Optical Properties of Superlattice Photonic Crystals

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SUMMARY

Photonic band gap materials, commonly referred to as photonic crystals (PCs), have been a topic of great interest for almost two decades due to their promise of unprecedented control over the propagation and generation of light. We report investigations of the optical properties of a new PC structure based upon a triangular lattice in which adjacent \([i, j]\) rows of holes possess different properties (refractive index or radius, \(r\)), creating a super-lattice (SL) periodicity. Symmetry arguments predicted “band folding” and band splitting behaviors, both of which are direct consequences of the new basis that converts the Brillouin zone from hexagonal (six-fold) to rectangular (two-fold). Plane wave expansion and finite-difference time-domain (FDTD) numerical calculations were used to explore the effects of the new structure on the photonic dispersion relationship of the SL PC. Electron beam lithography and inductively coupled plasma dry etching were used to fabricate 1 \(\mu m \times 1 \mu m\) SL PC areas (lattice constant, \(a = 358\) nm and 480 nm) with hole radius ratios ranging from 1.0 (triangular) to 0.585 \((r_2/r_1 = 73.26\) nm/125.26 nm) on Silicon-on-insulator wafers. The effects of modifying structural parameters (such as hole size, lattice constant, and SL strength) were measured using the coupled resonant band technique, confirming the SL symmetry arguments and corroborating the band structure calculations. Analysis of the dispersion contours of the static SL (SSL) PC (a hole radius modulated SL PC) predicted both giant refraction \((\Delta \theta_r \approx 110^\circ \text{ for } \Delta \theta_i = 8^\circ)\) and superprism behavior \((\Delta \theta_r \approx 108^\circ \text{ for } \Delta \omega_n = 12\%\) in these structures. Dynamic control of these refraction effects was also investigated by incorporating electro-optic and nonlinear materials into the SSL PC structure. Wavevector analyses on these structures predicted \(\Delta \theta_r > 96^\circ\) when the refractive index inside of the holes of the structure changed from \(n=1.5\) to 1.7. Through this investigation, the first successful measurement of the band folding effect in multidimensional PCs as well as the first explicit measurement of the dielectric band of a 2D PC were reported. In addition, the SL PC’s impact on new opto-electronic devices was explored.
CHAPTER I

INTRODUCTION

Materials with a periodicity in their dielectric constant have been admired and studied since man began collecting precious gems like opal. In fact, Lord Rayleigh was the first to formulate a theory to explain the behavior of these gem stones in 1887 [77, 32]. Fabricating such structures in the laboratory and with periodicities on the length scale of hundreds of nanometers (the wavelength of visible light) has also been a great challenge for man. However, great progress in this field has been made in recent years thanks to two proposals in 1987 that sparked fervent activity in a field that melds solid state physics, optics, and electromagnetic theory: the study of photonic crystals (PCs) or photonic band gap materials. It was 100 years after Lord Rayleigh’s work that in 1987 that both Eli Yablonovitch and Sajeev John, independently and simultaneously, proposed the possibility of photon confinement and the suppression of spontaneous emission by materials possessing a dielectric constant that was periodically modulated in three-dimensions [103, 28]. To understand how an optical material could possibly trap or confine photons, we briefly discuss a man-made periodic structure that is related to those proposed by Yablonovitch and John and that has been thoroughly studied and fully integrated into our everyday lives: the quarter-wave stack (Figure 1.1(a)).

These structures are made by a deposition of two materials of different refractive index, \( n_1 \) and \( n_2 \) onto a surface so that the layers alternate between high and low refractive index as indicated by the different shading in Figure 1.1(a). The different layers have thicknesses of \( a \) and \( b \), which are typically equivalent to \( \lambda_i/4 \), where \( \lambda_i \) is the wavelength of light in the \( i = 1, 2 \) layer, and one period of the structure is the thicknesses \( a + b \). In operation, certain ranges of electromagnetic (EM) energy can be totally reflected, as shown in Figure 1.1(b), according to the dielectric constants of the layers and their thicknesses (high transmission is possible as well, but for photon confinement we are interested only in total reflection).
Figure 1.1: (a) Schematic of a quarter-wave stack showing total reflection of an beam at normal incidence. (b) Plot of reflectivity spectrum of a 15-period Bragg stack at various incident angles. (c) Typical dispersion relation of a Bragg stack at normal incidence (adapted from [108]).
Thus, the quarter-wave stack has uses as selective band-pass filters, beam splitters, mirrors, or elements in distributed feedback lasers (high reflection) or as anti-reflection coatings on eye glasses and camera lenses (high transmission).\(^1\) High reflection/transmission effects are possible in the quarter-wave stack because of scattering events that occur at each layer interface where a portion of the incident wave is either reflected back to the light source or transmitted to the next layer. For a particular wavelength range of EM radiation, the sum of the scattered events results in total destructive interference of transmitted waves (all waves out of phase by 180°), and total constructive interference of reflected waves (all waves in of phase). Thus, light is not transmitted through the structure and is perfectly reflected. This frequency range of zero transmittance is called a photonic band gap (PBG) in the dispersion relation (Figure 1.1(c)), and is analogous to an electronic band gap in semiconductors. In fact, there are so many analogous concepts between solid state physics and PCs, that they are often referred to as “semiconductors for light”, as we will explore in Chapter 2.

If a photon were surrounded by perfect mirrors, to form an optical cavity, and the photon’s energy was within the PBG of the mirrors, it would be confined to the optical cavity since it could not propagate through any of the walls. So, why not make a box with quarter-wave stack walls? Unfortunately, geometrical reasons limit the quarter-wave stack structures to operate optimally as mirrors only at angles where the incident and reflected light are in-phase, which is not at all incident angles for a single frequency range. Any tilt in the propagation direction changes the path length the waves travel, which changes the interference between the waves. And since the photon is free to travel in any direction it wishes in the box, the quarter-wave stack walls are not always the perfect mirrors that an optical cavity needs to confine photons. This is where the proposals of Yablonovitch and John offered a solution to this problem thereby extending the capabilities of periodic dielectric structures in optical applications. Instead of a periodic modulation in a single direction, both proposals hypothesized that a material with a periodic modulation in all three directions would introduce new optical phenomena, including photon confinement. Yablonovitch

\(^1\)For a rigorous analysis of periodic layered thin films see [13] or [108].
hypothesized that if the PBG overlapped the electronic band edge, spontaneous emission would be prevented since radiation from the excited atoms inside the material would be forbidden to propagate in any direction [103]. John suggested that a 3D lattice with a moderately disordered superlattice would result in strong photon localization due to geometric Bragg resonances [28]. Both of these effects rely upon a PBG that extends in all directions, a full PBG. Yet, achieving such a goal is not easy. Luckily, as we will see in this work, photonic crystals offer many more useful optical phenomena outside of a full PBG.

1.1 The search for the full PBG

Nature offers many stunning examples of PBG materials, yet the challenge facing researchers was to fabricate these structures at length scales on the order of the wavelength of visible light. Perhaps the most common example of a natural PBG structure (Figure 1.2) that can be replicated by man is the opal (Figure 1.3) [39], in which spheres of silica on the order of 200-300nm in diameter are arranged in a close-packed fashion (the face-centered cubic (FCC) lattice). For an opal, the two contrasting dielectric materials are the silica spheres ($n \sim 1.46$) and air ($n = 1$), where the periodicity comes from the families of planes formed by the FCC structure. As the gem is rotated in white light, many bright colors are observed at certain viewing angles. These bright reflections occur because of constructive interference from the reflections off families of planes of silica spheres, also known as the Bragg peak. Although these reflections are quite stunning, they are only unidirectional peaks, occurring for light incident in a specific crystallographic direction, rather than in all directions. Thus, opals cannot suppress radiation or localize photons as Yablonovitch and John proposed, and the search for the lattice structure that would have a full PBG would continue.

In 1990, Ho et al. were the first to theoretically predict a structure that would have a full PBG [26]. Their structure consisted of a diamond lattice of dielectric spheres in an air background, or vice versa. Shortly after, in 1991, Yablonovitch et al. successfully demonstrated, in the microwave regime, the first structure to have a full PBG, later called “Yablonovite” (Figure 1.4) [104]. Yablonovite was made by mechanically drilling holes in a
Figure 1.2: Example of a natural opal gem stone [90].

Figure 1.3: Example of a fabricated opal (2 cm × 2 cm area) when viewed at three different angles—90°, 22.5°, and 45° (from top to bottom) [39].
Figure 1.4: Schematic showing the fabrication of the Yablonovite structure [104].
Figure 1.5: Montage of various structures showing a full 3D PBG, clockwise from upper-left: (a) silicon inverse opal [12], (b) log pile [63], (c) chiral [91], and (d) modified layer by layer structure [34].
dielectric slab along three of the axes of the diamond lattice. A mask defining a triangular array of points was placed on the surface of the slab and three holes were drilled at each point at an angle of 35.26° tilted from the surface normal and rotated such that they were separated by 120° on the azimuth. Figure 1.5 presents a montage of other full 3D PBG structures that would soon follow, such as the inverse opal [12], the woodpile [63], and others [22, 16, 91, 36, 37, 34], each with their own caveats and solutions to the challenges of fabrication, PBG robustness, bandwidth, and increasing the PBG width.

Indeed, having a full PBG in all directions requires a complicated structure, and even more complicated fabrication techniques. However, reducing the dimensionality to confine light propagation within a plane, significantly reduces the complexity, and PCs may show a full PBG within the two allowed directions of propagation.

1.2 Two-dimensional PC structures

In the field of PCs, dimensionality refers not to the spatial representation of the structures (since all of these structures have length, width, and height), but rather the number of directions the periodic modulation extends. An easy way to visualize this is shown in Figure 1.6 which presents three structures with modulations in 1, 2, and 3 dimensions (from left to right) as indicated by the different colored regions [27]. The 1D PC is the familiar quarter-wave stack that was mentioned earlier for which light will experience a PBG only if propagating in the $x$-direction, since light propagating in the $y$ or $z$-directions would not experience any modulation in the dielectric constant, $\epsilon$. In the 2D modulated structure, light traveling in a direction that lies within the $x$-$y$ plane will experience a periodic modulation in $\epsilon$. Finally, in the 3D modulated structure, light traveling in any direction will experience a periodic modulation in $\epsilon$. Additionally, in all of these structures, a minimum refractive index contrast is required to observe PBG effects. Following these guidelines, Figure 1.7 presents examples of 2D and 3D PC structures, respectively: (a) a triangular array of air holes in a dielectric slab and (b) the inverse opal structure where air spheres are arranged in a FCC lattice in a dielectric background (Yablonovite is another example of a 3D PC). Both of these PC structures plus the quarter-wave stack block EM
**Figure 1.6:** Illustration of PC dimensionality which is defined by the number of directions the periodic modulation in refractive index extends [27]).

**Figure 1.7:** Illustrations of (a) the slab waveguide and (b) the inverse opal, example of 2D and 3D PC structures, respectively.
radiation from propagating if the frequency falls within the PBG of the material and the light is propagating in the direction of the modulated $\epsilon$.

### 1.2.1 The square and triangular lattices

As mentioned previously, the complicated structures of 3D PCs can be simplified by removing an allowed propagation direction, as can be shown by the two structures in Figure 1.7. In 1991, Plihal et al. were the first to propose the existence of a PBG in the simple square and triangular lattices depicted in Figure 1.8(a) and (b) [74, 73]. Both consist of arrays of infinitely long dielectric rods, $\epsilon_c$ embedded in a dielectric background, $\epsilon_b$. The rods have circular cross sections of radius $r$ and their intersections with a plane perpendicular to the rod axes produces either a square or equilateral triangular array of circles that are separated by the lattice constant, $a$. Both show a full PBG for light traveling in the plane perpendicular to the rod axes when the appropriate parameters of design ($r$, $\epsilon_c$, $\epsilon_b$, and $a$) and excitation (frequency and polarization) are chosen. However, the square lattice requires a large dielectric contrast ($\epsilon_c - \epsilon_b > 12.3$) to open a full PBG for both TE ($E$ perpendicular to the rod axis) and TM ($E$ parallel to the rod axis) polarizations [94], whereas the triangular lattice only requires a contrast of 7.2 [52]. In 1992, Meade et al. confirmed the existence of a PBG in these two lattices experimentally by drilling holes ($r = 0.992\text{cm}, a = 1.044\text{cm}$) in a block of material with $\epsilon \sim 13 - 15$ and measuring the transmission spectra in the GHz frequency range. Later in 1993, Wendt et al. used electron-beam lithography and reactive-ion-beam etching to fabricate a triangular lattice of air holes in a GaAs/AlGaAs heterostructure which operated at optical wavelengths [97].

Along with their structural simplicity and scalability, 2D PCs are compatible with top-down fabrication techniques that have been extensively used in the microelectronics industry to design patterns on a sub-micron length scale. Lattice patterns can be drawn in a polymer based photoresist using photo- or electron beam lithography [97, 100], or by laser interference patterns [10, 95, 85]. These patterns can then be used as masks as the underlying material is subjected to etching. What remains is a regular array of holes or pillars that form the 2D PC structure at the desired length scale. Since these fabrication techniques are
Figure 1.8: Schematics of (a), square and (b), triangular 2D PC lattices.
very mature, a high degree of precision and accuracy in the fabrication of the structures can be achieved. In addition, by nature of these fabrication techniques, 2D PCs can be readily integrated into pre-existing opto-electronic devices all on the same silicon wafer, eliminating the need for extra fabrication steps or solutions to coupling different device components on different wafers.

Fabrication is not the only simplification that 2D PCs offer over their 3D counterparts. Computations and theoretical analyses are simplified as well. The removal of an independent variable (a spatial direction) in Maxwell’s equations simplifies many computational algorithms and greatly decreases the computational time and power necessary to solve for photonic band structures or EM field profiles. The analysis is also simplified since only two independent spatial variables are present. In a 3D PC, EM field profiles must be analyzed either volumetrically, or by taking multiple slices in multiple directions through the structure. However, in a 2D PC structure, the field profiles are identical in any plane that contains the propagating field; thus only one slice in the plane of the structure is needed to view the field profiles (another slice parallel to the hole axis is necessary if the PC is finite in height). Additionally, analysis of the dispersion surface is simplified. The dispersion surface is analogous to the Fermi surface in solid state physics and it represents all solutions to Maxwell’s equations for a given structure in terms of $k$-space and frequency. In a 3D PC structure, the dispersion surfaces are complicated 3D surfaces that resemble thin membranes of constant frequency [75]. Thus, to view multiple frequencies at one time is time consuming and computationally taxing. In a 2D PC, the dispersion surfaces can be represented as planes in a plot of frequency vs. the in-plane $k$-vector. This dramatically simplifies the interpretation of the information in the dispersion surfaces, allowing accurate predictions of the optical response of the PC such as refraction or dispersion effects [80, 42, 5].

As with 3D PCs, research on 2D PCs initially focused on the full PBG effect and using it to block light, as in a filter, and to manipulate light through intentional lattice defects. As in semiconductor physics, a defect in the lattice allows an energy state to exist within the band gap where, analogous to solid state physics, the density of states (DOS) is zero.
A defect creates a spike in the zero DOS region, allowing an electron/photon with the same energy as the defect state to exist within the band gap. In the same way, a defect in a PC lattice creates a localized state within the PBG, allowing a photon with the defect mode frequency to exist within the localized area of the lattice defect [20, 53, 86, 87]. Many applications result from this effect, for example in 1996, Villeneuve et al. reported that a point defect within a triangular lattice could operate as a high-Q cavity [93] which can be used for laser applications [4, 64]. In 1991, Meade et al. reported that a line defect created by removing a row of rods or holes in a 2D PC structure strongly confines a propagating mode to within the defect line [53], and if the defect line bends, low losses are possible even around sharp corners [54, 92]. And shortly after in 2000, Noda et al. proposed a channel drop filter device that combines elements of line and point defects [60]. In all of these devices, the operating wavelength lies within the PBG of the defect-free lattice. Thus, the light is strongly confined into the defect regions through a mechanism different from total internal reflection, as in optical fibers or waveguides. In fact, using this alternative confinement mechanism, PC researchers have shown high transmission (< 35 dB loss) in waveguide bends of 120° and zero radius of curvature [92], a performance that optical fibers and integrated optic waveguides could never achieve using total internal reflection.

1.3 Beyond the full PBG: Refraction effects in PCs

In the infancy of PC research, the full PBG was the ultimate goal for many researchers. However, PCs offer a far richer pallet of optical phenomena, as was noticed by Dowling and Bowden in 1994 [21] when they proposed a giant refractive property due to the highly nonlinear dispersion relation near the band edge. Through an analytical expression for the effective index of refraction in a simple 3-D photonic crystal, they deduced that at the photonic band edge the phase velocity, $v_p$, tends toward infinity, implying that the index of refraction approaches zero since the index of refraction is defined by $n \equiv c/v_p$.

The ramifications of a less than unity index of refraction is best illustrated using Snell’s law as shown in Figure 1.9 and as described below mathematically:

$$\sin \theta_2 = \frac{n_1}{n_2} \sin \theta_1, \quad (1.1)$$
Figure 1.9: Snell’s Law in (a) a homogeneous, isotropic dielectric medium and in (b) a photonic crystal [21].
where $n_1$ and $n_2$ are the refractive indices of the media in region 1 and 2 and $\theta_1$ and $\theta_2$ are the angles of propagation in each media as measured from the normal line of the interface between region 1 and 2. As shown in Figure 1.9(b), $n_2 < 1$ leads to a dramatic increase in $\theta_2$ in a PC when compared to a homogeneous material, Figure 1.9(a). In 1996, Lin et al. demonstrated the hypothesis of Dowling and Bowden showing that large refraction effects do exist in PCs, giving them the ability to divert EM radiation greatly from its original path [49]. The experiment was conducted in the millimeter wavelength range (75-110 GHz) using alumina rods ($r = 0.1525$ mm, $\epsilon = 8.9$) arranged in a 2D triangular lattice ($a = 0.81$ mm). Their results showed a $46.5^\circ$ deflection of the incident EM radiation, corresponding to an estimated effective index of refraction of, $n_{eff} = 1.58$ from the formula:

$$\delta = \theta_1 + \sin^{-1}\left\{ \left(\sin\alpha\right)\left[n^2 - \sin^2\theta_1\right]^{1/2} - \sin\theta_1 \cos\alpha \right\} - \alpha, \quad (1.2)$$

where $\theta_1$ is the angle of incidence of the beam, $\alpha = 60^\circ$ is the interior angle of the array of rods, $\delta$ is the beam deviation angle (the angular difference between the incident beam and the beam exiting the prism, which is different than $\theta_2$), and $n$ is the refractive index of the alumina rods. This ‘prismatic’ derivation assumes the PC behaves as an isotropic, homogeneous dielectric medium with an $n_{eff}$ derived from the slopes in the dispersion relationship, or band diagram. The value of this experiment is apparent when we recall the linear nature of Maxwell’s equations which allows the properties of photonic devices at larger length scales to be directly scaled to smaller dimensions to operate at shorter wavelengths. Thus, Lin et al. estimated that a scaled version of their structure operating in the visible at $\lambda = 700$ nm would have a lattice constant of 300 nm and occupy a $18 \mu m \times 18 \mu m$ area – a length scale reduction of 2,700 [49].

### 1.3.1 Superprism and giant refraction effects

Another key advancement in the study of refraction behavior in 2D-PCs came in 1998 when Kosaka et al. succeeded at visualizing negative refraction of a near-infrared (NIR) beam propagating inside the 3D PC structure shown in Figure 1.10 [42]. The structure was fabricated by first patterning a substrate with a triangular lattice of pits by electron beam (e-beam) lithography and dry etching, followed by bias sputtering deposition of alternating
Figure 1.10: Schematic of 3D autocloned PC structure [42].

Figure 1.11: Image of beam propagation in 3D autocloned PC structure [42].
layers of Si/SiO$_2$. The sputtering method used preserves the corrugated pattern in the substrate, an effect called “autocloning”, so that the resulting Si/SiO$_2$ structure resembles the graphite structure [35]. Figure 1.11 shows the resulting top-plane image when a 0.956 $\mu$m laser beam is incident on the side of the 500 $\mu$m $\times$ 500 $\mu$m structure. As shown, a change in the incident angle of 14° results in a large swing (140°) of the refracted beam inside of the PC. Also, their structure exhibited a large frequency dispersion where a change of 10 nm in the wavelength of the incident beam changed the propagation direction by 30° [42], and in a later paper they reported this effect to be as high as 50° [40]. Collectively they named their observations the superprism effect. In addition to the superprism effect, Kosaka et al. observed a beam divergence behavior in the propagating beam where the PC acted as either a collimator or a lens depending only upon the propagating angle and independent of the divergence of the incident beam [42, 43]. These findings show that the PC behaves as a highly anisotropic medium and cannot be described by an $n_{eff}$. Thus, they distinguished their results from previous works by saying that the origin of their superprism effect results from a strong modification of the group velocity, $v_g$, rather than the phase velocity, $v_p$ [42, 41, 40, 43]. Consequently, beam propagation behavior must be predicted using wavevector analysis of the dispersion surface, just as it is done in traditional optics and in planar waveguide gratings on the index ellipsoid. In 1996, Russell et al. described this procedure [80] as it applies to PCs, which will be covered in more depth in Chapter 6 of this work.

The findings of Kosaka et al. in 1996 drew attention to the dispersive nature of PCs, and paved the way for countless proposals of integrated optical devices such as wavelength-division multiplexers/demultiplexers [41, 7, 100] and beam collimators [43, 99, 106]. Additionally, work has continued to fully characterize refraction effects in PCs such as quantifying the resolution of the superprism effect [5] and considering beam behavior at the exit facet of the PC region [7, 50].
1.4 Tunable PC structures

As we have discussed, PCs possess many interesting optical properties that affect the transmission, reflection, confinement, and propagation of light. In a typical PC, these propagation effects are passive since they depend upon refractive index, lattice period, and feature size. However, the ability to dynamically alter propagation properties by actively changing one of these parameters while under excitation can lead to many new effects. For example, the refractive index of the structure can be modified through the use of electro-optic (EO) or nonlinear materials (NL) [69, 14, 48, 65, 84, 102, 110] or mechanical deformation can modify the lattice period [67, 109]. The first to propose these effects were Busch and John, who, in 1999, proposed that the frequency of the PBG of an inverse opal that is infiltrated with a liquid crystal (LC) can be shifted by an applied bias [14, 29]. In 2D-PC structures, Leonard et al. demonstrated that infiltrating a 2D triangular lattice of air pores in silicon with LC allowed temperature dependent tunability of the air band edge frequency. However, the maximum theoretical tuning of the air band edge was not achieved because pinning of the LC molecules limited the alignment of the director to an escaped-radial configuration, which reduced the E7 refractive index tuning to below the maximum $\Delta n$ of 0.2 [48].

