}.
\]  

(B.53)
Denoting the submatrices of $t^{(s)}$ by

$$t^{(s)} = \begin{bmatrix} t_{11}^{(s)} & t_{12}^{(s)} \\ t_{21}^{(s)} & t_{22}^{(s)} \end{bmatrix},$$

it is easy to show from Eq. (B.51) and Eq. (B.53) that

$$t_{uu}^{(s)} = t_{11}^{(s)} - t_{12}^{(s)} [t_{22}^{(s)}]^{-1} t_{21}^{(s)}$$ (B.54)

From the definitions of $\phi^{(s)}$ and $t^{(s)}$ in Eq. (B.50) and Eq. (B.51), we note that the exponentially growing term $e^{-i\lambda^{(s)} ds}$ appears in $t_{12}^{(s)}$ and $t_{22}^{(s)}$, while it is inverted in $t_{11}^{(s)}$ and $t_{21}^{(s)}$. One can then easily see from Eq. (B.54) that this term appears inverted in the $S^{(s)}$ matrix. In this manner, the numerical instability resulting from the repeated application of Eq. (B.51) is avoided.

Manipulation of Eq. (B.52) for $S^{(s-1)}$ and Eq. (B.53) gives recursion relations for $S^{(s)}$:

$$T_{uu}^{(s)} = t_{uu}^{(s)} [1 - R_{ud}^{(s-1)} R_{du}^{(s)}]^{-1} T_{uu}^{(s-1)}$$ (B.55)

$$R_{ud}^{(s)} = r_{ud}^{(s)} + t_{uu}^{(s)} [1 - R_{ud}^{(s-1)} R_{du}^{(s)}]^{-1} R_{ud}^{(s-1)} t_{dd}^{(s)}$$

$$R_{du}^{(s)} = R_{du}^{(s-1)} + T_{dd}^{(s-1)} [1 - r_{du}^{(s)} R_{ud}^{(s-1)}]^{-1} r_{du}^{(s)} T_{uu}^{(s-1)} T_{dd}^{(s-1)}$$

The recursion can be initialized by setting $S^{(0)} = s^{(0)}$. In our case, and indeed for most problems of this type, $u_q^{(0)} = 0$ for all $q$. Therefore, only $R_{ud}^{(n)}$ and $T_{dd}^{(n)}$ need to be calculated. It is then beneficial to use the fact that $[1 - XY]^{-1} X = X [1 - YX]^{-1}$ and write:

$$R_{ud}^{(n)} = r_{ud}^{(n)} + t_{uu}^{(n)} R_{ud}^{(n-1)} [1 - r_{du}^{(n)} R_{ud}^{(n-1)}]^{-1} t_{dd}^{(n)}$$ (B.56)
minimizing the number of matrices which must be calculated. Finally, the reflected and transmitted modes emanating from the phase mask, \( u_q^{(s+1)} \) and \( d_q^{(0)} \), respectively, can be obtained by initializing \( d_q^{(s+1)} \) according to the incident beam, and computing

\[
\begin{align*}
\begin{bmatrix} u_q^{(s+1)} \\ d_q^{(0)} \end{bmatrix} &= R_{ud}^{(n)} \begin{bmatrix} d_q^{(s+1)} \end{bmatrix} \\
&= T_{dd}^{(n)} \begin{bmatrix} d_q^{(s+1)} \end{bmatrix}.
\end{align*}
\] (B.57)

### B.7 Application to Optical Phase Masks

Here, we summarize the steps involved in using the RCWA method to calculate the diffraction-interference patterns from optical phase masks.

1. **Calculate Layer Matrices**

For each layer \( (s) \) in the problem (including layer \( (n + 1) \) corresponding to the semi-infinite region from which the incident beam emerges, and layer \( (0) \) corresponding to the photoresist), calculate the matrix

\[
W^{(s)} = \begin{cases} 
\begin{bmatrix} E_1^{(s)} & E_1^{(s)} \\ E_2^{(s)} & E_2^{(s)} \\ H_1^{(s)} & -H_1^{(s)} \\ H_2^{(s)} & -H_2^{(s)} \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -C_m^{(s)} & A_m^{(s)} & C_m^{(s)} & A_m^{(s)} \\ B_m^{(s)} & C_m^{(s)} & -B_m^{(s)} & -C_m^{(s)} \end{bmatrix} & \text{if } (s) \text{ is a grating layer} \\
\end{cases}.
\] (B.58)
and the diagonal matrix

\[
\phi(s) = \begin{cases} 
\begin{bmatrix} e^{i\lambda_q(s)x^3} & 0 \\
0 & e^{-i\lambda_q(s)x^3} \\
e^{i\gamma_{mn}(s)x^3} & 0 & 0 & 0 \\
0 & e^{i\gamma_{mn}(s)x^3} & 0 & 0 \\
0 & 0 & e^{-i\gamma_{mn}(s)x^3} & 0 \\
0 & 0 & 0 & e^{-i\gamma_{mn}(s)x^3} 
\end{bmatrix} & \text{if } (s) \text{ is a grating layer} \\
\end{cases}
\]

For grating layers, the submatrices \(E_{1mnq}\) and \(E_{2mnq}\) are obtained from the eigenvectors of the eigenvalue equation Eq. (B.40). The values \(\lambda_q\) are the eigenvalues from Eq. (B.40).

The submatrices \(H_{1mnq}\) and \(H_{2mnq}\) are obtained from Eq. (B.41). For homogeneous layers, the diagonal submatrices \(A_{mn}^{(s)}\), \(B_{mn}^{(s)}\), and \(C_{mn}^{(s)}\) are defined in Eq. (B.49), and \(\gamma_{mn}^{(s)}\) are defined in Eq. (B.45). We truncate the Fourier expansions by taking \(-m_{\text{max}} \leq m \leq +m_{\text{max}}\) and \(-n_{\text{max}} \leq n \leq +n_{\text{max}}\). Typically, the choice \(m_{\text{max}} = n_{\text{max}} = 12\) is sufficient for convergence.

2. Calculate Transmission Matrices

For each layer except layer \((n + 1)\), calculate the transmission matrices

\[
t(s) = [W^{(s+1)}]^{-1} W^{(s)} \phi(s) = \begin{bmatrix} t_{11}^{(s)} & t_{12}^{(s)} \\
t_{21}^{(s)} & t_{22}^{(s)} \end{bmatrix}.
\]

3. Calculate Layer Scattering Matrices

For each layer except \((n + 1)\), calculate the scattering matrix components

\[
t_{uu}^{(s)} = t_{11}^{(s)} - t_{12}^{(s)} [t_{22}^{(s)}]^{-1} t_{21}^{(s)} \\
\]

\[
r_{ud}^{(s)} = t_{12}^{(s)} [t_{22}^{(s)}]^{-1} \\
\]

\[
r_{du}^{(s)} = -[t_{22}^{(s)}]^{-1} t_{21}^{(s)}
\]
4. Calculate System Scattering Matrix

Calculate the relevant scattering matrices for the system using the recursion relations

\[ R_{ud}^{(n)} = r_{ud}^{(n)} + t_{uu}^{(n)} R_{ud}^{(n-1)} \left[ 1 - r_{du}^{(n)} R_{ud}^{(n-1)} \right]^{-1} t_{dd}^{(n)} \]

\[ T_{dd}^{(n)} = T_{dd}^{(n-1)} \left[ 1 - r_{du}^{(n)} R_{ud}^{(n-1)} \right]^{-1} t_{dd}^{(n)} . \]

The recursions can be initialized by taking \( R_{ud}^{(0)} = r_{ud}^{(0)} \) and \( T_{dd}^{(0)} = t_{dd}^{(0)} \).

5. Calculate Transmitted and Reflected Modes

Finally, calculate the transmitted modes in the photoresist, \( d_q^{(s+1)} \), and the reflected modes in the substrate, \( u_q^{(s+1)} \), from

\[
\begin{bmatrix}
  u_q^{(s+1)} \\
d_q^{(0)}
\end{bmatrix} = R_{ud}^{(n)} \begin{bmatrix}
  d_q^{(s+1)} \\
  d_q^{(0)}
\end{bmatrix},
\]

Here, \( d_q^{(s+1)} \) denotes the incident E-field components.
Appendix C

Finite-Difference Time-Domain
Simulation of Electromagnetic Wave Propagation in PBG Waveguides