While actively shifting the PBG will lead to many new devices such as tunable filters, an idea more central to the theme of this work is the dynamic tuning of bulk propagation effects such as the superprism effect. In 2002, we proposed that a LC infiltrated silicon triangular lattice PC would allow tuning of the giant refraction effect by switching the bias on or off between the top and bottom planes of a PC [68, 66]. We predicted a change in refractive index from 1.5 to 1.7 for the LC in the holes would produce a change in beam propagation of 3-10°. In 2003, two groups [84, 102] proposed an opposite configuration where the background material is an EO material such as lead lanthanum zirconate titanate (PLZT). They also predicted large changes in the propagation direction when the bias on the structure was switched. However, the calculations reported were on pure 2D systems which neglected the finite thickness of the waveguide layer which will reduce the degree of tunability in these structures [70].
Figure 1.12: Schematic of LC infiltrated superlattice PC [70]
1.5 The superlattice PC structure

In 2002, Park and Summers proposed to overcome the limitations introduced by a finite slab thickness with a superlattice PC configuration which is more sensitive to changes in refractive index [66, 57, 70]. Figure 1.12 illustrates their structure, which is a triangular lattice of holes in silicon that is infiltrated with LC and has an interdigitating addressing scheme on the top surface and a planar addressing scheme on the bottom surface. This allows rows to be biased/unbiased independently, thus adjacent rows of holes can possess different refractive indices. If the rows are biased in an alternating manner, as shown in Figure 1.12, then a longer range periodicity is introduced in the lattice, forming a superlattice. The superlattice dramatically alters the optical properties of the PC because of symmetry reduction and other effects that were illuminated through this current work. However, the superlattice strength of the LC structure above is also limited by the index tunability of the refractive index of the LC, which in principle can range from $0 < \Delta n < 0.6$ [38]. We address this in the current work by presenting several new lattice structures with dynamic refractive index tuning that offer significant improvements over the triangular lattice and which allow greater control over the superlattice strength due to a superlattice periodicity formed by using holes of two different radii together with the use of EO or NL materials.

1.6 Goal of this work

The optical properties of PCs outside of the PBG offer great flexibility in controlling the propagation of light, and these propagation effects are strongly tied to the lattice structure of the PC. Currently, a detailed analysis has not been conducted on the properties of 2D-PC structures containing a superlattice periodicity, and herein lies the goal of this work. Chapter 2 will establish a theoretical and experimental background of PC research, some of which was applied to the SSL PC structure in this work. The theoretical aspects and consequences of a 2D SL on the photonic band properties of a PC are discussed in Chapter 3 and 4, respectively, while Chapter 5 investigates the photonic band properties experimentally. The refractive properties of the 2D SSL PC is characterized through calculations in Chapter 6, and a survey of tunable SSL PC structures is presented in Chapter 7. Finally,
Chapter 8 will conclude the work and offer some suggestions for future directions of research in superlattice structures.
CHAPTER II

BACKGROUND

One of the many intellectual beauties of PCs is the way multiple disciplines in physics are melded together to describe their properties. As an EM phenomena, Maxwell’s equations are the main platform for explaining the behavior of photons when encountering PCs. However, the ‘crystal’-like properties of PCs leads to descriptions that parallel many solid state physics concepts. At the same time, their photonic properties are analyzed with well known optical concepts such as wavevector diagrams describing the applications and relationships of these three disciplines to PCs is the goal of this chapter.

First, we examine Maxwell’s equations and how they can be cast in a manner reminiscent of the Schrödinger equation, which leads to many parallels between the description of PCs and electronic materials. Next, we briefly elucidate the numerical methods commonly employed to solve Maxwell equations in a periodic system; in particular the plane-wave expansion (PWE) and finite-difference time-domain (FDTD) methods, both of which are heavily employed in this work. A natural progression is the discussion of the analysis methods used to decipher the data given by PWE and FDTD calculations. This includes propagation properties determined from analyzing the photonic dispersion surfaces and quantifying this performance.

2.1 The Maxwell equations and PCs

Maxwell’s unified theory of EM behavior was a triumph of science in 1864. Through four coupled equations, all EM phenomena could be explained, including that of light and other radiation. In this work, we assume all materials are linear, isotropic, and lossless. In addition, we assume the materials have a frequency independent dielectric constant, that the magnetic permeability is equal to unity, and that there are no sources. With these assumptions and the constitutive relations $\mathbf{D} = \epsilon \mathbf{E}$ and $\mathbf{B} = (1/\mu)\mathbf{H}$, the Maxwell equations
\[ \nabla \cdot \mathbf{H}(\mathbf{r}, t) = 0, \quad \nabla \times \mathbf{E}(\mathbf{r}, t) + \frac{1}{c} \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t} = 0 \]  
(2.1)

\[ \nabla \cdot \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}, t) = 0, \quad \nabla \times \mathbf{H}(\mathbf{r}, t) - \frac{i \omega}{c} \epsilon(\mathbf{r}) \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} = 0. \]

These equations are linear, and as a consequence, we can separate out the time dependence by expressing \( \mathbf{E} \) and \( \mathbf{H} \) as a set of harmonic plane waves:

\[ \mathbf{H}(\mathbf{r}, t) = H_0 e^{i \mathbf{k} \cdot \mathbf{r}} e^{i \omega t} \]
\[ \mathbf{E}(\mathbf{r}, t) = E_0 e^{i \mathbf{k} \cdot \mathbf{r}} e^{i \omega t}, \]

(2.2)

where \( \mathbf{k} \) is the wavevector, \( \mathbf{r} \) is the position vector, and \( t \) is the time. Substituting these equations into Equation (2.1) gives:

\[ \nabla \cdot \mathbf{H}(\mathbf{r}) = 0, \quad \nabla \times \mathbf{E}(\mathbf{r}) + \frac{i \omega}{c} \mathbf{H}(\mathbf{r}) = 0 \]

(2.3)

\[ \nabla \cdot \mathbf{D}(\mathbf{r}) = 0, \quad \nabla \times \mathbf{H}(\mathbf{r}) - \frac{i \omega}{c} \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}, t) = 0, \]

where the divergence equations in the left column state that there are no point sources or sinks of displacement and magnetic fields in the material. Since we are using a plane wave solution, they also require that \( \mathbf{E} \) and \( \mathbf{H} \) are transverse, eg. \( \mathbf{E} \cdot \mathbf{k} = 0 \). The two curl equations in the right column relate \( \mathbf{E} \) to \( \mathbf{H} \) and can be cast in terms of only one field to give the equation:

\[ \nabla \times \left[ \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right] = \left( \frac{\omega}{c} \right)^2 \mathbf{H}(\mathbf{r}) \]

(2.4)

This equation will give all the information about the \( \mathbf{H} \) field in the material given the dielectric function \( \epsilon(\mathbf{r}) \). This solution can then be used to find the \( \mathbf{E} \) field by substituting \( \mathbf{H} \) back into Equation (2.3). Essentially, Equation (2.4) is an eigenvalue equation where an operation on a function on the left side equals the same function multiplied by a constant. But the most remarkable thing about this equation is its striking resemblance to another
famous eigenvalue equation which describes electron propagation in a periodic potential: the time-independent Schrödinger equation

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \Psi(r) = i\hbar \dot{\Psi}(r),
\]  

(2.5)

where \( V(r) \) is the potential, \( m \) is the electron mass, and \( \Psi(r) \) is the wave function of the electron. This similarity makes it possible to describe PCs using the same language as used in solid state physics. Yet, at the same time, PCs are also naturally described using optical concepts.

2.1.1 Solid state physics concepts in PCs

The forms of Equations (2.4) and (2.5) are similar, thus their solutions should be similar as well. Indeed, it is the similarities between Equations (2.4) and (2.5) and the periodicity in the structures that introduces the use of such concepts as reciprocal space, Brillouin zone, dispersion surface (Fermi surface), Bloch solutions, crystal symmetry, modal degeneracy, photonic band structure, density of states, and defect modes. However, there are significant differences in the solutions, the first of which is in the linearity of Maxwell’s equations.

Solutions to the Schrödinger equation for free electrons can take the form of plane waves,

\[
\Psi(r,t) = \psi_0 e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\omega t},
\]  

(2.6)

and have an energy dependence in direct proportion to the electron wavevector, \(|\mathbf{k}| = k = 2\pi/\lambda\), given by

\[
E(k) = \hbar\omega(k) = \frac{\hbar^2 k^2}{2m}
\]  

(2.7)

Likewise, photons have a similar dispersion relation since there are plane wave solutions (Equations (2.2)) to Maxwell’s equations. However, unlike the square law of Equation (2.7), photon dispersion in an isotropic medium is linear:

\[
\omega = \frac{ck}{\sqrt{\epsilon}},
\]  

(2.8)

where \( c \) is the speed of light in vacuum and \( \epsilon \) is the dielectric constant of the medium. Equation (2.8) is often called the light line, and has particular significance in describing the properties of 2D slab waveguide PCs.
In a PC, a periodicity in the dielectric function, $\epsilon(r)$, exists and can be defined as

$$\epsilon(r) = \epsilon(r + lT), \quad l = 0, \pm 1, \pm 2, \ldots,$$

(2.9)

where $T$ is a translation vector. This is analogous to the periodic potential created by the atomic nuclei in a crystalline material.

Though there exists many similarities between the mathematics of solid state physics and PCs, there are many important differences as well. For example, the Schrödinger equation describes scalar fields while the Maxwell equations describe vector fields. In addition, PCs are macroscopic systems, thus they do not possess a fundamental length scale such as the Bohr radius. This lack of a fundamental constraint allows the scalability of the Maxwell equations, permitting the prediction of the optical properties of a particular lattice configuration in terms of a normalized length scale. In fact, the frequency of the optical response scales inversely with the lattice constant, $a$, of the PC structure. Therefore, a structure can be designed and tested at longer wavelength ranges, where fabrication constraints are more tolerable. Then, the structure can be scaled according to the operating wavelength range of interest and the properties will remain unchanged.

### 2.1.2 Optics concepts

As mentioned in Chapter 1, the quarter-wave stack (which is a one-dimensional PC) was studied for 100 years before the proposals of Yablonovitch and John in 1987. A standard method of analysis in these structures is the use of transfer matrices [13, 108], which has been applied successfully to multi-dimensional PCs [82, 8, 71] to calculate transmission and reflection coefficients, which yields information about the PBG and DOS. However, the transfer matrix method is unable to simulate the bulk propagation properties of PCs, which are a central theme in this work. Instead, bulk propagation in PCs are studied using the finite-difference time-domain method and also by wavevector diagrams, common tools in optics which were first applied by Russell to one-dimensional periodic gratings [81] and later to multidimensional PCs [82, 80] in 1986 and 1995, respectively.

The analysis of wavevector diagrams begins with the dispersion surfaces which are, in fact, surfaces in multiple-dimensions just as the Fermi surface in solid state physics. In
2D PCs, they are three-dimensional, as in Figure 2.1(a), with the base plane defined by two in-plane $k$-vectors and the third dimension by the frequency, $\omega$. The intersection of a fixed $\omega$ plane with the dispersion surface yields contour lines of allowable wavevectors in the medium, referred to in this work as dispersion contours. For an isotropic, homogeneous medium, such as air, the dispersion surface is an inverted cone as shown (recall, the dispersion relation for an isotropic medium is given by $\omega = ck/\sqrt{\epsilon}$). Thus, the dispersion contours are congruent circles as shown in Figure 2.1(b) whose radii are given by $k = \omega n/c$, where $n$ is the refractive index of the medium. For an anisotropic birefringent medium, the dispersion contours are ellipses (Figure 2.1(c)), and for a PC, they are complicated two dimensional shapes (Figure 2.1(d)). From the dispersion contours, the photon group velocity and direction of propagation in the new medium can be obtained since it is given by the gradient of the contour:

$$v_g = \nabla k \omega(k),$$  \hfill (2.10)

where $v_g$ is a vector normal to the contour and points in the direction of increasing frequency. Further details into the derivation of the refraction response in PCs is discussed in Chapter 3.

### 2.2 Numerical analysis of PCs

The various numerical techniques employed to solve Maxwell’s equations in PCs are as numerous as the potential applications for PCs, and each has its own advantages and disadvantages, with no single method emerging as the penultimate. Because of the similarities between PCs and crystalline solids, the techniques used in solving electronic bands are also employed to find photonic bands in PCs. One important difference between the calculations used in solid state physics and those used in PC research is that while the calculations in solid state are by nature of the algorithms, approximations of the real systems, the calculations in PCs are, in principle, exact. Therefore, their accuracy is limited only by the accuracy and detail in the definition of the dielectric function $\epsilon(\mathbf{r})$ that is input at the start of a calculation. This difference in the solution accuracy arises because photons are non-interacting particles (bosons) whereas electrons are fermions that interact with one
Figure 2.1: (a) Dispersion surface of an arbitrary isotropic, homogeneous medium and dispersion contours of (b) an isotropic medium, (c) a birefringent medium, and (d) an arbitrary PC with a hexagonal shaped Brillouin zone.
another. In solid state physics, fermions are often approximated as bosons in order to reduce the complexity of the problem to arrive at a reasonable definition of a problem for computers to handle.

The two main classes of numerical methods for solving EM problems in PCs are frequency-domain based and time-domain based. Typically, frequency-domain methods, such as the plane-wave expansion (PWE), offer a speed advantage over time-domain based methods (such as the finite-difference time-domain (FDTD) method). However, the computational load of the former scales exponentially as the size of the computational domain increases, while the latter method scales linearly with domain size [107, 15, 89]. This section describes, in general terms, the two computational methods employed in this work and their respective advantages or disadvantages.

2.2.1 Plane wave expansion

In the plane-wave expansion (PWE) method, solutions to the eigenvalue equation, Equation (2.4), are found by expanding \( \mathbf{H} \) into plane waves using Bloch’s theorem to give:

\[
\mathbf{H}(\mathbf{r}) = \sum_{G} \sum_{\lambda=1}^{2} h_{\mathbf{G},\lambda} \hat{\mathbf{e}}_{\lambda} e^{i(k+G)\cdot\mathbf{r}},
\]  

(2.11)

where \( k \) is a wavevector in the Brillouin zone, \( G \) is a reciprocal lattice vector, and \( \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 \) are unit vectors that are perpendicular to \( k + G \) in order to satisfy the transversality requirement, \( \nabla \cdot \mathbf{H} = 0 \). This expansion by plane waves, Equation (2.11), is possible because \( \epsilon(\mathbf{r}) \) is periodic. The eigenvalue equation, Equation (2.4), is then expressed as a matrix equation:

\[
\sum_{G',\lambda'} H_{G',G}^{\lambda,\lambda'} h_{G',\lambda'} = \left( \frac{\omega}{c} \right)^2 h_{G,\lambda},
\]  

(2.12)

where

\[
H_{G,G'} = |k + G||k + G'|\epsilon^{-1}_{G,G'} \begin{pmatrix}
\hat{e}_2 \cdot \hat{e}_2' & -\hat{e}_2 \cdot \hat{e}_1' \\
-\hat{e}_1 \cdot \hat{e}_2' & \hat{e}_1 \cdot \hat{e}_1'
\end{pmatrix}
\]  

(2.13)

and \( \epsilon^{-1}_{G,G'} \) is the Fourier transform of the dielectric function [26]. Equation (2.12) can now be solved using standard matrix diagonalization methods to produce the normal mode coefficients and the mode frequencies which give the dispersion relation for the PC.
The PWE method is a powerful tool, but it is unable to do everything. For example, the PWE method cannot calculate time evolution of field profiles for beam propagation and calculating transmission or reflection coefficients requires extra steps in the algorithm. PWE has difficulty with three dimensional structures that are finite in dimension or that do not have periodicity in all directions, eg. slab waveguide PC structures. In PWE, the boundaries of the computational cell are always periodic, otherwise the $\mathbf{H}$ field could not be expanded into plane waves. Therefore, to calculate structures that are finite, a supercell is used in which a large area of freespace surrounds the dielectric structure so that when the computational cell is repeated, each dielectric structure in the resulting array is buffered and isolated from one another. Clearly a large computational cell must be used to achieve isolation of the dielectric structures; thus, the computations take much longer and are only accurate within the range of frequencies that can be confined by the dielectric structure. For example, accurate results for a slab waveguide are only possible within the guiding regime of the slab (under the light line of the cladding material). Thus, time-domain methods are indispensable for their ability to make up for what frequency-domain methods lack.

### 2.2.2 Finite-difference time domain

FDTD calculations have been used in EM problems for some time, finding their earlier applications in antenna and guided wave simulations in the microwave regime. Adapting the method to PCs is elementary since Maxwell’s equations are linear and a large catalog of boundary condition implementations is available. This was first done by Chan et al. in 1995 [15].

The FDTD method discretizes space into a mesh of points on which the $\mathbf{E}$ and $\mathbf{H}$ fields are solved using Maxwell’s equations, Equation (2.1), from a given initial field condition. In Cartesian coordinates, Equation (2.1) can be written as a set of six coupled equations:
\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right), \quad \frac{\partial E_x}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_y}{\partial z} - \frac{\partial H_z}{\partial y} - \sigma E_x \right)
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right), \quad \frac{\partial E_y}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_y \right)
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right), \quad \frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} - \sigma E_z \right)
\]

(2.14)

A set of finite-difference equations first introduced by Yee in 1966 is then used to calculate the derivatives with second-order accuracy, both spatially and temporally [107]. Following the notation used by Yee, a point on the mesh is denoted by

\[(i, j, k) = (i \Delta x, j \Delta y, k \Delta z)\]  

(2.15)

and any temporal function is denoted by

\[F^n(i, j, k) = F(i \Delta x, j \Delta y, k \Delta z, n \Delta t),\]  

(2.16)

where \(\Delta x, \Delta y, and \Delta z\) are the spatial increments, \(n\) denotes the time, \(\Delta t\) is the time increment, and \(F\) is equivalent to \(E\) or \(H\). Now, we use a Taylor series expansion of \(F\) at a fixed time, \(t_n = n \Delta t\), around the spatial point \(x_i\) to arrive at an expression for the spatial derivative

\[
\frac{\partial F^n(i, j, k)}{\partial x} = \frac{F^n(i + \frac{1}{2}, j, k) - F^n(i - \frac{1}{2}, j, k)}{\Delta x} + O[(\Delta x)^2],
\]

(2.17)

which shows the finite differences are taken over the interval \(\pm 1/2 \Delta x\) and where \(O[(\Delta x)^2]\) denotes the remainder term which approaches zero as the square of the increment. Similar expressions are derived for the partials in the \(y\) and \(z\) directions, and if the position is fixed at the space point \((i, j, k)\), the expression for the first time partial derivative is given by

\[
\frac{\partial F^n(i, j, k)}{\partial t} = \frac{F^{n+1/2}(i, j, k) - F^{n-1/2}(i, j, k)}{\Delta t} + O[(\Delta t)^2].
\]

(2.18)

Equations (2.17) and (2.18) are then substituted for the partial derivatives in Equation (2.14). The positions of the \(E\) and \(H\) components are spatially staggered on the mesh.
(the Yee cell) as shown in Figure 2.2 so as to achieve greater accuracy in Equation (2.17). Meanwhile, the computational accuracy of Equation (2.18) is achieved by evaluating $E$ and $H$ at alternate half-time steps.

After the substitution of Equations (2.17-2.18) into Equation (2.14), each equation of the coupled set takes a form similar to either:

$$
H_x^{n+1/2}(i, j + \frac{1}{2}, k + \frac{1}{2}) = H_x^{n-1/2}(i, j + \frac{1}{2}, k + \frac{1}{2}) + \Delta t \frac{\mu(i, j + \frac{1}{2}, k + \frac{1}{2}) \Delta x}{\mu(i, j + \frac{1}{2}, k + \frac{1}{2}) \Delta x} \left[ E_y^n(i, j + \frac{1}{2}, k + 1) - E_y^n(i, j + \frac{1}{2}, k) + E_z^n(i, j, k + \frac{1}{2}) - E_z^n(i, j + 1, k + \frac{1}{2}) \right]
$$

(2.19)

for the $H$ field components, or

$$
E_x^{n+1}(i + \frac{1}{2}, j, k) = \left[ 1 - \frac{\sigma(i + \frac{1}{2}, j, k) \Delta t}{\epsilon(i + \frac{1}{2}, j, k)} \right] E_x^n(i + \frac{1}{2}, j, k) + \Delta t \frac{\epsilon(i + \frac{1}{2}, j, k) \Delta x}{\epsilon(i + \frac{1}{2}, j, k) \Delta x} \left[ H_x^{n+1/2}(i + \frac{1}{2}, j + \frac{1}{2}, k) - H_x^{n+1/2}(i + \frac{1}{2}, j - \frac{1}{2}, k) + H_y^{n+1/2}(i + \frac{1}{2}, j - \frac{1}{2}, k) - H_y^{n+1/2}(i + \frac{1}{2}, j, k + \frac{1}{2}) \right]
$$

(2.20)

for the $E$ field components. With these full set of six equations, the values of the field vector components at a single time step increment can be updated to the future at any point on the Yee cell mesh. For example from Equation (2.19), we can find the $H_x$ field component at the next time step at the mesh point $(i, j + \frac{1}{2}, k + \frac{1}{2})$ from knowing only the value of the $H_x$ field at the same point during the previous time step and the previous values of the $E_y$ and $E_z$ field components at adjacent points in the mesh. Thus, after the initial field values are defined over the mesh, the time step is incremented until a sinusoidal steady state is achieved at each mesh point.

Naturally, accuracy and stability in the finite-difference equations is achieved by the choice of appropriate time and space increments. For accurate results, the spatial increment is required to be either a small fraction of the minimum wavelength expected in the simulation or a small fraction of the minimum dimension of a dielectric feature. This ensures that the field values do not change abruptly between two spatial increments and that the definition of the dielectric features is not too coarse. Stability of the time-stepping
Figure 2.2: Schematic of Yee cell and the positions of the field components.
algorithm is achieved by the appropriate choice of $\Delta t$ such that it satisfies

$$v_{max}\Delta t \leq \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-1/2}$$

(2.21)

where $v_{max}$ is the maximum phase velocity in the simulation. Typically in a PC calculation all values are normalized by the lattice constant, $a$, and the speed of light, $c$, thus $v_{max} = 1$.