C.1 Introduction

The finite-difference time-domain (FDTD) method is a well-established technique for simulating the time evolution of electromagnetic fields [151]. In this method, the electric and magnetic fields are discretized over the computational domain, and updated by time-stepping through Maxwell’s curl equations with space and time derivatives replaced with finite-difference expressions. This results in a flexible and scalable computational tool able to treat a large variety of problems. On the downside, FDTD calculations can become computationally intensive, and the generality of the method means that it can be difficult to distinguish certain features of a model that are easily obtained from frequency domain methods such as RCWA and PWEM. For example, the diffraction-interference patterns from optical phase masks can be calculated using FDTD, but the contributions from distinct beams cannot be easily isolated as they are in the RCWA calculation. In this appendix, we provide an overview of FDTD in the context of
Figure C.1: Positions of the electric (blue) and magnetic (red) field components on the FDTD computational grid. The left side shows the field components at a whole-integer index of the \( z \)-component, while the right side shows field components at a half-integer index. The \( E \)- and \( H \)-field components are arranged in a “leapfrog” configuration in time, with the \( H \)-field components being defined at whole integer time steps \( (n) \) and the \( E \)-field components at times halfway in between \( (n + 1/2) \).

the calculations used in this thesis.

C.2 Formulation of Time Stepping Equations

The FDTD method relies on the discretization of Maxwell’s curl equations,

\[
\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu} \vec{\nabla} \times \vec{E} \\
\frac{\partial \vec{E}}{\partial t} = \frac{1}{\epsilon} \vec{\nabla} \times \vec{H}
\]

on a spatial lattice introduced by Yee. Here, we are considering linear, isotropic, nondispersive, nonconducting, nonpermeable media.

Fig. C.1 shows the positions of the electric and magnetic field components on the Yee lattice. The \( E \)- and \( H \)-field component grids are shifted relative to one another by half of a lattice spacing. Additionally, the field components are arranged in a “leapfrog” configuration in time, with the \( H \)-field components being defined at whole integer time steps \( (n) \) and the \( E \)-field components at times halfway in between \( (n + 1/2) \). Assuming that the lattice spacing
in $x$, $y$, and $z$ dimensions are $\Delta x$, $\Delta y$, and $\Delta z$, respectively, and the time step is $\Delta t$, we use
\[
F_\sigma^n_{i,j,k} \equiv F_\sigma(j\Delta x, j\Delta y, k\Delta z, n\Delta t)
\] (C.2)
to denote a particular field component at a given grid point and time increment. By replacing the space and time derivatives in Eq. (C.1) with centered finite-difference expressions of the form
\[
\frac{\partial F_\sigma^n_{i,j,k}}{\partial x} \Bigg|_{i,j,k} = \frac{F_\sigma^n_{i+\frac{1}{2},j,k} - F_\sigma^n_{i-\frac{1}{2},j,k}}{\Delta x}
\]
(C.3)
\[
\frac{\partial F_\sigma^n_{i,j,k}}{\partial t} \Bigg|_{i,j,k} = \frac{F_\sigma^n_{i,j,k+\frac{1}{2}} - F_\sigma^n_{i,j,k-\frac{1}{2}}}{\Delta t},
\]
we obtain six time-stepping equations:
\[
E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} = E_x|_{i+\frac{1}{2},j,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon_{i+\frac{1}{2},j,k}} \left[ \frac{1}{\Delta y} \left( H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n} - H_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n} \right) \right] - \frac{1}{\Delta z} \left( H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n} - H_y|_{i+\frac{1}{2},j,k-\frac{1}{2}}^{n} \right)
\]
(C.4)
\[
E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} = E_y|_{i,j+\frac{1}{2},k}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon_{i,j+\frac{1}{2},k}} \left[ \frac{1}{\Delta z} \left( H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n} - H_z|_{i\frac{1}{2},j+\frac{1}{2},k}^{n} \right) \right] - \frac{1}{\Delta x} \left( H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n} - H_x|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n} \right)
\]
(C.5)
\[
E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} = E_z|_{i,j,k+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon_{i,j,k+\frac{1}{2}}} \left[ \frac{1}{\Delta x} \left( H_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n} - H_x|_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}^{n} \right) \right] - \frac{1}{\Delta y} \left( H_y|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n} - H_y|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n} \right)
\]
(C.6)
\[
H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} = H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n} + \frac{\Delta t}{\mu_0} \left[ \frac{1}{\Delta z} \left( E_y|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n} - E_y|_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}^{n} \right) \right] - \frac{1}{\Delta y} \left( E_z|_{i,j+1,k+\frac{1}{2}}^{n} - E_z|_{i,j,k+\frac{1}{2}}^{n+1} \right)
\]
(C.7)
\[
H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+1} = H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n} + \frac{\Delta t}{\mu_0} \left[ \frac{1}{\Delta z} \left( E_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n} - E_x|_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}^{n} \right) \right] - \frac{1}{\Delta x} \left( E_z|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n} - E_z|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n+1} \right)
\]
(C.8)
\[
H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = H_z|_{i+\frac{1}{2},j+k+\frac{1}{2}}^{n} + \frac{\Delta t}{\mu_0} \left[ \frac{1}{\Delta y} \left( E_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n} - E_x|_{i+\frac{1}{2},j+\frac{1}{2},k-\frac{1}{2}}^{n} \right) \right]
\]
(C.9)
The time evolution of the electromagnetic fields in a given computational domain are obtained by updating the $E$-field components, using Eq. (C.4)-Eq. (C.6), followed by the $H$-field components, using Eq. (C.7)-Eq. (C.9), in alternating fashion.

The formulation in Eq. (C.4)-Eq. (C.9) does not allow for the addition of energy into the system by way of explicitly-defined sources. To account for such sources, we amend Ampere’s Law, Eq. (C.2), to include an independent source of energy, $\vec{J}_{\text{src}}$:

$$\frac{\partial \vec{E}}{\partial t} = \frac{1}{\epsilon} \nabla \times \vec{H} - \vec{J}_{\text{src}}.$$ (C.10)

The time-stepping equations for the $E$-field components then become:

$$E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} = E_x|_{i+\frac{1}{2},j,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon|_{i+\frac{1}{2},j,k}} \left[ \frac{1}{\Delta y} \left( H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n} - H_z|_{i+\frac{1}{2},j-\frac{1}{2},k}^{n} \right) + J_{\text{src},x}|_{i+\frac{1}{2},j,k}^{n} \right]$$ (C.11)

$$E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} = E_y|_{i,j+\frac{1}{2},k}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon|_{i,j+\frac{1}{2},k}} \left[ \frac{1}{\Delta z} \left( H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n} - H_x|_{i,j+\frac{1}{2},k-\frac{1}{2}}^{n} \right) + J_{\text{src},x}|_{i+\frac{1}{2},j,k}^{n} \right]$$ (C.12)

$$E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} = E_z|_{i,j,k+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\epsilon|_{i,j,k+\frac{1}{2}}} \left[ \frac{1}{\Delta x} \left( H_y|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n} - H_y|_{i-\frac{1}{2},j+\frac{1}{2},k}^{n} \right) + J_{\text{src},x}|_{i,\frac{1}{2},k}^{n} \right]$$ (C.13)

### C.3 Absorbing Boundary Conditions

The simplest way to truncate the FDTD computational domain is to set the value of the electric $E$-field component at the boundary to zero at all times. This creates a perfect electric conductor boundary that acts as a perfect mirror for the electric field. Unfortunately, this is not a practical option for creating realistic models in most cases. Alternatively, depending on the periodicity
of the system, Bloch boundary conditions of the form
\[
E_y|_{n+\frac{1}{2}} = e^{i\vec{k} \cdot \vec{r}} E_y|_{n-\frac{1}{2}}
\]  
(C.14)
can be applied. For a non-periodic boundary, however, it is desirable to have a mechanism to suppress reflections back into the computational domain. In this thesis, we make use of an anisotropic, absorbing medium surrounding the computational domain known as a uniaxial “perfectly matched layer” (PML) that absorbs incident fields without reflection.