During the calculation, the field values are stored at mesh points randomly distributed in the computational domain. After the time stepping is complete, the fields are integrated in time, and a Fourier transform of the collected fields yields the resonant frequency components in the spectrum, which are then used to plot the dispersion relationship of the PC. Alternatively, the field components at all the mesh points can be stored for the purpose of visualizing their time-evolution.

### 2.3 Experimental analysis of PCs

Fabrication on length scales comparable to the wavelength of visible light ($< 800$ nm) requires ingenuity and mastery of state-of-the-art technologies. In addition, consideration must be given to the design of the structure according to which experiments will be used to measure the photonic properties of a PC.

#### 2.3.1 Fabrication

The scalability of Maxwell’s equations is an invaluable property to experimental investigations in PCs. In the infancy of PC research, experiments were designed at longer wavelengths, allowing structures with millimeter sized features to be fabricated and tested [105, 104, 51, 87, 49]. For 2D structures, fabrication involved machining holes in slabs of dielectric constant matching materials, or using arrays of alumina rods in air. As fabrication techniques became more complicated, feature sizes decreased as well as the operating wavelengths.

In 1993, Lehmann demonstrated the formation of regular arrays of high-aspect ratio macropores in n-type silicon by electrochemical etching [47]. First, the sites for the pore nuclei were defined on the wafer by photolithography and alkaline etching. Then, the wafer
was anodically etched in hydrofluoric acid (HF) while the backside was illuminated, forming deep macroscopic pores in the Si wafer.

In 1996, Grüning et al. used a slight modification of this technique to form triangular arrays of pores in a silicon wafer with \( a = 2.3 \, \mu m \), as shown in Figures 2.3(a-b) [25]. They modified the original process by adding a thermal oxidation and wet etch step to widen the pore diameter to 2.13 \( \mu m \) to achieve an air filling fraction that would maximize the PBG. Many advantages are present in this fabrication technique. For example, silicon has a high-dielectric contrast with air (which is desirable for PCs), it has low propagation loss in the NIR (the frequency range used in integrated optics and optical communications), and it is a commonly used materials system. Additionally, the exceptionally large pore depth allows the structure to be approximated as a pure 2D-PC for numerical calculations.

Optical measurements of the Grüning et al. structure showed a PBG in both TE and TM polarizations centered around 4.9 \( \mu m \) (Figure 2.3(c) and (d), respectively). Later, others used this electrochemical etching technique to fabricate PCs operating in the NIR [11, 78, 48, 83, 24], and in 2001, Schilling et al. pushed the PBG to 1.3 \( \mu m \) [83]. The Schilling et al. structure had a triangular array of pores with \( a = 0.5 \, \mu m \), \( r = 0.215 \, \mu m \), and depth, \( h = 100 \, \mu m \).

Further scaling of 2D PC structures was reported in 1993 by Wendt et al. who applied electron-beam lithography (EBL) and reactive-ion-beam etching (RIBE) to a GaAs/AlGaAs heterostructure [97]. They succeed in fabricating hole diameters of 245 nm to a depth of 0.6 \( \mu m \) in a triangular lattice with \( a = 295 \, \text{nm} \). EBL offers a high degree of precision and great flexibility in the design of the device and feature geometries. However, EBL requires expensive equipment and long operating times to pattern large areas. Despite these disadvantages, it remains a widely used technique in 2D-PC fabrication [42, 92, 100, 106], and is employed in this work to fabricate structures in silicon.

### 2.3.2 Optical characterization

Experiments to measure the optical properties of PCs typically involve a broad spectrum light source incident on the PC in a particular lattice direction and a detector appropriately
Figure 2.3: (a-b) Scanning electron micrographs of the triangular PC structure fabricated by Grüning et al. (c) TE and (d) TM polarization transmission spectra of the structure [25].
positioned to measure the transmission or reflection spectrum. For 3D [105, 104, 12] and pure 2D PCs [25, 49, 11] this is straightforward since orienting the structures in relation to the incident source can be accomplished with the source located externally to the PC. Beam propagation can also be measured by this method by viewing the out-of-plane scattering of the structure [42].

However, if the holes or rods of the 2D PC are not deep enough to be considered ‘infinite’ (a more realistic situation for integrated applications) then wave-guiding plays an important role in the optical properties of the PC [30]. In these structures, henceforth called 2D slab waveguide (SWG) PCs, the propagating beam is confined in the axial direction by a high index layer sandwiched by low index layers or surrounded by air. Consequently, the PBG and beam propagation effects of the PC are limited to the EM modes supported by the slab waveguide which will have a frequency range under the light line (\(\omega = ck/n\)) of the cladding layers. Modes of all other frequency can couple and decay into the cladding layers. Thus, the photonic properties of the 2D-SWG-PC must be measured using different experiments: those that use mode confinement and those that do not. Thus, the 2D-SWG-PC structure poses an experimental challenge to fully characterize their optical properties. However, several solutions have been offered and are presented in the next sections.

### 2.3.3 Guided in-plane excitation measurements

The first method implemented to measure the transmission/reflection properties of 2D-SWG-PCs used a rib waveguide to deliver an external excitation source (via coupling to the waveguide) to the PC (Figure 2.4) [44]. This technique measures the PBG [44] directly from dips in the transmission spectrum as well as the bulk propagation properties of the PC [100, 101, 99] from scattered light imaged from above the PC or from relative intensity values in the output waveguides. However, this technique is limited in the bandwidth of the excitation source due to the fixed dimensions of the rib waveguide. Also, the waveguides themselves introduce a level of uncertainty in the actual propagation behavior of the beam because of their fixed locations. Another experimental method is to place an active source region inside the waveguide layer of a planar heterostructure and excite the region by an
Figure 2.4: (a) Device configurations for input/output waveguide transmission measurement method. (b) Measured transmission spectrum for device in (a) [44]
Figure 2.5: (a,b) Experimental configuration for in-plane transmission measurements where the excitation source is located inside the waveguide layer. (c) Transmission spectrum using technique in (a,b) [45]
external source (Figure 2.5) [6, 45, 46]. The light generated by the source will be confined by the slab waveguide and interact with the PC structure, which is patterned in the waveguide layer. Then the transmission spectrum can be measured at the opposite end of the structure at a cleaved facet, giving information regarding the PBG of the structure. This technique is limited by the complicated growth process of the active layer and by the lack of directional control of the excitation; however, one advantage of this technique is that a large excitation frequency range can be probed. Both of the techniques presented above are limited in that they can only measure the guided photonic bands of the PC, *eg.* the bands that are below the light line, while the technique described below is capable of just the opposite.

### 2.3.4 Resonant band coupling technique

Just as eigenstates of a 2D-SWG-PC that are under the light line can only be measured using an excitation that is also confined by the SWG, PC modes above the light line can only be measured by an excitation outside of the guiding regime. This was confirmed in 1996 by Peng and Morris [72] and also in 1999 by Astratov *et al.* [3] when out-of-plane reflectivity measurements of two-dimensional gratings showed resonant anomalies in measured diffraction spectra. Peng and Morris concerned themselves only with a single resonant reflection peak from a square array of holes in a photoresist layer on a Si$_3$N$_4$ thin film, while Astratov *et al.* sought to directly probe the band structure of a triangular lattice of air holes patterned in a Al$_x$Ga$_{(1-x)}$As SWG. Astratov *et al.* coupled to the resonant bands of the SWG-PC using a collimated, broad-band excitation source incident from above the sample. Figure 2.6(a) shows the reflectivity spectrum with an inset showing the geometry of the experiment. The dips in the reflectivity signify coupling of the incident beam to the allowed bands of the PC structure that are above the light line and are plotted in Figure 2.6(b). Previous to their report, the same technique was employed in the study of shallow etched gratings [98] (for a review see [79]). However, since their work, the technique has been used in both reflection and transmission configurations to probe the dispersion surfaces of 1D PCs [2], 2D square lattice PCs [23, 106], and PC structures in different materials systems [17, 106]. In 2004, Coquillat *et al.* successfully applied the resonant coupling technique to
Figure 2.6: (a) Experimental setup and reflectivity spectrum of the resonant band coupling technique. (b) Band structure plot from data collected by (a) [3].
measure the dispersion contours (or ‘equifrequency surfaces’) of a GaN-based triangular lattice PC, thereby demonstrating the versatility of this technique [18]. Consequently, the resonant band coupling technique was applied to the structures fabricated in this work.
CHAPTER III

THE SUPERLATTICE PHOTONIC CRYSTAL STRUCTURE

In 2002, Park and Summers [66] presented a dynamically tunable PC structure that improved the magnitude of tunability of optical properties in 2D PCs through an interdigital biasing scheme of the triangular lattice as shown in Figure 3.1. This biasing scheme allows adjacent [1 0] rows of the triangular lattice to be biased individually such that an additional periodic modulation of refractive index is introduced in the lattice when biased in an alternating manner, as indicated by the different colors in Figure 3.1. As in crystallography [19], this type of long-range periodicity overlaid upon a shorter range periodicity creates a superlattice (SL), which modifies the optical response of a PC through symmetry reduction and other effects.

An interdigital biasing scheme is not the only method of creating a SL. In fact, finer control and a larger magnitude of the SL modulation can be accomplished by changing the hole diameters in adjacent rows as shown in Figure 3.2 [59, 55]. We label this structure the static superlattice (SSL) since the SL is ‘hardwired’ into the structure as opposed being dynamic like that of Park and Summers. This chapter will use the SSL configuration to investigate the general properties of SL PCs. These concepts are used in later chapters to characterize the optical properties of various SL configurations including the SSL and other tunable SLs. Naturally, this analysis can be extended to the structure originally proposed by Park and Summers.

3.1 Real space and reciprocal space representations

3.1.1 The triangular lattice

We begin our analysis by discussing the structural parameters of the triangular lattice [73] since it is underlying the SL structure in this work. Figures 3.3(a) and (b) show the real
Figure 3.1: Schematic of the interdigital biasing scheme that forms a superlattice by modulating the refractive index in adjacent [1 0] rows of a 2D triangular lattice PC.

Figure 3.2: Schematic of the static superlattice where a modulation in the hole radius between adjacent [1 0] rows of a 2D triangular lattice PC forms a SL.
space and reciprocal space representations of the triangular lattice, respectively, and the
defining parameters in each. In real space, cylindrical features (either rods or holes) with a
dielectric constant $\epsilon_c$ and a circular cross section of radius $r$ are arranged in a background
dielectric, $\epsilon_b$, at the vertices of an equilateral triangle whose sides are the lattice constant, $a$,
as indicated by the dashed triangle. In this work, these cylindrical features are referred to
as ‘holes’ since they are typically a lower index of refraction than the background. The two
basis vectors, $a_1$ and $a_2$ are separated by 60° and have endpoints at $(1,0)$ and $(1/2,\sqrt{3}/2)$,
respectively. From crystallography [19] or solid state physics [1], the reciprocal lattice
vectors of any real space structure are defined by the relationships:

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)}$$

$$b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot (a_2 \times a_3)}$$

$$b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot (a_2 \times a_3)}.$$  \hspace{.5cm} (3.1)

Since we are only concerned with 2D structure, eg. $a_3 = (0, 0, 1)$, these equations reduce to

$$b_1 = \frac{2\pi}{(a_{1,x}a_{2,y} + a_{1,y}a_{2,x})}(a_{2,y}, -a_{2,x})$$  \hspace{.5cm} (3.2)

$$b_2 = \frac{2\pi}{(a_{1,x}a_{2,y} + a_{1,y}a_{2,x})}(-a_{1,y}, a_{1,x}),$$  \hspace{.5cm} (3.3)

where $a_{j,x}$ and $a_{j,y}$ are the $x$ and $y$ coordinate of the $j = 1, 2$ point. Thus, from Equations
(3.2) and (3.3), the primitive reciprocal lattice vectors $b_1$ and $b_2$ are given by

$$b_1 = \frac{2\pi}{a}(1, -\frac{\sqrt{3}}{3})$$  \hspace{.5cm} (3.4)

$$b_2 = \frac{2\pi}{a}(0, \frac{2\sqrt{3}}{3}).$$  \hspace{.5cm} (3.5)

As shown in Figure 3.3(b), the reciprocal lattice is also triangular, as indicated by the
dashed triangle, and has a hexagonal first Brillouin zone (BZ) as indicated by the light-
shaded region enclosed in solid lines. The symmetry of the lattice allows all reciprocal space
points ($k$-points) to be represented by the points in the irreducible BZ which is indicated
by the darkly shaded right triangle. For convenience, the high symmetry directions of the
Figure 3.3: (a) Real space and (b) reciprocal space representations of the triangular lattice.
structure, which correspond to the sides of the irreducible BZ, are labeled in Figure 3.3(b) as Γ, M, and K. These high symmetry directions are also shown on the real lattice as a reference.

3.1.2 The static superlattice

Figure 3.4 presents the real space representation of the SSL-PC, defining the relevant quantities in the structure. As mentioned, the underlying structure is a triangular lattice of holes with lattice constant \( a \), as shown by the dotted triangle. However, one out of the three holes that form the triangle has a different radius than the other two such that \( r_2/r_1 \leq 1 \) and \( \Delta r = r_1 - r_2 \). Repeating this pattern of hole sizes creates two distinct adjacent rows of holes, \( i \) and \( j \), that consist of holes of a single radius, either \( r_1 \) or \( r_2 \), respectively. As shown, the \([i, j]\) rows introduce a long range periodicity into the lattice in the \( y \)-direction.

To incorporate this additional periodicity into the real space unit vectors, a lattice with a two-point basis is used so that the new basis vectors are

\[
\begin{align*}
\mathbf{a}_1 &= a(0, \sqrt{3}) \\
\mathbf{a}_2 &= a(1, 0).
\end{align*}
\]

These vectors define a rectangular unit cell, as shown by the dashed rectangle in Figure 3.4, where \( r_1 \) holes are at the corners of the rectangle, and an \( r_2 \) hole is located at the center.

As a consequence of the new unit cell definition, the reciprocal lattice also changes as defined by Equations (3.2) and (3.3):

\[
\begin{align*}
\mathbf{b}_1 &= \frac{2\pi}{a}(0, \frac{1}{\sqrt{3}}) \\
\mathbf{b}_2 &= \frac{2\pi}{a}(1, 0).
\end{align*}
\]

The new reciprocal lattice is also rectangular and is shown in Figure 3.5 where the light-shaded region is the first BZ, the dark-shaded region is the irreducible BZ, the new symmetry directions are indicated, and the open and closed circles represent reciprocal lattice points possessing different structure factors as discussed below.

The rectangular reciprocal lattice definition is valid only if there exists Bragg reflections at these points, which is true as long as the holes in rows \( i \) and \( j \) have different properties,
Figure 3.4: Schematic defining parameters in the real space representation of the static superlattice.
Figure 3.5: Reciprocal lattice representation of the SSL.
such as different $r$ or $\epsilon_c$. Validation of the new reciprocal space definition is confirmed by examining the \textit{geometrical structure factor}, $S_K$, as in solid-state physics [1]. For a polyatomic lattice with an $n$-atom basis, the structure factor is given by

$$S_K = \sum_{j=1}^{n} f_j(K)e^{iK \cdot d_j}, \quad (3.10)$$

where $K$ is a reciprocal lattice vector, $f_j$ is the form factor, and $d_j$ is the coordinate of the $j^{th}$ hole as shown in Figure 3.4. The SSL has two different radii, thus $n = 2$ and the form factors, $f_1$ and $f_2$ are dependent upon the radius of the hole, i.e. if $r_1 = r_2$ then $f_1 = f_2$. Since any reciprocal lattice vector can be written as a linear combination of $b_1$ and $b_2$, a general expression for $K$ is given by

$$K = n_1 b_1 + n_2 b_2, \quad (3.11)$$

where $n_1$ and $n_2$ are integers. Substituting Equation (3.11) into Equation (3.10) and using $d_1 = (0, 0)$ and $d_2 = (a/2)(1, \sqrt{3})$ gives

$$S_K = f_1(K)e^{i(n_1 b_1 + n_2 b_2) \cdot d_1} + f_2(K)e^{i(n_1 b_1 + n_2 b_2) \cdot d_2}
= f_1(K) + f_2(K)e^{i(\pi n_1 + \pi n_2)}
= f_1(K) + (-1)^{n_1 + n_2} f_2(K). \quad (3.12)$$

If $r_1 = r_2$, then $f_1 = f_2 = f$ and Equation (3.12) shows that

$$S_K = f(K) (1 + (-1)^{n_1 + n_2})
= \begin{cases} f(K), & \text{if } n_1 + n_2 \text{ odd}, \\ 0, & \text{if } n_1 + n_2 \text{ even.} \end{cases} \quad (3.13)$$

Thus, the structure factor vanishes for those reciprocal lattice points whose coordinates are an odd sum with respect to the primitive lattice vectors and are shown as the open circles in Figure 3.5. Since no Bragg reflection is associated with these points, the rectangular reciprocal lattice is converted into the triangular reciprocal lattice which is indicated by the dotted hexagons in Figure 3.4. Thus, if the holes in adjacent rows are indistinguishable, the two-atom basis rectangular lattice reduces to a single-atom basis triangular lattice, and the reciprocal space representation is consistent with the derivation in Section 3.1.1.
When the SL is present, it lowers the symmetry of the lattice from six-fold to two-fold because now both the unit cell and first BZ are rectangular rather than hexagonal. In addition to the first BZ being rectangular, the irreducible BZ of the SL is also rectangular and comprises 1/4 of the first BZ as indicated by the dark-shaded region in Figure 3.5. The letters at the apex points, $\Gamma$, $M$, $X$, $Y$, define the high symmetry points of the structure. Only four of the six original $M$ points remain equivalent to one another, while the other two $M$ points become equivalent to $\Gamma$ points of the SL. At the midpoint between these new $\Gamma$ points (along the $\Gamma - M$ of the triangular lattice) the symmetry point, $Y$, is introduced. This high symmetry direction defines the real space lattice direction that points along the long side of the rectangle, \textit{i.e.} along $a_1$. Only two of the six $\Gamma - K$ directions of the original lattice remain as high symmetry directions. These two directions are parallel to $b_2$ as shown in Figure 3.5, and they are the real space directions that point along the shortest side of the unit cell. However, notice that the $K$ symmetry points along these directions lie outside of the SL BZ. Thus, a new symmetry point, $X$, is defined in this direction located on the boundary of the 1st BZ. The final result is there are now two equivalent $Y$ and $X$ points and four equivalent $M$ points in the first BZ [70, 66, 69].

3.2 The Brillouin zone folding effect

The symmetry reduction is a direct result of the new primitive lattice vectors and the resulting reciprocal lattice vectors. Both introduce the BZ folding effect to the hexagonal BZ of the triangular lattice. In this effect, the $k$-points that lie outside of the 1st BZ of the SL, but within the hexagon of the triangular BZ they are translated into the SL first BZ by an integer multiple of $b_1$ or $b_2$ as defined by the Bloch theorem and the use of the reduce zone representation. Thus, these points are ‘folded’ back into the rectangular BZ, which is smaller and less circular than the hexagonal BZ of the triangular lattice.

The BZ folding effect results in unique band diagrams and dispersion contours, and it is best illustrated by examples of each from a triangular lattice on which we place an artificial SL (an infinitesimal $\Delta r$). The easier to visualize of the two are the dispersion contours, which are instrumental in predicting the refraction behavior of PCs.
Figure 3.6: Typical dispersion contour of the second band in a triangular lattice PC with the SL BZ superimposed and translated contours indicated by dashed lines.

Figure 3.7: SL dispersion contour resulting from BZ folding effect on the triangular lattice.
3.2.1 BZ folding in dispersion contours

Figure 3.6 shows the first BZ for the triangular lattice (solid hexagon) and the SL (dashed rectangle) superimposed on one another. Also in Figure 3.6, the psuedo-hexagonal shape (blue solid lines) represents a typical dispersion contour for the second band of a triangular lattice of air holes in a dielectric material. Since the SL BZ is smaller than the triangular lattice BZ, portions of the triangular dispersion contour lie within the rectangular SL BZ, while other portions lie outside of it. As a consequence of Bloch’s theorem (and the definition of the reduced zone scheme) [1], the \( k \)-points that lie outside of the first BZ are translated back into the BZ by an integer multiple of \( b_1 \) or \( b_2 \), as indicated by the downward arrow. Repeating this process for all \( k \)-points outside of the rectangle results in the portions of the SL dispersion contour shown by the dashed red lines in Figure 3.6. Because of the shape of the SL BZ in relation to the hexagon, the curves appear to ‘fold’ over the SL BZ boundary lines, as indicated by the curved arrows. Hence, we call this the band folding effect. In addition, there are portions of the psuedo-hexagon that fall inside of both the triangular and SL BZ’s, thus they do not need any translation. As a result, the full dispersion contour of the SL is a combination of the dashed red lines and solid blue lines inside of the rectangle, and is given in Figure 3.7. This example uses a fixed normalized frequency and the same structure, i.e. \( S_K = 0 \), thus the two contours should be indistinguishable when they are folded. This requires that the dashed lines and the solid lines in Figure 3.6 share common points on the boundary of the SL BZ (Y – M and M – X), as highlighted by the ellipses in Figure 3.7. However, when the SL is present, \( S_K \neq 0 \), this is no longer true, and the contour lines will separate along the BZ boundary lines, with their separation directly proportional to the SL strength as we will discuss in Section 3.3.

3.2.2 BZ folding in band structures

The band folding effect can also be seen in the band structures of the SL. Figure 3.8 shows the TE polarization band structure for a triangular lattice of air holes (\( r = 0.35a, \epsilon_c = 1.0 \)) in a dielectric material (\( \epsilon_b = 12.0 \)) while Figure 3.9 shows the band diagram with an infinitesimal \( \Delta r \). From Figure 3.6, the lattice directions of the triangular lattice affected
Figure 3.8: Band structure of a triangular lattice of air holes ($r = 0.35a$) in a background of silicon.

Figure 3.9: Band structure of a superlattice of air holes ($r = 0.35a$) in a background of silicon.
the most by BZ folding are the two \( \Gamma - M \) and the two \( \Gamma - K \) directions that are normal to the rectangular boundary.