The PML region is characterized by permittivity and permeability tensors \( \bar{\varepsilon} = \varepsilon(\vec{r}) \bar{s} \) and \( \bar{\mu} = \mu_0 \bar{s} \), where \( \varepsilon(\vec{r}) \) is the dielectric constant of the photonic crystal at point \( \vec{r} \) and
\[
\bar{s} = \begin{bmatrix}
s_y s_x & 0 & 0 \\
0 & s_x s_y & 0 \\
0 & 0 & s_x s_y
\end{bmatrix},
\]  
(C.15)
with \( s_\rho = 1 + \sigma_\rho / i\omega \) for \( \rho \in \{x, y, z\} \). The strength of the absorption of the PML is determined by the parameters \( \sigma_\rho \), which are non-zero only in the directions perpendicular to the boundary in question. For example, for the PML regions at the \( x \)-boundaries of the computational domain, \( \sigma_x \) is non-zero while \( \sigma_y = \sigma_z = 0 \), except those zones where there is overlap with the PML regions at the \( y \)- or \( z \)-boundaries. Furthermore, the PML absorption strength, corresponding to a \( \sigma_\rho \) value, is gradually increased from zero, at the interface between normal computational space and the PML region, to some maximum value, at the far surface of the PML. This is done to prevent reflections from the PML surface due to discretization error.

In the PML regions, the time-stepping equations Eq. (C.4)–Eq. (C.9) cannot be used due to the frequency dependence in the \( \bar{\varepsilon} \) and \( \bar{\mu} \) tensors. Instead, we introduce the fields \( \vec{D} \) and \( \vec{B} \), given by
\[
\vec{D}(\vec{r}) = \varepsilon(\vec{r}) \begin{pmatrix}
s_x E_x \\
s_y E_y \\
s_z E_z
\end{pmatrix}
\]  
(C.16)
which allows us to decouple this frequency dependence. This results in a set of two-step time-stepping equations for the PML regions. For the $\vec{E}$-fields, these are

\[
D_{x}^{n+\frac{1}{2},j,k} = \left(\frac{2 - \sigma_{x}\Delta t}{2 + \sigma_{x}\Delta t}\right) D_{x}^{n-\frac{1}{2},j,k} + \frac{2\Delta t}{2 + \sigma_{x}\Delta t} \times \left[\frac{1}{\Delta y} \left( H_{x}^{n+\frac{1}{2},j+\frac{1}{2},k} - H_{x}^{n+\frac{1}{2},j-\frac{1}{2},k} \right) - \frac{1}{\Delta z} \left( H_{y}^{n+\frac{1}{2},j,k+\frac{1}{2}} - H_{y}^{n+\frac{1}{2},j,k-\frac{1}{2}} \right) \right]
\]

(C.17)

\[
D_{y}^{n+\frac{1}{2},j,k} = \left(\frac{2 - \sigma_{y}\Delta t}{2 + \sigma_{y}\Delta t}\right) D_{y}^{n-\frac{1}{2},j,k} + \frac{2\Delta t}{2 + \sigma_{y}\Delta t} \times \left[\frac{1}{\Delta z} \left( H_{x}^{n+\frac{1}{2},j,k+\frac{1}{2}} - H_{x}^{n+\frac{1}{2},j,k-\frac{1}{2}} \right) - \frac{1}{\Delta x} \left( H_{x}^{n+\frac{1}{2},j,k+\frac{1}{2}} - H_{x}^{n+\frac{1}{2},j,k-\frac{1}{2}} \right) \right]
\]

(C.18)

\[
D_{z}^{n+\frac{1}{2},j,k} = \left(\frac{2 - \sigma_{z}\Delta t}{2 + \sigma_{z}\Delta t}\right) D_{z}^{n-\frac{1}{2},j,k} + \frac{2\Delta t}{2 + \sigma_{z}\Delta t} \times \left[\frac{1}{\Delta x} \left( H_{y}^{n+\frac{1}{2},j,k+\frac{1}{2}} - H_{y}^{n+\frac{1}{2},j,k-\frac{1}{2}} \right) - \frac{1}{\Delta y} \left( H_{x}^{n+\frac{1}{2},j,k+\frac{1}{2}} - H_{x}^{n+\frac{1}{2},j,k-\frac{1}{2}} \right) \right]
\]

(C.19)

and

\[
E_{x}^{n+\frac{1}{2},j,k} = \left(\frac{2 - \sigma_{x}\Delta t}{2 + \sigma_{x}\Delta t}\right) E_{x}^{n-\frac{1}{2},j,k} + \frac{1}{\epsilon_{i,j+\frac{1}{2},k}} \left[ \left(\frac{2 - \sigma_{x}\Delta t}{2 + \sigma_{x}\Delta t}\right) D_{x}^{n+\frac{1}{2},j,k} - \left(\frac{2 - \sigma_{x}\Delta t}{2 + \sigma_{x}\Delta t}\right) D_{x}^{n-\frac{1}{2},j,k} \right]
\]