Figure 3.10(a) presents two BZs of the triangular lattice (dashed-line hexagons) and three of the SL (bold-line rectangles). The Y point of the SL bisects the line connecting \( \Gamma_0 \) and \( \Gamma_1 \) (which is an M point of the triangular lattice), thus a vertical line is drawn at the Y point in the band structure of the triangular lattice in Figure 3.10(b) to represent this boundary. As explained in the previous section, the \( k \)-points outside of the rectangle are translated back into the rectangle to give the appearance of the bands folding across the Y line as indicated by the curved arrow in Figure 3.10(c), giving the SL band structure for the \( \Gamma - Y \) direction in Figure 3.10(d). Arriving at the resultant band shape can be thought of in another way: when traveling along on the \( \Gamma - M \) line from \( \Gamma_0 \) to M (eg. \( k \)-vectors increasing in length along \( \Gamma - M \)), the first band increases in frequency. In the BZ of the SL, we are traveling to the \( \Gamma_1 \) point after reaching the Y point, resulting in the second band to increase in frequency from Y to \( \Gamma \) as indicated by the arrows in Figure 3.10(d). If this procedure is repeated for the other bands of the triangular lattice for the \( \Gamma - M \) segment, the higher-order bands can be derived.

The same technique can be applied to the \( \Gamma - K \) section of the triangular lattice to derive the \( \Gamma - X \) section of the SL band structure, as illustrated in Figure 3.11. However, notice that the new symmetry point X does not bisect the \( \Gamma - K \) line as before, and continuing on this line towards the next \( \Gamma_2 \) point of the SL continues along a \( K - M \) line of the triangular lattice. Appropriately, we must consider the \( \Gamma - K \) and \( K - M \) portions of the triangular lattice that fold over the X point in Figure 3.11(b) to reconstruct the SL band structure which is shown in Figure 3.11(d).

As with the dispersion contours, the band structure analysis follows intuitively when the structure factor is zero, but when \( S_K \neq 0 \), the bands experience multiple crossings, anti-crossings, and splitting of degenerate states, all of which complicate the band structure greatly. The latter of these effects, the splitting of degenerate states, has many important consequences which will be described later in Section 4.4.
Figure 3.10: Folding scheme of the triangular band structure to the SSL band structure in the Γ – M direction.
Figure 3.11: Folding scheme of the triangular band structure to the SSL band structure in the $\Gamma - K$ direction.
3.3 Quantifying the superlattice strength

As shown in the previous sections, the SL effects are only observed when \( S_K \neq 0 \). A non-zero structure factor is only possible if \( f_1 \neq f_2 \), which states that the holes in rows \( i \) and \( j \) have different properties, such as a different radius or dielectric constant. The greater the difference between the structural properties of the holes, the stronger the SL effect on the optical properties of the PC. To quantify this difference the concept of the superlattice strength was introduced [59, 55]. Since all of the holes are the same size in the dynamic SL of Park and Summers [66], the SL strength in that structure is directly related to the difference in refractive index, \( \Delta n \), between the holes. On the other hand, the SL strength in the SSL is directly related to the difference between the hole sizes, \( \Delta r \). Thus to quantify the properties of the SSL and to compare it with the dynamic SL, an effective index approximation was developed as presented in the following section.

3.3.1 The effective index approximation

In the SSL, the strength of the SL modulation is controlled by \( \Delta r = r_1 - r_2 \) and is characterized by the radius ratio, \( r_2/r_1 \), which incorporates the relative sizes of the two holes. For the structures in this work, \( r_1 \) was held constant at 0.35\( a \) while \( r_2 \) ranged from 0.35\( a \) to 0.15\( a \). However, the majority of the results presented are from two SL strengths: \( r_2/r_1 = 0.30/0.35 = 0.857 \) and \( 0.20/0.35 = 0.571 \). Thus, as \( r_2/r_1 \) decreases, the SL strength increases. In the effective index approximation, the additional dielectric material appended to the structure as \( r_2 \) is decreased is averaged over the area or the volume of the original hole. This produces an \( \epsilon_c \) value for a \( r_2 \) hole which translates to an effective index, \( n_{\text{eff}} \). For a pure 2D structure, this involves averaging the dielectric constant of the area of material added over the entire area of a \( r_1 \) hole, while for a 3D structure, this involves averaging the volume of the added material over the volume of the entire hole. In the former, if we assume the additional material has the same dielectric constant as the background material, then \( n_{\text{eff}} \) of a row \( j \) hole is given by

\[
 n_{\text{eff}} = \left[ \frac{\epsilon_b A_\delta + \epsilon_c A_j}{A_i} \right]^{1/2} \quad (3.14)
\]
Figure 3.12: Schematic describing the effective index method used on the SSL.

Figure 3.13: Plot of effective index of refraction as a function of SL strength in the SSL.
\[ = \left[ \epsilon_b \frac{r_1^2 - r_2^2}{r_1^2} + \epsilon_c r_2^2 \right]^{1/2} \]  
\[ = \left[ \epsilon_b \left( 1 - \left( \frac{r_2}{r_1} \right)^2 \right) + \epsilon_c \left( \frac{r_2}{r_1} \right)^2 \right]^{1/2} \]  
(3.15)  
(3.16)

where \( \epsilon_c \) is the dielectric constant inside a hole, \( \epsilon_b \) is the background dielectric, and \( A_\delta \) is the change in area due to \( \Delta r \) as defined in Figure 3.12.

Equation (3.16) is plotted in Figure 3.13 assuming air holes \( (\epsilon_c = 1.0) \) in two different background media \( \epsilon_b = 12.0 \) and \( \epsilon_b = 6.0 \). Figure 3.13 clearly shows that the magnitude of the refractive index modulation between rows in the SSL is directly related to the difference between the hole sizes. For example, for air holes in a background material of \( \epsilon_b = 12 \), a change in \( r_2 \) of \( \Delta r = 0.05a \), i.e. a SL strength of 0.857, is equivalent to having a SL in which the holes have the same radius, \( r_1 \), but row \( j \) holes have \( \epsilon_c = 3.918 \). In terms of the dynamic SL, this is equivalent to a \( \Delta n = 0.979 \) between rows \( i \) and \( j \). For a SSL with a strength of 0.571, the index modulation increases to \( \Delta n = 1.90 \), clearly showing that the SL strength in a SSL configuration is unprecedented in comparison to the dynamic SL which is limited by the tunable \( \Delta n \) of the NL or EO material infiltrated into the holes [70, 88].

In actuality, the effective index method is an oversimplification of the actual physical changes of the SSL structure. However, it is included for comparison with the dynamic SL structure and for illustrative purposes. The main shortcoming of the effective index method is that it neglects the actual change in the dimensions of the air/dielectric interface for each hole. For this reason, the radius modulated SSL is unique in its impact on the optical properties of PCs. Thus, the effective index method was not employed in the calculations, but more appropriately, the hole radii were defined in the calculations to accurately model the SL structure.
CHAPTER IV

PHOTONIC BAND PROPERTIES OF THE STATIC SUPERLATTICE PC

In this chapter we present the analysis of the photonic band properties of the SSL structure through numerical studies. First, the effect of the SL strength on the band structure was analyzed for 2D and 2D-SWG PC structures. In both structure, many effects were observed when the SL strength is increased, such as the removal of modal degeneracies due to the reduction of the lattice symmetry. In this effect, several singular bands of the unmodulated SL split into two bands. We explain the origin of this effect through the visualization of the EM field profiles and their power distributions. Next, the dispersion surfaces of the 2D SSL are presented as three-dimensional surfaces and as contour plots, which are the convenient form of presentation for the analysis of beam propagation behavior in PCs. However, the beam propagation analysis is left for Chapter 6.

4.1 Numerical Methods

As mentioned in Chapter 2, two numerical methods were employed in this work to investigate the properties of SL PC structures. The first of these was the PWE method via a freely available software package called MPB (MIT Photonic Bands) [33]. This code has the capability of calculating structures in 1-, 2-, or 3-dimensional space, and it is a modified PWE algorithm that utilizes a preconditioned conjugate-gradient Rayleigh-quotient minimization method for the iterative eigensolver algorithm. At the beginning of the calculation, a user-defined control file is passed to the main program that defines the spatial geometry of the dielectric structure and the desired output parameters, such as field profiles, power densities, or the Poynting vector. The computational space can have an arbitrary coordinate system, but typically this is chosen to match the periodicity of the PC structure. The calculation then iterates until the change in solutions between iterations is below a
certain tolerance level, which is defined in the control file. The results are the frequencies (eigenvalues) of the EM modes (eigenstates) at a single value of $k$.

Many EM quantities can be calculated by MPB, such as the band structure, defect states, field profiles, and energy distributions. For a more exhaustive list, the reader is directed to the online-manual and tutorial maintained by the software developer [33].

The second numerical method was FDTD, for which two codes were used. The first was a heavily modified version of Andrew Ward’s Order-N code called ONYX [96]. Just as in MPB, the ONYX code can work in any arbitrary coordinate system. This is ideal for systems in which it is convenient to define a non-orthogonal basis such as the triangular lattice. The code contains Bloch and metallic boundary conditions, the former allows the simulation of infinite structures. However, for our purposes, the code was modified to include a Berenger-type perfectly matched layer (PML) as an absorbing boundary condition [9, 111] and a mirror boundary condition, both of which were necessary to accurately simulate a slab waveguide structure, which are infinite in the 2D plane, but finite in height. Also, the subroutine which defined the dielectric function was modified to suit our needs. ONYX was used for band structure calculations, while the second FDTD code was used for visualizing beam propagation in the SSL PC. This second FDTD code is described in Chapter 6, where it is implemented for EM field propagation calculations. Since MPB and F2P are available on the Web, only the ONYX code is provided in the Appendix. However, example input files that were used in all three codes are presented in the Appendices.

4.2 Photonic bands of the pure 2D SSL

For the 2D SSL, calculations were performed using the PWE method for air holes in a high dielectric constant material ($\epsilon_b = 12.0$) such as silicon or gallium arsenide. The radius of row $i$ holes were held constant at either 0.4$a$, 0.35$a$, or 0.3$a$ while $r_2$ was decreased from $r_1$ to 0.15$a$, resulting in a variety of SL strengths in the calculations. The calculation results for the first eight bands in TE and TM polarization are presented in Figures 4.1 and 4.2, respectively. The three plots, (a), (b), and (c), in each figure show the band structures for three different SL strengths when $r_1$ held constant at 0.35$a$: (a) $r_2/r_1=1.0$, (b) $r_2/r_1=0.857$, ...
Figure 4.1: Photonic band diagrams for TE polarization in 2D SSL structures \((r_1 = 0.35a)\) calculated using the PWE method for (a) \(r_2/r_1=1.0\), (b) 0.857, and (c) 0.571.
Figure 4.2: Photonic band diagrams for TM polarization in 2D SSL structures ($r_1 = 0.35a$) calculated using the PWE method for (a) $r_2/r_1=1.0$, (b) 0.857, and (c) 0.571.
and (c) $r_2/r_1=0.571$. As expected, for $r_2/r_1 = 1$, the band structures were identical to the conventionally defined triangular lattice after accounting for the BZ folding effect. However, increasing the SL strength greatly influenced the band structures and several effects were observed.

One of the most pronounced effects is the rapid decrease in the width of the full PBG for TE polarization as the SL strength increases. This effect is indicated by the shaded boxes in Figure 4.1. The origin of this effect is the decrease in the air filling fraction of the structure as $r_2$ decreases, pushing the air bands to lower frequencies, whereas the effect is much smaller for the dielectric band. The effect of lowering the air band frequencies is also seen in the TM case, however there is not a closing of a PBG for TM polarization because a full PBG does not exist for $r_1 = r_2 = 0.35a$. The decrease in the full PBG in TE polarization as the SL strength is increased is summarized in Figure 4.3 for different initial values of $r_1 0.4a, 0.35a$, and $0.3a$. For example, for a SL strength of $r_2/r_1 = 0.857$, the full PBG reduces in width by 31.5%. This increases to a reduction of 77.9% when the SL strength increases to 0.571. In addition, the band separation at the M point more than doubles in magnitude when the SL strength is increased from 0.857 to 0.571.

The second observation was that certain bands split into two different bands at many places in the BZ. This occurs for both polarizations and is especially evident at the M point for the third lowest band in the unmodulated SL (Figure 4.5(a)). The area of interest is highlighted by the dashed ellipses in the TE polarization band structures in Figure 4.5, and the split bands are labeled $3s$ and $3p$. For a SL strength of unity, the two modes are degenerate at the M point as shown by the two bands that come together at the M point along the $\Gamma - M$ direction. However, as the SL strength increases, the degeneracy is removed and the bands separate into the $3s$ and $3p$ bands which have different frequencies. In addition, the magnitude of the separation between the two states is directly proportional to the SL strength. An explanation of the band splitting behavior can be found in the EM field patterns and EM energy densities (Section 4.4), both of which show that the lifting of the degeneracy at the M point is caused by mode reshaping and EM energy redistribution.
Figure 4.3: Plot showing the effect of the SL strength on the width of the full PBG for $r_1$ values of 0.3, 0.35, and 0.4$a$. 
Figure 4.4: Dependence of the frequency gap between the 3s and 3p bands at the M point upon SL strength for $r_1$ values of 0.3, 0.35, and 0.4a.
Figure 4.5: TE polarization band structures for three SL strengths (a) 1.0, (b) 0.857, and (c) 0.571, showing the band splitting effect introduced by the SL modulation, $r_1 = 0.35a$. 

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4.3 Photonic bands of the 2D slab waveguide SSL

In the slab waveguide PC configuration, the PC structure is patterned in a high dielectric material that has a finite height, \( h \), as shown in Figure 4.6. The structures investigated in this section were air-bridge SWG structures (dielectric slabs surrounded by an air cladding) with \( h = 0.5a \), \( \epsilon_b = 12.0 \), and \( \epsilon_c = 1.0 \). Both FDTD and PWE calculations were performed on the structures; however, only the FDTD calculations were accurate for all solutions since the PWE solutions only fully describe modes within the guiding regime of the SWG, i.e. under the light line [30].

Since the PWE method always employs periodic boundary conditions (BCs) on all sides of the computational domain, a computational supercell (Figure 4.6) was required to correctly model the finite height of the SWG. As a consequence, the periodic BCs create a system of infinitely extended dielectric planes stacked parallel to one another and separated by air. In SWG PCs, light can couple into extended states out of the plane of the PC because of the guiding condition of the SWG which is dictated by the cladding material and indicated in the band structures by the light line [30]. Unguided modes (those that are above the light line) can radiate into the air regions in between the slabs and possibly couple and interact with the modes from a neighboring slab. Thus, a critical parameter in supercell calculations is the amount of space between the SWGs, which must be large enough to minimize the interaction of radiated modes between slabs. A conservative value of \( 4a \) was used for the supercell height in this work. Regions of the dielectric function in Figure 4.6 appear blurred because of the 1) the volumetric rendering of the graphics software, and 2) because of the smoothing of the dielectric function at materials interfaces which provides stability and accuracy to the calculations. Large, abrupt changes in the dielectric constant will lead to discontinuities in the calculations. An iso-value skin is also shown in Figure 4.6 to aid in the visualization of the structure. Inside of the skin, \( \epsilon_b \geq 10.0 \), showing that only a small portion of the structure has \( \epsilon_b < 10 \).

In comparison to the PWE calculations, the FDTD computational cell has a perfectly-matched layer (PML) absorbing BC on one end of the cell (Figure 4.7). Thus the unguided modes radiate into the air space above the SWG and are absorbed by the PML, providing
Figure 4.6: Three-dimensional plot of the dielectric function used in the PWE calculations showing the supercell height, $4a$, and the slab waveguide thickness, $h = 0.5a$. 
accurate solutions for both above and below the light line. Opposite the PML, bisecting the slab, is a mirror BC which was used to reduce the computational domain by one-half, thereby decreasing the computational time by 50%. A mirror BC can be used in the calculations by assuming that the modes of the SWG PC have either even (TE-like) or odd (TM-like) symmetry through the center of the slab. This holds true if the slab is sandwiched between identical materials, as in the air-bridge structure. Figure 4.7 shows the typical values used for the dimensions of the FDTD domain. Note the dielectric slab thickness is 0.25a in the computational domain. Due to the mirror BC, this is equivalent to the slab thickness in the MPB supercell calculation, $h = 0.5a$.

Figure 4.8 is the band diagram for a silicon ($\epsilon_b = 12.0$) SSL SWG PC ($h = 0.5a$) with a SL strength of $r_2/r_1 = 0.3a/0.35a = 0.857$ as calculated by the PWE (solid lines) and FDTD (scattered points) methods for even modes. The shaded region represents the extended states above the light line that are not guided in the SWG. Agreement between the results from the two different calculation methods was obtained for bands under the light line for reasons explained earlier; however, outside of the light line, only the FDTD method is accurate.

As in the 2D SSL, the influence of the SL strength on the photonic band properties manifests itself in a reduced PBG and the splitting of degenerate bands as shown in Figure 4.9 which plots the band structures for three SL strengths in a silicon SSL SWG: (a) 1.0, (b) 0.857, and (c) 0.571. (Note, a full PBG is not possible because the light line allows extended states over many regions in the BZ.) The PBG is indicated by the shaded regions, the band splitting is highlighted by the ellipses, and the 3s and 3p bands are labeled as in the band structure plots in the previous section. Again, the width of the PBG and the magnitude of the band separation at the M point were calculated when $r_1$ was held constant at 0.4a, 0.35a, or 0.3a. These results are plotted in Figure 4.10(a) and (b), respectively, where second degree polynomials (solid lines) were fitted to the raw data (scattered points) from the band structure calculations. As shown, the PBG decreases by 28.3% when the SL strength was increased from 1.0 to 0.857 and by 75% for an increase from 1.0 to 0.571 when $r_1 = 0.35a$. As in the 2D SSL, the magnitude of the band separation at the M point more
Figure 4.7: Plot of the computational domain used in FDTD calculations when mirror symmetry through the slab waveguide is assumed.
Figure 4.8: Photonic band structures of the even modes as calculated by the FDTD (scattered points) and PWE (solid lines) methods for a silicon ($\epsilon_b = 12.0$) SSL SWG PC ($h = 0.5a$) with a SL strength of 0.857, $r_1 = 0.35a$. The shaded region represents the extended states above the light line that are not guided in the SWG.
Figure 4.9: Band structures for three SL strengths (a) 1.0, (b) 0.857, and (c) 0.571 as calculated using the FDTD method, $r_1 = 0.35a$, $\epsilon_b = 12.0$, $h = 0.5a$. 
Figure 4.10: Graphs showing the influence of the SL strength on (a) the PBG width and (b) the band separation at the M point in a SSL SWG where $r_1$ was held at 0.3$a$, 0.35$a$, or 0.4$a$ while $r_2$ was decreased to 0.15$a$. The data (scattered points) was fitted with second degree polynomials (solid lines) to show their trends.
than doubles when the SL strength is increased from 0.857 to 0.571.

Our calculations confirm that the SL effects predicted for the band structures of the 2D SSL are also manifested in the 2D SWG configuration. The impact of this corroboration is invaluable because the 2D SWG PC is more amendable to planar photonic devices and circuits than the pure 2D PC. Thus, it is important to show that the influence of the guiding condition does not remove the unique optical phenomena associated with the SL structure. In addition, this confirmation affirms the value of our 2D analysis of the SSL structure to the implementation of optical devices.

4.4 The splitting of degenerate states

As shown in Figure 4.1 by the areas highlighted by dashed ellipses, the M point is one of the symmetry points where pronounced band splitting occurs. To investigate and identify the cause of this phenomenon, the TE field patterns and time-averaged energy densities were calculated at the M point using the PWE method for SL strengths of 1.0, 0.857, and 0.571. The $H_z$ component of the TE field was used to visualize the fields and their energy density distributions because $H_z$ is normal to the 2D plane of the PC structure in TE polarization, which has field components $E_x$, $E_y$, and $H_z$. Figure 4.11 presents the results of the calculations for a SL strength of 1.0. The air holes are outlined by circles, and rows $i$ and $j$ are labeled appropriately, according to the SL definition. For the field profiles (Figures 4.11(a)-(c)), regions of positive or negative field amplitude are labeled and shaded, while the zero crossings (nodes) are indicated by white values. In the energy density plots (Figures 4.11(d)-(f)), regions of higher energy are indicated by white, while the darker areas are regions of lower energy.

Figures 4.11(a) and (d) are the field profile and energy density, respectively, of the second band of the triangular lattice when a triangular unit cell was used for the calculation. As expected, a harmonic field pattern is formed that has phase fronts normal to the $\Gamma$ – M direction. The field has nodes in the air holes, with the field amplitude modulating between positive and negative values along a single row $i$ or $j$, as indicated in Figures 4.11(a-c). The energy density plot (Figure 4.11(d)) shows that the fields are more concentrated in
Figure 4.11: Field profiles (a-c) and time-averaged magnetic-field energy density (d-f) of the $H_z$ field component for the second TE band of the triangular lattice, $r = 0.35a$, $\varepsilon_b = 12.0$. 
the dielectric region surrounding each hole, with 95.9% of the H-field power and 68.2% of the D-field power of band 2. In Figures 4.11(b-c) and (e-f), the rectangular unit cell of the SL is used in the calculations, rather than the triangular unit cell. These fields result from the bands numbered ‘band 3’ and ‘band 4’ in the output of the program. In both bands, field nodes are located in the air holes horizontally and vertically. Band 3 has horizontal nodes along row i and vertical nodes in row j, and band 4 has the opposite scenario. Additionally, the field modulates along row j in band 3 and along row i in band 4, rather than in both rows simultaneously, as in the second band of triangular lattice.

The relationship of the field patterns in Figures 4.11(b-c) to that of the triangular lattice is clearly seen by summing the fields together. The result of this sum is the field pattern in Figure 4.11(a), and this is also true for the energy densities. The modes in Figures 4.11(d), (e), and (f) have the same fraction of energy density (95.93%, 95.96%, and 95.93%, respectively) concentrated in the dielectric regions of the structure. This is clear evidence that band 3 and band 4 (Figures 4.11(b-c) and (e-f)) are degenerate modes of the triangular lattice that are indistinguishable under translational symmetry. However, this degeneracy changes when the SL strength increases, as we show below.