(C.20)

\[
E_{y}^{n+\frac{1}{2},j,k} = \left(\frac{2 - \sigma_{y}\Delta t}{2 + \sigma_{y}\Delta t}\right) E_{y}^{n-\frac{1}{2},j,k} + \frac{1}{\epsilon_{i,j+\frac{1}{2},k}} \left[ \left(\frac{2 - \sigma_{y}\Delta t}{2 + \sigma_{y}\Delta t}\right) D_{y}^{n+\frac{1}{2},j,k} - \left(\frac{2 - \sigma_{y}\Delta t}{2 + \sigma_{y}\Delta t}\right) D_{y}^{n-\frac{1}{2},j,k} \right]
\]

(C.21)

\[
E_{z}^{n+\frac{1}{2},j,k} = \left(\frac{2 - \sigma_{z}\Delta t}{2 + \sigma_{z}\Delta t}\right) E_{z}^{n-\frac{1}{2},j,k} + \frac{1}{\epsilon_{i,j+\frac{1}{2},k}} \left[ \left(\frac{2 - \sigma_{z}\Delta t}{2 + \sigma_{z}\Delta t}\right) D_{z}^{n+\frac{1}{2},j,k} - \left(\frac{2 - \sigma_{z}\Delta t}{2 + \sigma_{z}\Delta t}\right) D_{z}^{n-\frac{1}{2},j,k} \right]
\]

(C.22)

At a given time step, the $E$-field components can be updated by first computing the updated $D$-field component, then using the updated value along with the previous value to calculate the
then computing

\[
B_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} = \left(\frac{2 - \sigma_y \Delta t}{2 + \sigma_y \Delta t}\right) B_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n - \frac{2 \Delta t}{2 + \sigma_y \Delta t} \times \left[ \frac{1}{\Delta y} \left( E_x|_{i,j+1,k+\frac{1}{2}}^n - E_x|_{i,j,k+\frac{1}{2}}^n \right) - \frac{1}{\Delta z} \left( E_y|_{i,j+1,k+1}^n - E_y|_{i,j,k}^n \right) \right]
\]

(C.23)

\[
B_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+1} = \left(\frac{2 - \sigma_z \Delta t}{2 + \sigma_z \Delta t}\right) B_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n - \frac{2 \Delta t}{2 + \sigma_z \Delta t} \times \left[ \frac{1}{\Delta z} \left( E_x|_{i+\frac{1}{2},j+1,k+\frac{1}{2}}^n - E_x|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n \right) - \frac{1}{\Delta x} \left( E_z|_{i+1,j+\frac{1}{2},k}^n - E_z|_{i,j+\frac{1}{2},k}^n \right) \right]
\]

(C.24)

\[
B_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = \left(\frac{2 - \sigma_x \Delta t}{2 + \sigma_x \Delta t}\right) B_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n - \frac{2 \Delta t}{2 + \sigma_x \Delta t} \times \left[ \frac{1}{\Delta x} \left( E_y|_{i+1,j+\frac{1}{2},k}^n - E_y|_{i,j+\frac{1}{2},k}^n \right) - \frac{1}{\Delta y} \left( E_x|_{i+\frac{1}{2},j+1,k}^n - E_x|_{i+\frac{1}{2},j,k}^n \right) \right]
\]

(C.25)

then computing

\[
H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} = \left(\frac{2 - \sigma_z \Delta t}{2 + \sigma_z \Delta t}\right) H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n + \left[ \left(\frac{2 + \sigma_x \Delta t}{2 + \sigma_x \Delta t}\right) B_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+1} - \left(\frac{2 - \sigma_x \Delta t}{2 + \sigma_x \Delta t}\right) B_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n \right]
\]

(C.26)

\[
H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+1} = \left(\frac{2 - \sigma_x \Delta t}{2 + \sigma_x \Delta t}\right) H_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n + \left[ \left(\frac{2 + \sigma_y \Delta t}{2 + \sigma_y \Delta t}\right) B_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^{n+1} - \left(\frac{2 - \sigma_y \Delta t}{2 + \sigma_y \Delta t}\right) B_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n \right]
\]