When the SL strength increases, the symmetry of the triangular lattice is broken, and the EM energy redistributes itself according to the electromagnetic variation principle [27] which states that higher energy radiation will concentrate its energy in the higher dielectric regions. Figures 4.12 and 4.13 show the effect of the SL on the field profiles and energy densities for SL strengths of 0.857 and 0.571, respectively. The columns in Figures 4.12 and 4.13 represent consecutive bands that are output from the calculations as ‘band 3’ and ‘band 4’. In a previous section, we introduced the nomenclature 3s and 3p, to describe these split bands at the M-point (Figure 4.1). The rational behind this designation was due to the shapes of the energy density profiles in each band, which we borrowed from the designation of orbital shapes as in solid-state physics. As \( r_2 \) decreases, the dielectric area surrounding holes in rows i and j increases, thereby influencing the shape of the modes and their energies. In row j, the holes are decreasing in size, thus the area between adjacent holes becomes wider, allowing the mode to concentrate its energy more in between the holes.
Therefore, the energy distribution becomes more rectangular (or ellipical) in shape than in the triangular lattice as shown in Figures 4.12(c) and 4.13(c). Thus, we observe from the energy density shape and the band structure that the mode centered in row $j$ becomes lower in energy and more circular, just as a $s$-orbital is circular and has lower energy. On the other hand, the area between row $i$ holes does not change with the increase in SL strength, but rather, the area adjacent to the holes above and below the row increases. This pulls energy away from the space between the row $i$ holes, resulting in a mode that assumes a bow-tie shape as the SL strength increases (Figures 4.12(d) and 4.13(d)). This behavior of the mode centered in row $i$ resembles a $p$-orbital, which is higher in energy and bowtie in shape. Thus, in our notation the numeral indicates the band number and the letter indicates the mode field shape.

The change in the EM energy density was calculated for the $D$-field and the $H$-field as a function of the SL strength for a constant $r_1 = 0.35a$. The results are presented in Figure 4.14 for the fractional magnetic-field and electric-field energy densities in the dielectric (solid lines) and the air regions (dashed lines) of the 3$s$ and 3$p$ bands. As observed in the energy density plots, the 3$s$ band contains a greater power density of both the $H$- and $D$-fields in the dielectric regions than the 3$p$ band. Additionally, as the SL strength increases, the fraction of energy in the dielectric region increases in all four cases. This too was expected since the amount of dielectric region for the fields to concentrate in is increasing with increasing SL strength. The increasing SL strength does more than shift the EM energy in the structure, it also affects the shape of the dispersion surface, as we discuss in the following section.

4.5 Dispersion contours of the superlattice

The photonic band structure plots the dispersion relation only along the boundaries of the BZ. However, the dispersion relation for a 2D PC is a three dimensional surface in $k$-space, called the dispersion surface, where the $k$-vector components $k_x$ and $k_y$ are in the base plane and the normalized frequency, $\omega_n$ is the vertical axis. To completely understand the optical properties of a PC structure beyond the PBG, analysis of the dispersion surface is essential. While these surfaces can be visualized as three dimensional plots, it is convenient
Figure 4.12: Field profiles (a-b) and time-averaged magnetic-field energy density (c-d) of the $H_z$ field component for the $3s$ and $3p$ TE bands of the SSL with a strength of 0.857, $r_1 = 0.35a$, $\epsilon_b = 12.0$. 
Figure 4.13: Field profiles (a-b) and time-averaged magnetic-field energy density (c-d) of the $H_z$ field component for the 3s and 3p TE bands of the SSL with a strength of 0.571, $r_1 = 0.35a$, $\epsilon_b = 12.0$. 
Figure 4.14: Time-averaged magnetic-field (a-b) and electric-field (c-d) energy density in the air (dashed line) and the dielectric (solid line) regions of the 2D SSL as a function of SL strength for the 3s and 3p bands, $r_1 = 0.35a$, $\epsilon_b = 12.0$. 
and instructive to plot them in surface relief as contour maps. From the contour maps, the prediction of bulk propagation optical properties of a PC structure is made possible through wavevector analysis. We rely upon wavevector analysis heavily in Chapter 6, therefore this section is dedicated to the description of the dispersion surface in the 2D SSL PC structure and the effects of the SL strength on its properties as a foundation for later chapters.

4.5.1 Numerical method

The PWE method was used exclusively for the calculation of the dispersion surfaces of the 2D SSL structures. A major advantage of the PWE method over the FDTD method is that the solutions are automatically categorized according to band number, and there are virtually no spurious points in the solutions. In the FDTD method, the fields at a single $k$-point are stored in memory in the time-domain, then a Fourier transform (FT) is performed on the data. The peaks in the FT spectrum give the frequencies of the allowed bands at that particular $k$-point. Thus, the band structure is susceptible to erroneous points given by a poor filter or windowing function during the spectral analysis. On the other hand, the PWE method solves for the eigenstates of an eigenvalue equation. Thus, each data set output from the calculation is categorized according to its order from the first band. An array of these data sets are easily converted into matrices, which can be readily analyzed graphically and numerically. Thus, the irreducible portion of the BZ (1/4 of the first BZ that describes the entire BZ) of the SL was divided into a $k$-point mesh of $150 \times 150$ points, and the frequencies of the first four bands were calculated at each mesh point.

4.5.2 Calculated dispersion surfaces

Figures 4.15(a) and (b) show the dispersion surfaces of the triangular lattice and the SSL with a strength of 0.857, respectively, in the irreducible BZ of the respective structures. The dispersion surface of the triangular lattice is relatively straightforward with an inverted conical plane below the PBG that represents the dielectric band, and more complicated surfaces above the PBG representing the air bands. In contrast, in the SL, there are two surfaces below the PBG. The lower surface is the dielectric band as in the triangular lattice, but the upper band is a folded band as described earlier in Section 3.2.2. In addition, just
Figure 4.15: Dispersion surface plots of (a) the first three bands of the triangular lattice $r = 0.35a$ and (b) the first four bands of the SSL, strength of 0.857.
above the PBG, the surface representing the second band of the triangular lattice splits into two surfaces in the SL, the 3s and 3p bands, as described earlier. These two dispersion surfaces show dramatically different refraction behavior than the triangular lattice.

As mentioned previously, a convenient form of representing the dispersion surface is a contour map. In Figure 4.15, the intersection of a constant frequency plane with the dispersion surface produces a complex curve that represents the dispersion contour at that fixed frequency. Figure 4.16 presents the dispersion contours of the first four bands in the entire first BZ of a SSL of air holes in a dielectric background of $\epsilon = 12.0$, a SL strength of 0.857, and $r_1 = 0.35a$. The contours involve more complicated shapes than those of the triangular lattice, except for the first band, which is expected to be an inverted cone, radiating from the Γ point. For the second band, the contours radiate from the Y point while the contours generally radiate from the M point for the 3s and 3p bands. The dispersion surfaces of bands 3s and 3p lie close to one another in frequency range; and for a range of frequencies, a single equifrequency plane will intersect both of these surfaces, creating a complicated optical response.

4.5.3 The contour repulsion effect

In Section 3.2, we illustrated how the triangular lattice dispersion contours are affected by BZ folding. For an infinitesimal modulation in the hole radii between rows $i$ and $j$, the SL dispersion contours can be derived by simply ‘folding’ the contours of the triangular lattice over the SL BZ boundaries. However, when the SL strength increases, folding the contours in this manner does not give the correct shapes for the dispersion contours because the degenerate states of the triangular lattice are separated into the 3s and 3p states which experience different geometries and areas of the dielectric material that supports mode formation. This results in the contours to have quite different shapes.

Figures 4.17(a) and (b) show the change in the dispersion contours as $r_2$ is gradually decreased from 0.35$a$ to 0.33$a$, commensurate with increasing the SL strength from 1.0 to 0.943. In Figure 4.17(a), the contours are a combination of 3s and 3p contours at a single fixed normalized frequency of $\omega_n=0.3445$, while the contours in Figure 4.17(b) are from
Figure 4.16: Contour maps of the dispersion surface in the first Brillouin zone for the first four bands of a SSL PC structure with SL strength of 0.857, $r_1 = 0.35a$, $\epsilon_b = 12.0$. (a) Band 1, (b) band 2, (c) band 3s, and (d) band 3p.
three different frequencies ($\omega_n = 0.345, 0.3415,$ and $0.3317$ as the SL strength increases) so that their shapes align. In Section 3.2.1 we emphasized that the curves must connect at the BZ boundaries in the unmodulated SL at the points labeled A and B. However, as the SL strength increases, the bands are split, and the curves appear to ‘repel’ one another, changing their curvature dramatically in a localized region near the BZ boundary. As the SL strength increases, the strength of the repulsion also increases, eventually affecting the curvature of the entire contour.

In Figure 4.17(a), the contours are plotted at the same normalized frequency, and since the bands are lowered in frequency due to the increasing SL strength, the contours are shifted, relative to the base triangular lattice (solid lines). On the other hand in Figure 4.17(b), the frequency was adjusted for each SL strength so that the curves overlap one another as closely as possible. This was done to directly compare and visualize the changes in contour shapes as the SL strength was increased. Clearly, the curvature of the contour labeled ‘C’ in Figure 4.17(b) was most affected by the SL strength since this curve crosses the BZ boundary at two places, the Y – M and M – X boundaries. Thus, both ends of the curve are affected by the ‘repulsion’ effect, greatly changing the curve shape.

The curve repulsion effect is a result of two mechanisms. Firstly, the Bloch condition requires that the contours are continuous and smooth across the BZ boundaries. Thus, for waves traveling in any periodic crystal, the dispersion contours must intersect the BZ boundary at a 90° angle. This effect is equivalent to the Fermi surface in electronic crystals bulging out to make contact with the faces of the BZ when the surface lies near the zone edges (Figure 4.18) [1]. In the unmodulated SL PC (solid line in 4.17(a)), the contours are permitted to cross the BZ boundaries of the SL (the Y – M and M – X lines) at an angle other than 90° because they are not the true BZ boundaries for the structure, since the primitive lattice is triangular. Hence, the BZ is a hexagon (Figure 3.3) and different lines from Y – M and M – X define the boundaries. However, when the SL is present ($S_K \neq 0$), the rectangular BZ representation is correct. Thus, the contours must obey the Bloch condition, resulting in strong, localized modifications of the contours near the BZ boundaries such that the curves are bent to intersect the Y – M and M – X lines at 90°
Figure 4.17: Effect of superlattice strength on the dispersion contours relative to the base triangular lattice. (a) Change in contour shape at a constant frequency $\omega_n = 0.3445$ for different SL strengths. (b) Change in contour shape using a variable frequency to fix the position of the contours.
Figure 4.18: Illustration of the free electron sphere bulging out to touch the BZ faces in the $(111)$ directions [1].
(dashed and dotted lines in Figure 4.17(a)). Thus, the contours that were once “joined” along the $Y-M$ and $M-X$ lines now appear to repel one another. Additionally, the repulsion effect appears to increase in magnitude as the SL strength increases (Figure 4.17(b)). This was attributed to the increasing frequency gap between the $3s$ and $3p$ bands as the SL strength increases (Figures 4.1 and 4.4). The contour repulsion effect dramatically modifies the curvatures of the dispersion contours making it a powerful tool for creating a desired optical response to suit a specific application.

4.5.4 Dispersion contour families

Figure 4.19 shows a family of dispersion contours of the $3s$ and $3p$ bands for three SL strengths (1.0, 0.857, and 0.571) as indicated next to each row. The contours are labeled with the normalized frequencies and the gray scale shifts from dark to light with increasing frequency. Several changes are observed in both bands and are described in this section.

In the unmodulated SL, the band $3s$ contours along the $Y-M$ and $M-X$ lines curve toward the M point, but they change their curvature away from the M point when the SL is present. This is exemplified greatest by the contours in the upper right corner of the BZ, near the M point, because these curves cross the BZ boundary twice, as discussed earlier. For example, when the SL strength increases, the contour labeled 0.335 in Figure 4.19(a) changes from a lobe shape to a corner shape as shown by the contour labeled 0.301 in Figure 4.19(c). This effect is the opposite for the contours of band $3p$ which are modified to curve toward the M point as the SL strength increases. As shown in Figure 4.19(b) at $\omega_n=0.345$, the curvature of the contour in the upper right corner of the BZ is relatively flat around the $\Gamma-M$ line when the SL strength is 1.0. However, as the SL strength increases, the contours are modified and now have some curvature across the $\Gamma-M$ line (see Figure 4.19(d) at $\omega_n = 0.324$). These effects in the $3s$ and $3p$ bands introduce interesting refraction behavior into the SL, which will be discussed in Chapter 6. Another way to visualize the dispersion contours of the SSL is by plotting them as a function of frequency rather than band number.

Figure 4.20(a-f) shows the same family of dispersion contours as in Figure 4.19, but plotted at single frequencies, as indicated in the upper left corner of each plot, rather than
Figure 4.19: Family of dispersion contours of the 3s and 3p bands of a SSL of air holes in a $\epsilon = 12.0$ background with increasing SL strength of 1.0, 0.857, and 0.571 (top to bottom), $r_1 = 0.35a$. 

(a) SSL 1.0
(b) Band 3p
(c) SSL 0.857
(d) Band 3p
(e) SSL 0.571
(f) Band 3p
by individual bands. To distinguish contours originating from each band, the $3s$ contours are represented by solid lines, while the $3p$ are dash-dotted lines. In the unmodulated SL (Figure 4.20(a-b)), the $3s$ and $3p$ bands are not split, thus they intersect along the $Y-M$ and $M-X$ lines as described earlier. The relationship of the $3s$ and $3p$ band contours are shown in the remaining four plots as the SL strength increases (middle and bottom rows), and as the frequency increases (left and right columns).

Since the $3s$ and $3p$ bands separate when the SL strength increases, these surfaces can occupy different frequency ranges (whereas these bands in the unmodulated SL occupy the same frequency range because they are essentially one band). For a certain range of frequencies, dependent upon the SL strength, an equifrequency plane will intersect only the $3s$ band. Figures 4.21(a) and (b) plot these $3s$ contours for SSL strengths of 0.857 and 0.571 in the frequency ranges of 0.287–0.312 and 0.230–0.271, respectively.
Figure 4.20: (Left column): Family of dispersion contours showing curves from the third and fourth bands simultaneously at the same frequency. (Right column): Dispersion contours that have only contributions from the third band at a single frequency.
Figure 4.21: Plots of the frequency ranges which only have dispersion contours from the 3s band in a SSL of strength (a) 0.875 and (b) 0.571, $r_1 = 0.35a, \epsilon_6 = 12.0$. 
CHAPTER V

EXPERIMENTAL INVESTIGATION OF PHOTONIC BAND PROPERTIES OF THE SSL

The photonic band properties of the SSL structure were investigated by fabricating 2D SWG PCs in silicon using electron-beam lithography (EBL). This section briefly outlines the fabrication technique (the details of which can be found in Reference [106]), the structural characteristics of the samples, as measured by scanning electron microscopy, and their photonic band properties, as determined by the coupled resonant band technique described in Section 2.3.4.

5.1 Fabrication method

For 2D PC structures operating in the VIS–NIR wavelength region, EBL is an ideal fabrication method since the feature sizes are on the order of tens to hundreds of nanometers. However, this remains true only if the PC area is on the order of millimeters or less since EBL facilities typically charge a fee per hour of writing time. Thus, fabricating larger area PCs using EBL would not be cost effective, and an alternative would be holographic methods. However, the structures investigated in this work are ~1 mm square, thus fabrication by EBL is feasible. In addition, patterning the different hole diameters is accomplished with great ease through the superior control and precision of EBL, which can pattern virtually any 2D shape or combination of shapes. This flexibility is attributed to the operating principles of an EBL system, which is essentially a modified SEM.

Basically, an EBL system uses an electron beam (e-beam) to write patterns in a thin layer of polymer resist that coats the sample surface, just as an air brush is used to draw patterns on a canvas. The e-beam spot diameter can be controlled to create fine or large features, while the position of the e-beam is controlled using magnets in the gun column, or by controlling the position of the sample stage. In addition, the beam current and dwell...
time at a particular area on the sample controls the size of the features drawn. For example, a larger beam current or dwell time increases the electron dosage to the sample, thereby increasing the interaction between electrons and the resist, which increases the size of the features drawn as the electrons ‘bleed’ into adjacent areas. This is not a desirable effect for small, fine features; however, it is useful for smoothing rough edges of the shapes drawn. For example, the EBL system does not draw filled arcs or filled circles, but rather, it draws multiple filled polygons in close proximity to create an arc. Using the appropriate beam dosage blends the edges of the polygons, forming a smooth arc.

Photonic crystal patterns were fabricated in single crystal silicon on insulator (SoI) wafers purchased from Silicon Genesis Corporation. The wafers consisted of a 297.9–300.1 nm thick single crystal Si layer bonded onto a 1.000 ± 0.005 \( \mu m \) thick SiO\(_2\) bottom oxide (BOX) layer on a Si substrate. The PC patterns are first rendered in AutoCAD 2004 using the ‘DONUT’ command with an inside radius of zero and an outside radius equal to the desired hole radius. Figure 5.1 presents an example of a CAD design of the twelve patterns designed for these experiments. The different colors indicate different layers in the drawing, which were used to control electron beam dosages to the sample. The measurements are in units of microns, and the hole diameters given are the actual radius values of the holes. The CAD files are saved in DXF format, which was then transformed into the GDSII format by a program called LinkCAD. The GDSII file can then be converted into a pattern file by the EBL system.

A JEOL JBX-9300FS EBL system, which is capable of a spot size of 4 nm to 200 nm and an addressing resolution of 1 nm, was used to write the SL PC patterns into a polymer resist layer (ZEP-520A supplied by Zeon Chemicals) by chain scission. In this process, the focused electron beam interacts with the polymer chains, breaking the linkage which then allows the unlinked polymer to dissolve in a developer solution. Because the areas of the polymer that were exposed to the electrons were washed away, ZEP-520A is a ‘positive’ resist. Due to the limited field size and available memory of the EBL system, large areas must be patterned using either a lower magnification, which reduces resolution, or by repeating a smaller area in an array, which requires longer writing times. The latter
Figure 5.1: Detailed view of a SSL PC CAD design used as the input writing pattern for the JOEL EBL system. Measurements are in microns and the indicated hole dimensions are the radii.
method was chosen because of the required precision in the feature sizes, and the resulting patterned areas were approximately 1 mm × 1 mm in size.

After developing the pattern in the resist, they were transferred to the silicon layer by inductively coupled plasma (ICP) dry etching using a Plasma-Therm Dual ICP. A chlorine/C4F6 recipe [106] was used that maintained a vertical sidewall profile through the thickness of the Si layer. After etching, the remaining resist was removed using a heated oxygen plasma in a Gasonics Aura 1000 Asher stripper.

Two pattern sets were designed, one with a lattice constant of $a = 358$ nm and the other with $a = 480$ nm. Because of the file size limitations of the EBL system, the patterns were limited to an area of $58 \mu m \times 62 \mu m$ and $36 \mu m \times 118 \mu m$, respectively. Hence, each set was labeled x58y62-N and x36y118-N, respectively where $N$ is the sample number. The design parameters are summarized in Table 5.1 which gives $r_1$, $r_2$, $a$, the filling fraction $f$ (the ratio of the exposed to unexposed regions), the target radii, and the target SL strength. The target radii are the actual hole sizes desired after taking into consideration that a beam overdose would be used to smooth the edges of the holes. The planned increase in hole size was 15% and 25%. The final patterned areas were $986 \mu m \times 992 \mu m$ and $972 \mu m \times 944 \mu m$ for the x58y62-N and x36y118-N sets, respectively. As a precaution to preserve hole size uniformity across the sample, a 50 $\mu m$ thick frame was used around the perimeter of the PC writing area. Within this region, a smaller beam dosage was used to balance the charge dissipation at the edge of the patterned area, which can lead to smaller hole sizes if left unaccounted.

### 5.2 Structural characterization

The fabricated samples were characterized using a LEO 1530 thermally-assisted field emission scanning electron microscope (SEM) capable of 3nm resolution at 1 kV. A relatively low operating voltage of 5 kV was used to reduce sample charging since the samples were only mildly conductive. Figure 5.2, a micrograph taken at 100 X magnification, shows the entire patterned area which was approximately 1 mm × 1 mm. Figures 5.3, 5.4, and 5.5 show micrographs of three PC structures with different SL strengths: 1.0, 0.80, and 0.598,
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</tr>
<tr>
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<td>144.0</td>
<td>144.0</td>
<td>0.3265</td>
<td>25</td>
<td>180.0</td>
<td>1.0</td>
</tr>
<tr>
<td>x36y118-6</td>
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<td>144.0</td>
<td>144.0</td>
<td>0.3265</td>
<td>15</td>
<td>165.6</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table 5.1: CAD design parameters for the x58y62 and x36y118 families of structures. All measurements are in units of nm.
respectively, as measured from the median hole sizes. The microscope’s built-in size measurement tool was used to determine hole diameters and lattice spacings for two pairs of \( r_1 \) and \( r_2 \) holes at five different locations in the patterned area. Figure 5.4 shows a micrograph with the annotations used to measure the different structural parameters. As shown, hole diameters (DA1, DA2, DA3, and DA4), lattice constants (PA1, PA2, and PA4), and row spacing (PA3) were all measured in one micrograph, and at least five micrographs were taken for each sample: two at the edges of the sample and three within the area of the sample, to measure the uniformity of the hole sizes. Samples x58y62-N were measured at a magnification of 35 kX while 25 kX was used for measuring the x36y118-N samples.

Table 5.3.1 summarizes the average (\( \bar{r}_1, \bar{r}_2, \bar{a} \)), standard deviation (\( \sigma \)), and median (\( m \)) of the hole radii and lattice constants for the twelve fabricated samples. Overall, the samples showed excellent uniformity in feature sizes over the patterned area. This was attributed to the effectiveness of the 50 nm buffer frame surrounding the patterned area. However, errors were introduced by the equipment since the annotation tools are preset with discrete spatial increments. This explains the many multiple measurements of dimensions that were equivalent (see for example sample x58y62-4 which had a deviation in \( r_1 \) of \( \sigma(r_1) = 0 \)).

Table 5.3.1 summarizes the target radii, target SL strength, the average measured hole radii, and the measured SL strength for the twelve samples.

### 5.3 Optical characterization

#### 5.3.1 Measurement system and procedure

Optical measurements were performed using the coupled resonant band technique in the reflectivity configuration. Figure 5.6 presents a detailed schematic of the measurement system and sample orientation. White light from a tungsten halogen lamp (Mikropack DH-2000) was coupled to a multimode optical fiber (Ocean Optics). The fiber was attached to a variable angle arm equipped with an adjustable iris and two lenses that collimate the beam. A beam chopper (Spiricon) was mounted between the output end of the incident fiber and the iris. The variable angle arm allowed the incident angle, \( \theta \), of the beam to be adjusted from 20° to 65° with respect to the sample surface normal as shown in Figure 5.6. The
**Figure 5.2:** Plan view micrograph of sample x36y118-1 at 100 X magnification showing the dimensions of the area patterned by EBL.
**Figure 5.3:** SEM micrograph of the center of sample x58y62-1 at 35 kX magnification: target hole radius was 123.05 nm, average hole radius was 118.46 nm, \(a = 358 \text{nm}\), and SL strength was 1.0.
Figure 5.4: SEM micrograph of the center of sample x58y62-3 at 35 kX magnification: target hole radii were $r_1 = 123.05$ nm and $r_2 = 92.0$ nm, average hole radii were $r_1 = 124.03$ nm and $r_2 = 98.23$ nm, $a = 358nm$, and SL strength was $\sim 0.792$. 
Figure 5.5: SEM micrograph of the center of sample x58y62-5 at 35 kX magnification: target hole radii were $r_1 = 123.05$ nm and $r_2 = 60.95$ nm, average hole radii were $r_1 = 125.26$ nm and $r_2 = 73.26$ nm, $a = 358 nm$, and SL strength was $\sim 0.585$. 
Table 5.2: Summary of the average, standard deviation, and median values of $r_1$, $r_2$, and $a$ as measured from SEM micrographs of samples x58y62-N and x36y118-N. All measurements are in units of nm.

<p>| Sample name | Radius 1 | | Radius 2 | | Lattice constant | | SL strength |
|-------------|----------|---|----------|---|-----------------|---|
|             | $r_1$    | $\sigma(r_1)$ | $m(r_1)$ | $r_2$ | $\sigma(r_2)$ | $m(r_2)$ | $\bar{a}$ | $\sigma(a)$ | $m(a)$ | strength |
| x58y62-1    | 118.21   | 1.81 | 118.95   | —     | —     | —     | 362.44 | 5.33 | 364.0 | 1.0 |
| x58y62-2    | 122.70   | 2.22 | 123.95   | —     | —     | —     | 359.91 | 6.04 | 362.2 | 1.0 |
| x58y62-3    | 124.03   | 0.169| 123.95   | 98.23 | 2.13  | 99.15 | 359.35 | 6.11 | 357.9 | 0.792 |
| x58y62-4    | 128.9    | 0.0  | 128.9    | 105.59| 2.39  | 104.1 | 357.44 | 5.89 | 357.3 | 0.819 |
| x58y62-5    | 125.26   | 2.34 | 123.95   | 73.26 | 3.10  | 74.1  | 357.15 | 5.49 | 357.9 | 0.585 |
| x58y62-6    | 132.77   | 2.17 | 133.85   | 81.23 | 2.55  | 79.3  | 359.16 | 6.92 | 357.9 | 0.612 |
| x36y118-1   | 172.17   | 3.98 | 173.5    | 110.90| 9.37  | 111.05| 477.05 | 16.86| 478.9 | 0.644 |
| x36y118-2   | 167.49   | 2.13 | 166.85   | 100.77| 3.59  | 100.8 | 482.46 | 4.65 | 480.6 | 0.602 |
| x36y118-3   | 163.25   | 10.51| 166.55   | 131.85| 5.25  | 131.85| 477.53 | 6.45 | 476.1 | 0.808 |
| x36y118-4   | 163.77   | 3.59 | 166.55   | 131.85| 0     | 131.85| 476.97 | 3.06 | 478.6 | 0.805 |
| x36y118-5   | 165.56   | 2.51 | 166.55   | —     | —     | —     | 477.84 | 3.13 | 479.1 | 1.0 |
| x36y118-6   | 159.37   | 1.58 | 159.60   | —     | —     | —     | 479.33 | 9.44 | 479.1 | 1.0 |</p>
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<thead>
<tr>
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<th>Measured values</th>
</tr>
</thead>
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<tr>
<td>x36y118-6</td>
<td>165.6</td>
<td>—</td>
</tr>
</tbody>
</table>

**Table 5.3:** Summary of the target and average hole radii and the SL strength calculated from each. All measurements are in units of nm.
sample holder consisted of a rotation stage attached to an $xyz$ translation stage, allowing fine control of the sample orientation, especially the angle $\phi$ which is the azimuthal angle the plane of incidence makes with the $\Gamma - X$ direction (the direction parallel to rows $i$ and $j$). The collection fiber was also mounted on an adjustable arm with two lenses to focus the beam on the entrance end of the fiber. The collection fiber was then routed to a SpectraPro-150 spectrometer (Acton Research) equipped with a 600 g/mm grating that has a cutoff at 2800 nm. At the exit slit of the spectrometer, an indium gallium arsenide (InGaAs) detector (Thorlabs DET410) was placed to collect the spectrum within the 800 nm – 1700 nm operating range of the detector. The signal from the detector was fed to a preamplifier (EG&G model 181) which was then fed into a two-phase lock-in analyzer (EG&G model 5208) for preconditioning and synchronization with the signal chopper. Finally, the DC electrical signal was sent to a personal computer via an USB SpectraHub (Acton Research) for data collection and analysis.

Measurements were taken by first establishing a reference spectrum (Figure 5.7) of the lamp and detector by reflecting the incident beam at $\theta = 20^\circ$ off an aluminum coated mirror. The spectrum tails off at the extremes of the wavelength range scanned because of the sensitivity limits of the InGaAs detector. The large dip in the spectrum at $\sim 1384$ nm results from O-H bond absorption in the optical fibers. At each incident angle, the input arm assembly was fixed while the collection arm was adjusted to find the maximum reflectivity from the mirror. This ensured we were operating at specular reflectance, and not at a diffraction order of the SWG sample. Next, the beam spot was aligned on an unpatterned region of the sample and the spectrum was recorded. The spot was moved to a patterned area of the sample and the azimuthal orientation, $\phi$, was adjusted to $0^\circ$, $30^\circ$, or $90^\circ$ according to the lattice direction being measured–$\Gamma - X$, $\Gamma - M$, or $\Gamma - Y$, respectively. This procedure was repeated for multiple incident angles in the range of $20^\circ \leq \theta \leq 65^\circ$ in increments of $5^\circ$ and along the three lattice directions described. At the same time, the spectrometer scanned a wavelength range of 800 nm to 1700 nm at a rate of 2 nm/s. In post processing, the spectrum collected from each sample was divided by the reference lamp spectrum, producing the reflectivity spectrum used for analysis.
Figure 5.6: Schematic of the optical system used for resonant band coupling reflectivity measurements.
Figure 5.7: Reference reflectivity spectrum of the tungsten halogen white light source showing the sensitivity limits of the InGaAs detector.
5.3.2 Analysis of as-collected reflectivity data

Figures 5.8(a-c) compare the reflectivity spectra of an unpatterned area of a SoI wafer to that of an area patterned with a triangular lattice (sample x58y62-1: Γ − M direction), and an area patterned with a SSL with a strength of 0.792 (sample x58y62-3: Γ − M direction), from top to bottom. The smooth curving dips in Figure 5.8(a) resulted from thin-film interference effects and were also observed to be imprinted over the finely modulated spectra recorded for the patterned areas. However, the positions of these dips in the spectra of the patterned areas do not align with those of the unpatterned area and are moved to shorter wavelengths. This was a result of the lower effective index of the Si slab in the patterned areas due to the material removed to make the holes. In addition to the thin film dips, many sharp dips were observed in the reflectivity spectra recorded from the patterned areas (Figures 5.8(b) and (c)) indicating that the incident \( k \)-vector was coupled to a mode of the PC structure, as described by Astratov et al. [3]. Several of these spectral features are indicated by the short vertical dashes above each dip in the spectrum. Additionally, the spectra from the two patterned areas were quite different, indicating that the two samples have different lattice structures.

The reflectivity spectra were compared between the triangular lattice and the SSL in the three lattice directions measured, and Figures 5.9 and 5.10 present these comparisons for two samples from each pattern set, \( a = 358 \text{ nm} \) and \( a = 480 \text{ nm} \), respectively. In both figures, the rows are the different lattice directions (\( \Gamma − M \), \( \Gamma − X \), and \( \Gamma − Y \)) from top to bottom), while the columns represent the different SL strengths. Recall that in the triangular and SL lattices, the \( \Gamma − K \) and \( \Gamma − X \) directions are parallel (e.g. run along the same sample orientation \( \phi \)) as well as the \( \Gamma − M \) and \( \Gamma − Y \) directions. Thus the appropriate naming convention is used in the figures. In the triangular lattice of both pattern sets, sharp reflectivity dips appeared at the shorter wavelengths in the spectrum, while the spectra remained smooth at longer wavelengths. In addition, the spectra in the \( \Gamma − M \) and \( \Gamma − M(Y) \) directions (plots (a) and (e) in Figures 5.9 and 5.10) are remarkably similar, confirming that the measurements in these two directions (\( \phi = 30^\circ \text{and} 90^\circ \)) were of the same lattice direction. This established that the sample was indeed a triangular lattice.
Figure 5.8: Angle dependent reflectivity spectrum of (a) an unpatterned region of the Si sample, (b) a region patterned with a triangular lattice (sample x58y62-1; Γ – M direction), and (c) a region patterned with a SL of strength 0.792 (sample x58y62-3: Γ – M direction).
For the SSL PC, many features appear at longer wavelengths that are not in the triangular lattice, as shown in Figure 5.8(c) and in the right columns of Figures 5.9 and 5.10. These features are attributed to the lower order bands being folded out of the light line as a direct consequence of the new symmetry of the lattice as described in Section 3.2.2. To our knowledge, this was the first observation the BZ folding effect in 2D PC structures.

The spectra from different samples were compared to characterize the behavior of the spectral features as a function of lattice structure. The relative shifts in frequency of the spectral features as a function of lattice constant or hole radius were consistent with theory, confirming that the spectral features were indeed from photonic bands, rather than from any anomalous optical effect. Figures 5.11 and 5.12 compare the spectra for SSL structures with the same lattice constant, $a = 358$ nm and $a = 480$ nm, respectively, but with different SL strengths as indicated by the column headings. The samples paired for comparison were chosen because $r_1$ was relatively constant within each pair. As before, the three lattice directions are organized in rows within the figures. As shown in Figures 5.11 and 5.12, the shorter wavelength reflectivity features (higher order bands in the band structures) shift to longer wavelengths with increasing SL strength. For example, in Figure 5.11(a), the three spectral features indicated by the vertical dashes on the $\theta = 45^\circ$ spectrum are located at $\lambda = 1130$, 1168, and 1434 nm, from left to right. When the SL strength is increased from 0.792 ($r_1 = 124.03$ nm, $r_2 = 98.23$ nm) to 0.585 ($r_1 = 125.26$ nm, $r_2 = 73.26$ nm), these features shift to $\lambda = 1180$, 1254, and 1446 nm, respectively, as shown in Figure 5.11(b). This is consistent with the findings presented in Chapter 4, where the air bands shifted to lower frequencies with increasing SL strength. Additionally, in the x58y62 structure set, the longer wavelength reflectivity features of the SSL samples remain relatively stationary when the SL strength increases. This was observed in the numerical results for the dielectric bands, meaning that these observed spectral features correspond to the modes in the dielectric band. For the other SSL set (Figure 5.10, $a = 480$ nm) all of the spectral features are shifted to longer wavelengths with increasing SL strength. This is because the dielectric bands were not within the wavelength range of the detector for this structure. This is expected due of the larger lattice constant of the x36y118 SSL structures.
Figure 5.9: Reflectivity spectra of the triangular lattice (left column, \( r = 118.21 \) nm) and the SSL (right column, \( r_1 = 124.03 \) nm, \( r_2 = 98.23 \) nm, strength 0.792) for three lattice directions as measured by the resonant band coupling method on two samples from the pattern set x58y62, \( a = 358 \) nm. Note: The short vertical dashes indicate some of the spectral features identified with the PC structure.
Figure 5.10: Reflectivity spectra of the triangular lattice (left column, $r = 165.56 \text{ nm}$) and the SSL (right column, $r_1 = 163.77 \text{ nm}$, $r_2 = 131.85 \text{ nm}$, strength 0.805) for three lattice directions as measured by the resonant band coupling method on two samples from the pattern set x36y118, $a = 480 \text{ nm}$.
To our knowledge, at the time of preparation of this work, observation of the location of the top of the dielectric band of a 2D PC had only been accomplished with in-plane measurement techniques because of the restrictions of the light cone. Thus, the observation of the dielectric bands using out-of-plane measurements was a pioneering effort.

Two final comparisons were made using the reflectivity spectra of three SSL samples that had approximately the same SL strength \((\approx 0.8)\). For the first comparison, the lattice constant was increased between two samples, while in the second comparison, the hole size was increased between the samples. The former comparison can be done using the spectra of Figure 5.11(a,c,e) and Figure 5.12(a,c,e). However, the relative shift in the reflectivity features is so dramatic that it is difficult to correlate the data using these as-collected spectra. On the other hand, the relative shifting of the spectra when the hole size increases was quite apparent, as shown in Figure 5.13. Between the two SSL structures \(a\) was constant at 358 nm as well as the SL strength \((\approx 0.8)\), but both \(r_1\) and \(r_2\) increased approximately 4–7 nm. In the left column of Figure 5.13, \(r_1\) and \(r_2\) were 124.03 nm and 98.23 nm, respectively, while in the right column, \(r_1\) and \(r_2\) were 128.9 nm and 105.59 nm. As shown, the shorter wavelength features shifted to the left, corresponding to the air bands shifting to higher frequencies. For example, in Figure 5.13(a), the two spectral features indicated by the vertical dashes on the \(\theta = 45^\circ\) spectrum are located at \(\lambda = 1168\) and 1434 nm, from left to right. When the hole sizes are increased \(\Delta r_1 = 4.87\) nm and \(\Delta r_2 = 7.36\) nm, these features shift to \(\lambda = 1148\) nm and 1406 nm, respectively, as shown in Figure 5.13(b). This was remarkably consistent with PC theory where an increase in hole size decreases the effective index of the slab, which shifts the photonic bands to higher frequencies (shorter wavelengths).

### 5.3.3 Post processing: Band diagram analysis

Visualizing the reflectivity data and the effects of the structural parameters can be aided by filtering the spectrum and plotting the positions of the spectral features in the same format as a band diagram: \(\omega_n\) vs. \(k\). To perform this function, a post processing routine [106] was used that accurately detected dips in the reflectivity spectrum. First, a running
Figure 5.11: Reflectivity spectra for two different SL strengths of 0.792 and 0.585 (left and right columns, respectively) and three lattice directions (rows) in the x58y62 sample set, $a = 358$ nm. Sample x58y62-3: $r_1 = 124.03$ nm and $r_2 = 98.23$ nm. Sample x58y62-5: $r_1 = 125.26$ nm, $r_2 = 73.26$ nm.
Figure 5.12: Reflectivity spectra for two different SL strengths of 0.805 and 0.602 (left and right columns, respectively) and three lattice directions (rows) in the x36y118 sample set, $a = 480$ nm. Sample x36y118-4: $r_1 = 163.77$ nm and $r_2 = 131.85$ nm. Sample x36y118-2: $r_1 = 167.49$ nm, $r_2 = 100.77$ nm.
Figure 5.13: Comparison of the reflectivity spectra for two SSL structures with different hole sizes, but approximately the same SL strength and lattice constant ($a = 358$ nm). Left column: $r_2/r_1 = 98.23$ nm / 124.03 nm = 0.792. Right column: $r_2/r_1 = 105.59$ nm / 128.9 nm = 0.819.
Figure 5.14: Band structure of SSL sample x58y62-3 ($r_1 = 124.03$ nm, $r_2 = 98.23$ nm) in the $\Gamma - M$ direction as derived from the measured reflectivity spectra. The shaded region indicates the guided regime of the Si SWG layer.
average subtraction removed the average slope of the reflectivity data. Then, the central values of the dips were identified using the first and second derivatives. Using this running average technique was necessary in order to correctly isolate the sharp dips in the spectrum from the broader dips caused by thin film interference effects. The position of the dips were plotted on a band diagram using the wavelength, lattice spacing, and incident angle to calculate the normalized frequency vs. the in-plane $k$-vector, which is given by $k_{in} = k \sin \theta$.

Figure 5.14 presents the experimentally measured band diagrams for the x58y62-3 SSL PC structure as measured in the $\Gamma - M$ direction. The scattered dots represent the dips in the reflectivity spectra of the sample that were isolated by the post-processing routine. The light line is also plotted on the band structure as the sloped boundary line of the shaded region, indicating the guided regime of the Si SWG. Under the light line (within the shaded region) modes are guided in the SWG and coupling into and out-of these modes with an out-of-plane excitation is forbidden. However, modes above this line can be excited by an out-of-plane excitation and measured by an out-of-plane detector. Plotting the reflectivity data in the form of band diagrams allows direct visualization of the band structure outside of the light line, however the greatest advantage to presenting the data in this form is that numerical calculations can be used to corroborate the experimental observations.

Calculations were performed using the FDTD method because the measured bands are outside of the light line (the PWE method is accurate only for mode inside of the light line for SWG structures). Additional modifications were made to the ONYX code used in Chapter 4 to incorporate the substrate below the SWG which eliminates the mirror symmetry in the slab. Thus, the FDTD code required additional modifications to contain PML BCs both on the top and bottom of the computational cell. Also, the source condition was modified to include all directional components of the $H$ field during initialization since there are no even nor odd modes in the structure. Figure 5.15 presents the dielectric function used in the band structure calculation for the x58y62-5 SSL structure. This is an example of the computational domain used for the SSL calculations which was typically $18 \times 18 \times 125$ computational units in length, width, and height, where the unit length definitions were $1.0 \times \sqrt{3} \times 1.0$ to create a rectangular unit cell. For the triangular lattice, a unit cell
Figure 5.15: Dielectric function of the FDTD computational domain used for calculating the photonic band structure of sample x58y62-5.
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Table 5.4: Summary of the parameters used for the FDTD calculations of band diagrams for the fabricated samples. All dimensions in nm.

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</tr>
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<td>SSL 0.792</td>
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Table 5.5: Summary of Figures 5.16–5.27 including the samples they describe. SL strengths are calculated from the average hole sizes.
with non-orthogonal axes was used in the base plane, but the same parameters as the SSL calculation were used in the vertical dimension. The thickness of the patterned Si SWG matched that of the sample and was positioned on top of an approximately 1 nm thick SiO$_2$ oxide layer, $\epsilon = 2.09737$. Above the SWG an air layer was assumed that was at least the same thickness as the SWG. The sides of the computational domain were terminated with periodic BCs, while the top and bottom were terminated with PML. We assumed a native oxide layer coating of the SWG that effectively decreased the dielectric constant of the slab. The effective index of the slab was calculated by averaging the volume of SiO$_2$, $\epsilon = 2.90737$, with the volume of the Si layer, $\epsilon = 12.6736$. Four of the samples from the x58y62 set ($N=1, 2, 3, \text{ and } 5$) and three from the x36y118 set ($N=2, 4, \text{ and } 5$) were chosen for the FDTD calculations. Table 5.4 summarizes the parameters used in each band diagram calculation.

Figures 5.16–5.27 present the calculated and experimental band diagrams for three of the structures from both the x58y62 set and the x36y118 set. In all of the figures, the FDTD results are represented by square points and the experimental results by circular points. As before, the guided regime of the SWG is defined by the shaded region. Additionally, each structure is associated with two sets of figures. The first set plots the complete lattice directions of the respective structures for a large normalized frequency range, while the second set focuses on a smaller region of the band structure for detail. Table 5.3.3 summarizes the descriptions of the Figures.