(C.27)

\[
H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = \left(\frac{2 - \sigma_y \Delta t}{2 + \sigma_y \Delta t}\right) H_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n + \left[ \left(\frac{2 + \sigma_z \Delta t}{2 + \sigma_z \Delta t}\right) B_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} - \left(\frac{2 - \sigma_z \Delta t}{2 + \sigma_z \Delta t}\right) B_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n \right]
\]

(C.28)

### C.4 Transmission and Reflection Spectra

The transmission and reflection spectra for a waveguide bend or other scatterer can be calculated by sending a pulse through the bend and integrating the Poynting vector flux over planes at the input and output of the bend. We first show the details of finding the power through a plane. Let us consider the calculation of the power from a pulse travelling in the z-direction; extension to the x- and y- directions is trivial. We wish to consider the Poynting vector flux through a
planar surface $S$ parallel to the $x$-$y$ plane and containing the point $z$, with $x_{\text{min}} \leq x \leq x_{\text{max}}$ and $y_{\text{min}} \leq y \leq y_{\text{max}}$. At a given frequency $\omega$, the power through this plane is given by

$$P(\omega) = \text{Re} \left\{ \int_S \hat{n} \cdot \left[ \bar{E}_\omega^*(x, y, z) \times \bar{H}_\omega(x, y, z) \right] dx \, dy \right\}$$  \hspace{1cm} (C.29)$$

$$= \text{Re} \left\{ \sum_{i=i_{\text{min}}}^{i_{\text{max}}} \sum_{j=j_{\text{min}}}^{j_{\text{max}}} \hat{n} \cdot \left[ \bar{E}_\omega|_{i,j,k} \times \bar{H}_\omega|_{i,j,k} \right] \Delta x \Delta y \right\} ,$$

after discretization of space ($x = i \Delta x$, $y = j \Delta y$, $z = k \Delta z$ and so on). The Fourier transformed field $\bar{E}_\omega|_{i,j,k}$ is given at some time $t = n_{\text{max}} \Delta t$ by

$$\bar{E}_\omega|_{i,j,k} = \int_0^t e^{i\omega t} \bar{E}_\omega|_{i,j,k}(t) = \sum_{n=0}^{n_{\text{max}}} e^{i\omega n \Delta t} \bar{E}_\omega^n|_{i,j,k} \Delta t$$  \hspace{1cm} (C.30)$$
after time discretization; the Fourier transformed magnetic field is obtained in a similar manner. $\bar{E}_\omega|_{i,j,k}$ and $\bar{H}_\omega|_{i,j,k}$ are easily accumulated during the simulation, at each desired frequency and for all points comprising the flux surface. The power is calculated at the end of the simulation.

For a pulse with center frequency $\omega_0$ and bandwidth (full width at half maximum) $\Delta \omega$, we consider the transmission and reflection spectra to be reliable for frequencies in the range $[\omega_0 - \Delta \omega, \omega_0 + \Delta \omega]$.

The transmission and reflection spectra for a bend depend on the incident, transmitted, and reflected power. The transmitted power is simply obtained from the Poynting vector flux through a planar surface at the output of the bend. However, obtaining the incident and reflected power is more difficult due to the interference between the incident and reflected pulses. In order to obtain these values, we run two simulations, one with the bend in question, and one with only the incoming straight waveguide. The straight waveguide case allows for the calculation of the incident power; typically, the size of the computational domain can be reduced significantly without the bend. The reflected power is then obtained by calculating

$$P_r(\omega) = \text{Re} \left\{ \sum_{i=i_{\text{min}}}^{i_{\text{max}}} \sum_{j=j_{\text{min}}}^{j_{\text{max}}} \hat{n} \cdot \left[ \left( \bar{E}_\omega^*|_{i,j,k} - \bar{E}_\omega^*|_{i,j,k,0} \right) \times \left( \bar{H}_\omega|_{i,j,k} - \bar{H}_\omega|_{i,j,k,0} \right) \right] \Delta x \Delta y \right\} .$$  \hspace{1cm} (C.31)$$
It is necessary to subtract the incident field rather than the incident flux because of interference effects.