Overall, the calculated band structures match extremely well with the experimentally measured band structures for the normalized frequencies around 0.3. At higher frequencies, the FDTD calculations predicted bands at higher frequencies than measured. This was attributed to the frequency dependence of $\epsilon_b$, which can range from 12.3201 to 13.7641 over the wavelength (normalized frequency for $a = 358$ nm) range of 1700 nm (0.211) to 800 nm (0.323). Since the FDTD code assumes a frequency independent $\epsilon_b$, the calculations maintained accuracy only for a range of $\omega_n$. In fact, using a higher $\epsilon_b$ in the calculations showed better correlation with experimental results for the higher order bands; however, at the same time, the lower order bands shifted to lower frequencies. In addition, higher order bands are more difficult to isolate and characterize in both the calculations and experiments.
Figure 5.16: Full (a) $\Gamma - M$, (b) $\Gamma - M$ (measured in the $\Gamma - Y$ direction of the SSL), and (c) $\Gamma - K$ (parallel to the $\Gamma - X$ direction of the SSL) experimental (circular points) and calculated (square points) band diagrams of the $x5y62-1$ triangular lattice structure, $a = 358\text{ nm}$, $r = 118.21\text{ nm}$.
Figure 5.17: Detailed plot of the (a) $\Gamma - M$, (b) $\Gamma - M(Y)$, and (c) $\Gamma - K(X)$ experimental (filled circles) and calculated (open squares) band diagrams of the $x58y62-1$ triangular lattice structure, $a = 358$ nm, $r = 118.21$ nm.
Figure 5.18: Full (a) Γ − M, (b) Γ − Y, and (c) Γ − X experimental (circular points) and calculated (square points) band diagrams of the $x_{58}y_{62}-3$ SSL structure. SL strength $0.792$, $a = 358$ nm, $r_1 = 124.03$ nm, $r_2 = 98.23$ nm.
Figure 5.19: Detailed plot of the (a) $\Gamma - M$, (b) $\Gamma - Y$, and (c) $\Gamma - X$ experimental (filled circles) and calculated (open squares) band diagrams of the x58y62-3 SSL structure, SL strength 0.792, $a = 358$ nm, $r_1 = 124.03$ nm, $r_2 = 98.23$ nm.
Figure 5.20: Full (a) $\Gamma - M$, (b) $\Gamma - Y$, and (c) $\Gamma - X$ experimental (circular points) and calculated (square points) band diagrams of the x5y0.25 SSL structure, SL strength 0.585, $a = 358$ nm, $r_1 = 125$ nm, $r_2 = 32.26$ nm.
Figure 5.21: Detailed plot of the (a) $\Gamma - M$, (b) $\Gamma - Y$, and (c) $\Gamma - X$ experimental (filled circles) and calculated (open squares) band diagrams of the x58y62-5 SSL structure, SL strength 0.585, $a = 358$ nm, $r_1 = 125.26$ nm, $r_2 = 73.26$ nm.
Figure 5.22: Full (a) $\Gamma - M$, (b) $\Gamma - M(Y)$, and (c) $\Gamma - K(X)$ experimental (circular points) and calculated (square points) band diagrams of the $x_{36}y_{118}-5$ triangular lattice structure, $a = 480$ nm, $r = 165.56$ nm.
Figure 5.23: Detailed plot of the (a) $\Gamma - M$, (b) $\Gamma - M(Y)$, and (c) $\Gamma - K(X)$ experimental (filled circles) and calculated (open squares) band diagrams of the x36y118-5 triangular lattice structure, $a = 480$ nm, $r = 165.56$ nm.
Figure 5.24: Full (a) $\Gamma - M$, (b) $\Gamma - Y$, and (c) $\Gamma - X$ experimental (circular points) and calculated (square points) band diagrams of the x580y1.18-4 SSL structure, SL strength 0.805, $a = 480$ nm, $r_1 = 163.77$ nm, $r_2 = 131.85$ nm.
Figure 5.25: Detailed plot of the (a) $\Gamma - M$, (b) $\Gamma - Y$, and (c) $\Gamma - X$ experimental (filled circles) and calculated (open squares) band diagrams of the $x_{36}y_{118}-4$ SSL structure. SL strength 0.805, $a = 480$ nm, $r_1 = 163.77$ nm, $r_2 = 131.85$ nm.
Figure 5.26: Full (a) $\Gamma - M$, (b) $\Gamma - Y$, and (c) $\Gamma - X$ experimental (circular points) and calculated (square points) band diagrams of the x36y118-2 SSL structure, SL strength 0.602, $a = 480$ nm, $r_1 = 167.49$ nm, $r_2 = 100.77$ nm.
Figure 5.27: Detailed plot of the (a) $\Gamma - M$, (b) $\Gamma - Y$, and (c) $\Gamma - X$ experimental (filled circles) and calculated (open squares) band diagrams of the x36y118-2 SSL structure, SL strength 0.602, $a = 480$ nm, $r_1 = 167.49$ nm, $r_2 = 100.77$ nm.
Therefore, we focused our calculations on bands around $\omega_n = 0.3$.

As shown in Figures 5.16 and 5.22, the triangular lattice band structures do not display any bands below $\omega_n = 0.25$, which is consistent with the theoretical predictions that out-of-plane light as used in the measurements cannot couple to the dielectric band modes since they are within the light line. On the other hand, the SSL (Figures 5.18–5.21 and 5.24–5.27) possess photonic bands in the lower frequency regions in all three lattice directions. This was attributed to the folding of the bands of the triangular lattice out of the guided region by the new BZ, as described in previous chapters. The FDTD results confirmed that these folded bands are indeed from the dielectric bands due to their location in the band diagram. In the $\Gamma - M$ and $\Gamma - X$ directions, the lower bands are ‘flat bands’ at the top of the dielectric band that are practically horizontal. On the other hand, the lower bands in the $\Gamma - Y$ direction originate from the dielectric band in the $\Gamma - M$ folding over the Y-point (see Chapter 4), since the Y-point bisects the $\Gamma - M$ line.

Once again, we confirm the photonic band structures are indeed structurally dependent by comparing the relative shift in the band frequencies as a function of the change in SL strength, the hole radius, and the lattice constant. Figure 5.28 summarizes our findings by a comparison of the band structures in the $\Gamma - M$ direction of the different SSL structures under the aforementioned conditions. Figure 5.28(a) shows that for a fixed lattice constant ($a = 358$ nm) and fixed $r_1$ ($\approx 125$ nm), an increase in the SL strength from 0.792 (open triangles, sample x58y62-3) to 0.585 (circles, sample x58y62-5) shifts the bands to lower frequencies. For example, the points highlighted by the ellipse in Figure 5.28(a) shift from $\omega_n = 0.309$ to 0.306 for the increase in SL strength from 0.792 to 0.585. This was consistent with theoretical predictions since the decrease in $r_2$ from 98.23 nm to 73.26 nm increases the effective index of the SWG, which lowers the band frequencies. For a fixed SL strength ($\approx 0.8$) and lattice constant ($a = 358$ nm), a decrease in the hole radius (both $r_1$ and $r_2$) was predicted to shift the bands to lower frequencies. Figure 5.28(b) confirms this prediction for the SSL structures x58y62-4 (triangles, $r_1 = 128.9$ nm, $r_2 = 105.9$ nm) and x58y62-3 (circles, $r_1 = 124.03$ nm, $r_2 = 98.23$ nm). For example, the circled points in Figure 5.28(b) shift from $\omega_n = 0.315$ to 0.310 for the decrease in radii of $\Delta r \approx 5–7$ nm.
In the final comparison, Figure 5.28(c), the lattice constant was increased from 358 nm (circles) to 480 nm (open triangles) while the SL strength (∼0.8) was constant between the two structures, x58y62-3 ($r_1 = 124.03$ nm, $r_2 = 98.23$ nm, SSL 0.792) and x32y118-4 ($r_1 = 163.77$ nm, $r_2 = 131.85$ nm, SSL 0.805), respectively. Again, the band behavior in the measurements match that of the calculated band structures, in that the bands shift to higher frequencies (shorter wavelengths) with the increasing lattice constant. An arrow was drawn in Figure 5.28(c) to aid in the visualization of this effect showing the point from the same band shifting from $\omega_n = 0.250$ to 0.290 as $a$ increases from 358 nm to 480 nm.

The combination of the comparisons between the reflectivity spectra of the samples when structural parameters are shifted, the correlation of the FDTD calculations with the measured band structures, and the comparisons of the experimental band structures with the change in structural parameters validates our implementation of the SL structure in the calculations, and confirms the optical properties of the SSL that we predict. One of the more profound findings in this work was the measurement of the dispersion relationship of a dielectric band using out-of-plane measurements. As mentioned previously, these bands are normally inaccessible using the resonant band coupling method due to the light cone. In addition, in-plane transmission/reflection measurements can only infer the band structure of the dielectric band, rather than explicitly show the dispersion relationship as was demonstrated in this work with the SSL.

A final comparison is presented at this point to illustrate the application of the SSL to investigate the photonic band properties of the triangular lattice. Figure 5.29(a) shows the measured band structure in the $\Gamma-Y$ direction of sample x58y62-3 (filled squares) compared to the measured band structure of a triangular lattice (filled circles) that has the same $r_1$ as the SSL sample. As predicted by theory, the bands of the SSL are shifted to lower frequencies due to the decrease in $r_2$ between the two structures, increasing the effective dielectric constant of the SWG. On the other hand, Figure 5.29(b) compares the same measured band structure in the $\Gamma-Y$ direction of the SSL (filled squares) with that of the calculated band structure of a triangular lattice (open circles) that has an approximately 4% smaller $r_1$ than the SSL (118.96 nm as compared to 123.95 nm). Recall, the $\Gamma-Y$ direction of the SL is
Figure 5.28: Experimental band structures showing the relative shift of photonic bands as a function of the change in (a) SL strength, (b) hole radius, and (c) lattice constant.
parallel to a $\Gamma - M$ direction in the triangular lattice. When we assume a SL unit cell for the triangular lattice, the bands in the $\Gamma - M$ direction are folded/translated over the Y-point (as defined by the reduced-zone scheme) to create the bands in the $\Gamma - Y$ direction that are represented by the open triangles in Figure 5.29(b). Remarkably, the folded bands correlate very well with the measured bands of the SSL in the frequency range $0.2 < \omega_n < 0.35$. This is attributed to a similar averaged effective dielectric constant, $\epsilon_{avg}$ of the SWG between the two structures. This $\epsilon_{avg}$ was calculated by summing the weighted volumes of the air holes and the dielectric regions and averaging them over the entire volume of the SWG layer in a unit cell. For the triangular lattice presented, $\epsilon_{avg}$ was calculated to be 10.177, while $\epsilon_{avg}$ was 10.538 for the SSL. This evaluation was rather simplistic, however, the correlation between the measured and calculated band structures is quite remarkable. Perhaps future work will elaborate on optimizing the correlation between the SSL structure and the triangular lattice band structure beyond $\epsilon_{avg}$; but even with this simplistic approach, our results immediately show that the SSL coupled with the resonant band coupling measurement technique provide a new, powerful tool for measuring the dispersion relationship of the dielectric band, which to this date, has not been observed explicitly in any previous experiment.
Figure 5.29: Comparison of the SSL band structure in the $\Gamma - Y$ direction of sample x58y62-3 with the triangular lattice band structure from (a) experimental measurement (sample x58y62-2) and from (b) FDTD calculations (sample x58y62-1).
CHAPTER VI

REFRACTION EFFECTS IN THE SSL

As discussed in Chapter 1, PCs show interesting optical properties for frequencies outside of the PBG. In particular, as a result of their unique band structure, they exhibit anomalous refractive properties which differ significantly from the square and triangular lattices because of their complex-shaped dispersion surfaces. This chapter investigates the refractive properties of the SSL PC using numerical techniques. Two avenues to achieve an understanding of the behavior of propagating beams in the SSL are pursued. The first avenue exploits the information contained within the dispersion surfaces of the structure through wavevector or $k$-vector diagrams. The second avenue directly visualizes the propagation of a light beam in the PC by using the FDTD method. In this chapter we establish that both methods are valid, however, the former method offers greater detail in the analysis, while the latter method serves as a confirmation and direct visualization of the former.

6.1 Wavevector diagrams

The use of wavevector diagrams to predict refraction behavior at the interface between two materials is widely used in optics, and in 1996, Russell et al. [80] outlined the adaptation of this method to multi-dimensional PCs. First, we introduce this technique by considering the interface between two homogeneous, isotropic materials. Then, we apply the concept to the interface between a homogeneous, isotropic material and an arbitrary material that possesses a complex dispersion contour, such as a PC.

Consider an infinite plane wave with angular frequency $\omega$ that is incident at an angle $\theta_i$ at the interface between two homogeneous, isotropic media, Region 1 and 2, with refractive indices $n_1$ and $n_2$, respectively. Figure 6.1 defines this situation in $k$-space using the relationships

$$k_1 = \frac{n_1 \omega}{c},$$  

(6.1)
where \( c \) is the speed of light in vacuum. In addition, we assume that \( n_1 < n_2 \), the interface between the two regions is along the \( k_x \) direction, and the normal to the interface is along \( k_y \). Since the system possesses translational symmetry along the interface, the wavevector components of the incident wave, reflected wave, and refracted wave that are parallel to the interface, \( k_\parallel \), must be conserved when reflection or refraction occurs, as required by the conservation of momentum. This conservation condition is indicated by the *construction line* (the dashed line in Figure 6.1), which is drawn parallel to the normal line, \( k_y \), and at a distance from the origin equal to \( k_1\parallel \). Recall, the dispersion contours of a homogeneous, isotropic medium are circles, thus the semicircle in Region 2 indicates all of the possible wavevectors in Region 2 that have frequency \( \omega \), as defined by Equation (6.2). The endpoint of a wavevector that will satisfy the conservation condition in Region 2 is given by the intersection of the construction line with the dispersion contour. Thus, the wavevector inside the second medium, \( k_2 \), is drawn from the origin to the intersection point, making an angle \( \theta_2 \) with the normal line. However, the group velocity, \( v_g \), indicates the propagation direction of the wave in Region 2, and this is given by the gradient of the dispersion contour which is defined by

\[
 v_g = \nabla \omega(k) = \frac{\partial \omega}{\partial k}.
\]  

(6.3)

Thus, \( v_g \) is normal to the tangent of the dispersion contour at the point where the construction line and contour intersect and it points in the direction of increasing \( \omega \) and makes an angle \( \theta_r \) with the construction line. For the present case, \( v_g \) is in the same direction as \( k_2 \), since the radius of a circle is always normal to the tangent at any given point on the circle. Mathematically we have:

\[
 k_1\parallel = k_2\parallel
\]  

(6.4)

\[
 \frac{n_1\omega}{c} \sin \theta_i = \frac{n_2\omega}{c} \sin \theta_r
\]  

(6.5)

\[
 n_1 \sin \theta_i = n_2 \sin \theta_r
\]  

(6.6)

which shows that in the case of two homogeneous, isotropic media, wavevector analysis reduces to Snell’s law.
Figure 6.1: Illustration showing the use of wavevector diagrams to calculate the refraction of a plane wave at the interface of two different homogeneous, isotropic materials.
Figure 6.2: A wavevector diagram illustrating the calculation of refraction effects at the boundary of an isotropic, homogeneous medium and a medium with a complex dispersion surface, such as a PC.
However, Equation (6.5) is not always true for other materials such as birefringent materials or PCs. This is shown in Figure 6.2 where the wavevector technique is applied to an arbitrary dispersion contour, \( \omega = \omega(k) \), with a complex shape that could be possible in a triangular PC. Notice that when the conservation condition, Equation (6.4), is maintained, \( k_2 \) and \( v_g \) are not coincident. Thus, Equation (6.5) and Snell’s law are not valid for this system. The propagation direction of the refracted wave inside of the PC is given by \( v_g \) and the angle \( \theta_r \). Thus, the relationship between the direction of the refracted beam as a function of the direction of the incident beam can be derived by calculating the normal to the contour along its length. This is an important quantity that shows the sensitivity of the refracted beam to the properties of the incident beam. If the incident angle were fixed, rather than the incident frequency as in the previous case, we can also derive the sensitivity of the refraction angle as a function of the frequency of the incident beam. This is an important quantity in dispersive applications such as spectrometers or wavelength-division multi/demultiplexers.

Now, we are prepared to apply the wavevector diagram method to the SSL structure, which we will do in general terms before presenting the results of the calculations. Figure 6.3 shows the conventional setup of the system with Region 1 being the isotropic medium the wave is incident from and Region 2 being the SSL PC. Again, the interface line is parallel to the \( k_x \) direction, and the normal to the interface is parallel to \( k_y \). Here we have defined the \( \Gamma - M \) direction as being normal to the interface between the isotropic medium and the SSL PC, i.e. the light is traveling in a direction close to the \( \Gamma - M \) direction. (The reasons for this choice of incident direction will be discussed shortly.) The \( \Gamma \) point defines the origin which is the intersection of the normal and interface lines. As a consequence of the directional definition, the BZ of the SSL must be rotated 60° around the \( \Gamma \) point to match the conditions of the incident wave, as shown in Figure 6.3. In Figure 6.3, the dispersion contours are plotted in the repeated-zone scheme, where replications of the first BZ are placed adjacent to one another in order to fully represent the excitable modes from contours in proximity to the \( \Gamma \) point at the interface line. Multiple modes, represented by
Figure 6.3: Diagram illustrating the wavevector method as applied to the SSL structure, showing the excitation of multiple beams in the PC, $v_{g1}$ (backward propagating) and $v_{g2}$ (forward propagating)
\( v_g_1 \) and \( v_g_2 \), satisfy the conservation condition defined by the construction line\(^1\) as shown in Figure 6.3. However, the direction of \( v_g_1 \) indicates that this wave does not propagate forward into the PC structure, whereas the direction of \( v_g_2 \) indicates that it does. We call these the backward propagating and forward propagating modes, respectively, and the backward propagating modes are rejected from the PC.

As mentioned previously, the present work focused the behavior of light propagating along the \( \Gamma \rightarrow M \) direction of the SSL. This is for two reasons: First, the curves whose loci are at the M-point show anisotropic shapes across the \( \Gamma \rightarrow M \) line. This is in contrast to the other lattice directions where the curves are symmetric across the lattice direction line. This anisotropy introduces interesting refraction regimes such as refraction at normal incidence and the existence of positive and negative refraction at a single fixed frequency, as we have reported [88, 58, 55]. Second, in a SWG structure, the curves around the M-point are usually within the guiding regime of the SWG. In the BZ representation this is outside of the light circle, which is equivalent to saying the modes are below the light line in a band diagram. As the frequency of the excitation increases, the diameter of the light circle increases, enclosing more area of the BZ. Typically, the upper bands are used for refraction effects, thus the contours nearer the \( \Gamma \)-point are inside the light circle, indicating that these modes are not guided by the index contrast between the SWG and the cladding. On the other hand, modes excited from contours outside of the light circle are strongly confined within the SWG, rather than coupled to the extended states outside of the slab which decay rapidly. Since the M-point is furthest from BZ center, the contours near this point are typically within the guiding regime of the SWG. Obviously, contours in other directions (defined by the angle of the incident light) are also outside of the light cone, and many interesting effects occur along these directions, such as self-collimation, negative index lensing, and slowlight, however these effects are beyond the scope of this work and

\(^1\)In fact, there exist an infinite number of intersections between the construction line and the dispersion contours in the repeated-zone scheme. However, the angles of propagation, \( \theta_r \), of the excitations repeat themselves, thus an analysis of the contours near the first BZ is sufficient. On the other hand, the repeated-zone is necessary when considering the output interface of a finite PC region as discussed by Baba and Nakamura in 2002 [7]. However, the analysis of wave propagation at the output end of an SSL PC region is beyond the scope of this work.
are left for future investigations.

6.2 The refraction response of the SSL: wavevector calculations

The work presented in this section focuses on 2D SSL PC structures. Calculations of the refraction response through wavevector diagrams were performed using the PWE method to solve for the dispersion surfaces of the structure, which were then plotted as iso-contour maps of the BZ. Then, the refraction angles were calculated as discussed in the previous section. The angle sign convention used in this work was that a counter-clockwise angle from the interface normal is positive. The incident material was defined as either air or silicon, however changing media in which the incident light is traveling merely redefines the magnitude of the incident angle. This changes the sensitivity of the refraction effects to the incident angle, but it does not change the shape of the refraction curves as shown later. Therefore, calculating the refraction response for different incident materials can be accomplished simply by recalculating the incident angles accordingly, assuming the material is homogeneous and isotropic.

6.2.1 Numerical calculation procedure

The dispersion contours of the SSL were calculated with the PWE method using the same procedure outlined in Section 4.5 where the dispersion contours were first described. Figure 6.4 presents the graphical output from the calculation algorithm that performed wavevector analysis on the dispersion contours and outlines the step-by-step procedure followed to derive $\theta_i$ vs. $\theta_r$. After the dispersion surface of a individual band was reconstructed as an iso-contour map in the desired frequency range (Figure 6.4(a)), the data was cast in a repeated zone scheme to create a closed curve around the M-point. Next the curve was oriented properly so that the $\Gamma - M$ direction coincides with the $k_y$ axis (Figure 6.4(b)). Then the derivative of the rotated data was calculated (Figure 6.4(c)) to give the slopes of the tangent lines of the contour. Finally, the refraction angle as a function of incident angle was calculated from the conserved wavevector component and the derivative by the
equations:

\[ \theta_i = \frac{n_1 \cdot \sin^{-1}(k_{1\parallel})}{\omega}, \quad (6.7) \]

and

\[ \theta_r = \tan^{-1}\left(\frac{dk_y}{dk_x}\right), \quad (6.8) \]

where \( n_1 \) is the refractive index of the material in Region 1 and \( k_{1\parallel} \) is the conserved component of the incident wavevector with frequency, \( \omega \). The results of this calculation are plotted in Figure 6.4(d), which is an example of a calculation from the 3s band (TE polarization) of the SSL (strength of 0.857) patterned in silicon (\( \epsilon_b \)) with air in Region 1. For each structure, the frequency range of the calculation varied according to the minimum and maximum frequencies that showed a closed contour shape centered around the M-point. In this case, \( \omega_n \) ranged between 0.288 and 0.309 with a frequency spacing, \( \Delta\omega \), of 0.001, the chosen frequency spacing for all of the calculations presented, unless noted otherwise.

As mentioned, the current work focuses on refraction effects experienced by a wave propagating in the \( \Gamma - M \) direction of the SSL. More specifically, we have focused on the 3s and 3p bands and their dispersion surfaces because these two bands show unique dispersion contours, they are above the band gap, and portions of their bands are within the guiding regime when the implementation is a SWG configuration. As shown in Section 4.5.4, these bands possess unique contour shapes around the M-point. Figure 6.5(a) and (b) focus on the M-point and show examples of the contour shapes found around this point in the repeated-zone scheme for the 3s band and the 3p band, respectively. The 3s band possesses rectangular-like contours with curved sides and corner points within the BZ, while the 3p band has elliptically shaped contours with major and minor axes on the \( M - X \) and \( M - Y \) BZ boundary lines, respectively. The contours are rotated such that the \( \Gamma - M \) direction is vertical, along \( k_y \), as before, and both of the bands presented in Figure 6.5 are from a SSL with strength 0.857 and are within a frequency range of \( 0.295 \leq \omega_n \leq 0.309 \) for the 3s band and a range of \( 0.314 \leq \omega_n \leq 0.328 \) for the 3p band. In addition, for both bands, \( \omega_n \) increases as the contours radiate outward from M-point, thus \( v_g \) will point outward, away from the M-point.
Figure 6.4: Example of the graphical output during the calculation of refraction angles using the wavevector method on the 3s band (TE polarization, $0.288 \leq \omega_n \leq 0.309$) of a SSL with a strength of 0.857 ($r_1 = 0.35a$), $\epsilon_b = 12.0$, and a Region 1 of air. (a) Selection of the correct contour in the dataset, (b) rotated contour in the repeated-zone scheme, (c) slope of the contour tangent line, (d) plot of $\theta_r$ as a function of $\theta_i$. 
Figure 6.5: Dispersion contour plots centered around the M-point showing (a) the rectangular-like shape of the $3s$ band ($0.295 \leq \omega_n \leq 0.309$) and (b) the elliptical-like shape of the $3p$ band ($0.314 \leq \omega_n \leq 0.328$) when the repeated-zone scheme is used. Note: all dispersion contours make an orthogonal intersection with the BZ boundary lines M–X and M–Y.
Figure 6.6: Refraction response of the 3s band at $\omega_n = 0.299$: (a) results of the refraction analysis on (b) the entire rectangular contour shape around the M-point with forward (solid lines) and backward (dashed lines) propagating refraction response. (c) Refraction curves showing only the forward propagating response and the regions of positive and negative refraction. Labels indicate the material in Region 1.
6.2.2 The 3s band refraction response

The first shape type we consider is from the lower frequency range of the 3s band: the rectangular-like contours with moderately curved sides as shown in Figure 6.5(a). As the SL strength increases, the curves in the sides of the rectangle flatten, eventually becoming quite straight as seen Figure 4.19. The refraction angle as a function of incident angle was calculated using the wavevector method and the algorithm previously described for a SSL with strength \( r_2/r_1 = 0.3a/0.35a = 0.857 \). Figure 6.6(a) presents a detailed plot of the results of this calculation, showing the refraction angle response for all points along the rectangular-like contour at \( \omega_n = 0.299 \) (Figure 6.6(b)) for both silicon (dark lines) and air (light lines) in Region 1. As a consequence of the use of the entire contour shape, the refraction response of both the forward and backward propagating modes was calculated and are represented by the solid lines and dashed lines, respectively. These two responses are symmetric to one another through the \( y \)-axis. Notice the shape of the refraction curves for the different materials in Region 1 are scaled versions of one another. As shown, having silicon, or any high index material, in Region 1 increases the sensitivity of the refraction response to the incident beam direction because the magnitude of \( k_1 \) increases with the higher \( n \) (see Equation 6.2), which in effect increases \( k_\parallel \). This can be either an advantage or disadvantage, depending upon the specific system application containing the SSL PC, and it is a general property of all PCs.

Figure 6.6(c) shows only the forward propagating refraction response for the same structure and \( \omega_n \). In general, the forward propagating refraction response of the 3s band has a large slope at the two extrema of the \( \theta_i \) range. This high sensitivity of \( \theta_r \) with respect to \( \theta_i \) is a consequence of the corner regions of the rectangular-like dispersion contours where the slopes of the tangent lines approach infinity (see Figure 6.6(b)). As \( \theta_i \) increased from left to right in Figure 6.6(c), \( \theta_r \) stabilized at \(-30^\circ\) due to the long, flat contour that crosses the M–Y line. Next, \( \theta_r \) increases rapidly due to the corner of the contour, after which \( \theta_r \) dips slightly before increasing rapidly to \( 90^\circ \). This dip in \( \theta_r \) was attributed to the short-side of the rectangular-like contour which possesses a slight concavity in its curvature. The degree of this concavity increases as the contours move further from the M-point, \( i.e. \) as
\( \omega_n \) increases (see Figure 6.5(a)).

An interesting property of the SSL is that it possesses a non-symmetric refraction response across the \( \Gamma - M \) direction due to the rectangular BZ. In the triangular and square lattices, the refraction response of either \( \pm \theta_i \) across any lattice high-symmetry direction is symmetric through the origin of a \( \theta_r \) vs. \( \theta_i \) plot. This is due to the mirror symmetry of the BZ in those systems. This also observed in the SSL for the \( \Gamma - X \) and \( \Gamma - Y \) lattice directions since they too possess mirror symmetry. On the other hand, the SSL does not have mirror symmetry across the \( \Gamma - M \) direction, and thus the refraction response is not symmetric through the origin as shown in Figure 6.6(c).

When the BZ possesses folding symmetry across a lattice direction, as in the cases mentioned above, the structure can only exhibit either a positive or a negative refraction regime at a fixed normalized frequency, depending on the frequency of the excitation. We distinguish these two regimes in the following manner: A positive refraction regime is the response expected when Snell’s law is obeyed. In other words, in positive refraction, the sign of the incident and refracted angles match. When the signs differ, i.e. \( \theta_i \) is positive and \( \theta_r \) is negative, the situation is termed negative refraction. In negative refraction, the beam behaves as if the material in Region 2 has a negative index of refraction in order to obey Snell’s law. Because of the rectangular BZ and the lack of folding symmetry across the \( \Gamma - M \) direction, the SSL shows both positive and negative refraction at a fixed normalized frequency. This is indicated in Figure 6.6(c) by the labeling of the quadrants appropriately in the refraction plot. As shown, as \( \theta_i \) increased from quadrant III, the beam experienced positive, then negative, and finally positive refraction behavior.

Figures 6.7 and 6.8 present the refraction response of the 3s band (TE polarization) of two SSL PCs with SL strengths of 0.857 and 0.571 \((r_1 = 0.35a)\), respectively. In both figures, Region 1 was air, \( \epsilon_b = 12.0 \), and the entire frequency range of the 3s band that produced a closed curve around the M-point was plotted using a frequency interval, \( \Delta \omega_n \), of 0.004. As described earlier, the refracted beam steadily increased in \( \theta_r \) as \( \theta_i \) increased, with several of the contours having two flat regions, one at negative \( \theta_i \) and the other at positive \( \theta_i \), such as for the curve for \( \omega_n = 0.260 \). This indicated a refraction response
that is relatively stable under a wide range of incident angles, a valuable condition when considering a finite beam as in real device applications. At higher frequencies of the 3s band, the refraction response showed an inflection point in the positive refraction regime (quadrant I) in which the refracted beam decreased in $\theta_r$ with increasing $\theta_i$ before increasing once again, after which the forward propagating regime ceases. This effect was attributed to the concavity of the shorter sides of the contour shapes which increases with increasing $\omega_n$, moving the inflection point to larger $\theta_i$ and $\theta_r$ with increasing $\omega_n$. For example, in the 0.857 SSL (Figure 6.7), the inflection point moves from $(\theta_i = 25.4^\circ, \theta_r = 65.4^\circ)$ at $\omega_n=0.300$ to $(34.9^\circ, 83.4^\circ)$ at $\omega_n=0.308$. However, the concavity of the shorter sides decreased with increasing SL strength as shown in the inset of Figure 6.8 for the 0.571 SSL, resulting in a smaller shift in the inflection point position from $(29.4^\circ, 62.4^\circ)$ at $\omega_n = 0.248$ to $(36.7^\circ, 74.12^\circ)$ at $\omega_n = 0.256$. This represents a direct relationship between the refraction response and the SL strength, providing a route that enables greater flexibility in PC design.

Figures 6.9(a) and (b) present the refraction response of the SSL as a function of frequency at a constant incident angle for two SL strengths, 0.857 and 0.571, respectively. The medium in Region 1 was air, $\epsilon_b = 12.0$, $r_1 = 0.35a$, and the constant $\theta_i$ are indicated by the labels next to each curve. As shown, for normal incidence, the refraction response is fairly insensitive to the frequency of the incident beam. This is ideal for device applications where each frequency component of a beam having a broad spectral content must be refracted at the same angle. At negative incident angles, $\theta_r$ has a strong dependence on $\omega_n$ at the low-frequency extremes of the curves, however this dependence leveled off as $\omega_n$ increased. For example, at $\theta_i = -10^\circ$ in the 0.857 SSL, the change in the refraction angle was $\Delta \theta_r = 36.5^\circ$ ($\theta_r = -69.0^\circ$ to $-32.5^\circ$) for a change in frequency from $\omega_n = 0.2925$ to 0.2975 ($\Delta \omega_n = 0.005$). However, at a higher frequency range ($\omega_n = 0.2975$ to 0.3025), $\Delta \theta_r$ was only 4.7$^\circ$ ($\theta_r = -32.5^\circ$ to $-27.8^\circ$) for the same $\Delta \omega_n$. A similar response was observed at $\theta_i = -20^\circ$ in the 0.571 SSL where $\Delta \theta_r$ was 33.8$^\circ$ at the lower frequency range ($\omega_n = 0.2365$ to 0.2415) and $\Delta \theta_r = 5.4^\circ$ at the higher frequency range ($\omega_n = 0.2415$ to 0.2465). In addition, the refraction response was similar at other negative $\theta_i$. On the other hand, the refraction curves do not have a consistent shape at positive incident angles. For
Figure 6.7: Forward propagation refraction response of the 3s band, SSL 0.857 for multiple frequencies.
Figure 6.8: Forward propagation refraction response of the 3s band, SSL 0.571 for multiple frequencies. Inset shows the corresponding contours.
$\theta_i = 10^\circ$ in the 0.857 SSL, the change in refraction angle was larger, $\Delta \theta_r = 48.6^\circ$ (55.7$^\circ$ to 7.1$^\circ$), than at negative $\theta_i$ for the same change in frequency ($\Delta \omega_n = 0.005$) at the low-frequency range of $\omega_n = 0.289$ to 0.294. Also, at a higher frequency range, the slope does not flatten as at negative $\theta_i$. Thus, a larger $\theta_r$ is achievable if the frequency components of the incident beam have a large range, whereas at negative $\theta_i$, a threshold in $\Delta \theta_r$ is quickly reached because of the flat frequency response. In the 0.571 SSL, the $\Delta \theta_r$ increases slightly in comparison to the 0.857 SSL to $\Delta \theta_r = 49.3^\circ$ (67.4$^\circ$ to 18.1$^\circ$) for the frequency range $\omega_n = 0.2325$ to 0.2375. But at a higher frequency range, $\Delta \theta_r$ decreases slightly to 16.8$^\circ$ (18.1$^\circ$ to 1.3$^\circ$) for the frequency range $\omega_n = 0.2375$ to 0.2425.

6.2.3 The 3p band refraction response

The second shape type is from the lower frequency range of the fourth band and forms an elliptical-like shape in the extended BZ scheme as shown in Figure 6.5(b). At low SL strengths, the sides of the ellipse are relatively flat, forming more of a diamond shape; and as the strength increases, the sides become more curved and the overall shape becomes more elliptical with a major axis along the X–M–X line and a minor axis along Y–M–Y.

Figures 6.10(a) and (b) present the forward propagation refraction responses of the 3p bands under the same conditions as the two SSL structures in the previous section, SSL 0.857 and 0.571, respectively. As the SL strength increases, the beam was refracted more strongly in the negative direction when the incident beam is at normal incidence, as indicated by the y-intercept which lowers from $\sim \theta_r = -10^\circ$ to $\sim -20^\circ$, respectively. Additionally, the flattest regions of the curves are around normal incidence, while the refraction response shows a high gradient away from $\theta_i = 0^\circ$ at the $\theta_i$ extrema. For example, in the 0.857 SSL at $\omega_n = 0.320$, the refraction angle changes only $\Delta \theta_r \approx 8.1^\circ$ for a change in incident angle of $\Delta \theta_i \approx 5^\circ$ ($\theta_i = 0^\circ$ to 5$^\circ$), while at a higher $\theta_i$ (19.4$^\circ$ to 24.3$^\circ$), $\Delta \theta_r = 60.4^\circ$.

Examination of the $\theta_r$ vs. $\omega_n$ relationship (Figures 6.11) for the 3p band revealed that, just as in the 3s band, the refraction response of the 3p band is relatively insensitive to the frequency of the incident beam at higher $\omega_n$ ranges, and strongly dependent upon $\omega_n$ at lower frequency ranges. Unlike the 3s band, this was observed for both positive and
Figure 6.9: Forward propagation refraction response of the 3s band as a function of frequency for (a) SSL 0.875 and (b) SSL 0.571 at multiple incident angles, as indicated by the labels.
negative incident angles; and in both cases, the beam quickly changed from a high $\theta_r$ to a relatively constant $\theta_r$ as $\omega_n$ increased. For example, at $\theta_i = 20^\circ$ in the 0.857 SSL, the refracted beam rapidly moves from $\theta_r = 81.4^\circ$ to 19.6$^\circ$ ($\Delta \theta_r = 61.8^\circ$) when the beam scans a frequency range from 0.3175 to 0.3225 ($\Delta \omega_n = 0.005$).

### 6.3 Propagation visualizations of refraction effects

The analyses in the previous section assumed an infinite plane wave was incident on the SSL PC. Approximating this situation requires a large PC area in comparison to the incident beam width, which works against the ultimate promise of PCs: to reduce the dimensions of optical systems and devices by replacing bulky optical components. Thus, a more realistic situation is considered in this section, where the incident beam has a finite width. For this, FDTD calculations were performed to visualize the beam propagation and confirm the results of the wavevector analysis. While ONYX was used primarily for band structure calculations, a second FDTD code called F2P (Finite-difference time-domain 2D simulator for Photonic devices) was used for beam propagation visualizations. This code is also distributed freely on the worldwide web [76]. F2P is purely 2D, and it is similar to MPB in that the initial conditions are set by an input file which is read in at the beginning of the calculation. Many tools are available to the user including several different sources and detectors that can be placed anywhere in the computational domain. In addition, many geometrical shapes are available as well as several different boundary conditions. An example input file is available in the Appendix.

### 6.3.1 Numerical procedure

Figure 6.12 shows details of the computational domain used in the beam visualization calculations. The measurements were defined using the lattice constant, and an FDTD unit cell was defined as $0.05a \times 0.05a$. The entire domain was $70a \times 200a$ in size, with 12–40 FDTD cells of PML along all edges of the domain. The center of the line source was positioned at the middle of the domain in the vertical direction and $5a$ from the left edge of the domain, which is also $5a$ from the PC interface. The width of the line source (the beam width of the Gaussian excitation) was $24a$, and the beam was launched from left to
Figure 6.10: Forward propagation refraction response of the $3p$ band (TE polarization) as a function of incident angle, for (a) SSL 0.857 and (b) SSL 0.571 at multiple frequencies, $r_1 = 0.35a$, $\epsilon_b = 12.0$. 
Figure 6.11: Forward propagation refraction response of the 3p band (TE polarization) as a function of frequency for (a) SSL 0.875 and (b) SSL 0.571 at multiple incident angles, as indicated by the labels, $\theta_1 = 0.35 a$, $\epsilon_b = 12.0$. 

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right across the domain. The SSL-PC area was air holes patterned in silicon ($\epsilon = 12.0$); it was thick, and extended from the top to the bottom of the FDTD domain. The regions to the right and left of the patterned region were either air or silicon, depending on the calculation. In Figure 6.12, these areas are silicon. The SSL pattern was oriented with the $\Gamma - M$ direction parallel to the $x$-direction to match the conditions calculated using the wavevector method. As shown in the expanded view of a region of the SSL-PC area, the $[i, j]$ rows are tilted 30° below the horizontal to align the $\Gamma - M$ direction as described.

Two series of calculations were performed both with a total of 16,500 time steps in the calculation. The first series investigated incident beams with fixed frequencies and varying incident angles, while the second series focused on incident beams at fixed incident angles with varying frequency.

6.3.2 The 3s and 3p band refraction response

FDTD calculations were performed using the parameters described in Section 6.2.1 to confirm the findings of the wavevector analysis. Figure 6.13 shows the dispersion contour around the M-point for the 3s band at $\omega_n = 0.299$, the construction line (dashed line) corresponding to $\theta_i = 0^\circ$ and a silicon Region 1, the direction of propagation of the refracted beam (solid arrow), and an image of the $H_z$ field component from the FDTD calculation. The field snapshot was taken at the final time step of the calculation, $t = 16,500$, and the solid horizontal lines on the image indicate the boundaries of the SSL PC region. As shown, the refracted beam is steered approximately 34° from the $\Gamma - M$ direction, with remarkable beam collimation. This was in close agreement with the wavevector analysis (Figure 6.6(c)) which predicted $-30^\circ$. Figure 6.14 plots the results for $\theta_i = 4^\circ$. Again, the results of the beam visualization ($\theta_r \approx -3^\circ$) matches well with wavevector analysis ($\theta_r = 1^\circ$). However, the beam shows moderate spreading. This is due to the finite beam size and the curvature of the dispersion contour near the construction line. The beam spreading effect can be reduced by either operating at a flatter region of the dispersion contour, or by widening the excitation beam; however, the latter option increases device sizes. Figure 6.15 shows the refraction response for $\theta_i = 8^\circ$. The refracted beam is dramatically steered to $\theta_r = 73^\circ$, 162
**Figure 6.12:** Details of the computational domain used to for beam visualization calculations using the FDTD method.
which is almost a $\Delta \theta_r = 110^\circ$ change in the beam direction for only $8^\circ$ change in the incident angle. Wavevector analysis predicted only a $\Delta \theta_r = 88^\circ$ since $\theta_r = 58^\circ$ for $\theta_i = 8^\circ$. Also notice that the beam is well-collimated again. This is due to the relatively flat curvature of the contour in proximity to the construction line at this particular incident angle, as shown in Figure 6.15.

The FDTD calculations were repeated for a Region 1 consisting of air to confirm the results of the wavevector analysis, and to confirm that the results were not unique to the silicon and SSL-PC system. Using air in Region 1 shortens $k_{1\parallel}$ with respect to the Si system, which in turn increases $\theta_i$ in order to achieve the same magnitude in $k_{\parallel}$ as the Si system. Incident angles were chosen to match the position of the construction lines in Figures 6.13- 6.15, $\theta_i = 0^\circ, 14^\circ,$ and $31^\circ$, respectively. Figure 6.16 summarizes the results with all three construction lines in the contour plot and the beam images in sequence from bottom ($0^\circ$) to top ($31^\circ$). As shown, the results are practically identical to the silicon-PC system, confirming that the refraction response is valid for multiple materials systems.

Figure 6.17(a) and (b) presents a comparison of the results of the beam propagation calculations and the wavevector analysis for the $3s$ and $3p$ bands of the SSL 0.857 with air in Region 1. The scattered points represent the angles measured through the center of the refracted beam. Error in the measurements was caused by uncertainty in the beam direction due to beam divergence or weak coupling of the incident beam to the excited beam. For the $3s$ band, there was fair agreement between the wavevector method and the beam visualizations, unlike the results for the $3p$ band where adequate correlation was only found near $\theta_i = 0^\circ$. This is attributed to the curvatures of the contours in the respective bands. The $3s$ band has two regions of relatively flat curvature facing different directions that provides a forward propagating beam. Thus, a finite beam width will be well collimated as it is refracted. On the other hand, the $3p$ band has two flat regions that are not facing significantly different directions. The remaining regions of the $3p$ contour show high curvature which destroys the collimation of the incident beam.

The results presents show that a finite beam size impacted the refraction results. In particular, regions of the contours that have large amounts of curvature cause the incident
Figure 6.13: Beam propagation visualization of the refraction response of the 3s band of the SSL (strength 0.857) at normal incidence ($\theta_i = 0^\circ$) along the $\Gamma - M$ direction at a normalized frequency of 0.299.
Figure 6.14: Beam propagation visualization of the refraction response of the 3s band of the SSL (strength 0.857) at $\theta_i = 4^\circ$ off of the $\Gamma - M$ direction at a normalized frequency of 0.299.
Figure 6.15: Beam propagation visualization of the refraction response of the 3s band of the SSL (strength 0.857) at $\theta_i = 8^\circ$ off of the $\Gamma - M$ direction at a normalized frequency of 0.299.
Figure 6.16: Beam propagation visualization of the refraction response of the 3s band of the SSL (strength 0.857) at $\theta_i = 0^\circ$, $14^\circ$, and $31^\circ$ off of the $\Gamma - M$ direction at a normalized frequency of 0.299 for air in Region 1.
Figure 6.17: Comparison of the results of beam propagation visualization (scattered points) and wavevector analysis (lines) of the refraction response of (a) the 3s band and (b) the 3p band of the SSL (strength 0.857) at various $\omega_n$. 
beam to spread and deteriorate within the PC. However, the 3s band showed good collimation and beam steering greater than 100° for a change in incident angle of 8°. As mentioned earlier, the degree of beam divergence can be reduced by increasing the beam width. In the calculations presented, if $a = 358$ nm, the beam width was $\approx 12 \, \mu\text{m}$. However, increasing the beam width requires a larger PC area, thus there exists trade-off between device size and performance.
CHAPTER VII

TUNABLE SUPERLATTICE PC STRUCTURES

Up to this point, the optical response of the PC structures discussed has been dictated by the lattice periodicity, the fill fraction, and the dielectric constant of the structures. These parameters are fixed at a single excitation frequency and intensity, thus light propagation effects are passive, and once the structure is fabricated, the optical properties cannot change. However, the ability to dynamically alter propagation properties by actively changing one of these parameters while under excitation will result in many new properties and applications. For example, the refractive index of the structure can be modified through the use of electro-optic (EO) or nonlinear materials (NL) [14, 110, 48, 65, 84, 102, 70] or mechanical deformation can modify the lattice period [109, 67].

Busch and John were the first to propose the dynamic tuning of the PBG by using an index tunable material, such as liquid crystal (LC), to coat the interior of an opal structure [14]. Experimentally, Leonard et al. found that infiltrating a 2D PC structure of air pores in silicon with LC allowed temperature dependent tunability of the air band edge frequency of 70 nm. However, the maximum theoretical tuning of the air band edge of 113 nm was not achieved because pinning of the LC molecules limited the alignment of the director to an escaped-radial configuration, which limited the E7 refractive index tuning to below the maximum change in index of refraction, $\Delta n$, of 0.2. Regardless, the amount of tunability was sufficient to allow applications as tunable filters, microcavities, waveguides, or lasers.

The tunable optical properties of PCs are not only limited to PBG effects, and in 2002, Park et al. proposed that refraction effects could be tuned using NL or EO materials infiltrated in a triangular lattice PC structure [66]. The pure 2D triangular lattice offered a considerable degree of tunability, however this effect decreased when examined in a 2D slab waveguide configuration. Coupling this decrease in effectiveness with the pinning effect mentioned previously, and the magnitude of the tunability become quite limited [70]. To
overcome this, Park and Summers proposed a 2D SL PC configuration which was more sensitive to changes in refractive index [70]. While the refraction sensitivity was increased with their structure, the superlattice strength still was limited by the index tunability of the refractive index of the LC infiltrate (Δn from 0 to 0.4). We proposed a solution to this by hybridizing the SSL structure of the previous chapter with various dynamic PC structure schemes [59, 58, 56]. In this way, a greater superlattice strength was possible through the design of the hole diameters, allowing a greater range of tunability. Also, the blending of the superlattice structure with a nonlinear background (such as PLZT) will increase switching speeds in comparison to LC.

In this chapter we review the potential of these different schemes. In particular this research has focused on characterizing the tunability of three active SL structures presented in Figure 7.1: a) the E/O static superlattice (ESSL), b) the infiltrated static superlattice (ISSL), and c) the hybrid superlattice (HSL). Common to all three structures is the SSL formed as in the previous chapter by modulating hole radii in adjacent [0 1] rows. Figure 7.1 (a), air holes are patterned into an EO material such as lead lanthanum zirconium titanate (PLZT) [59], while the structures in Figure 1(b) and (c) are patterned in silicon and infiltrated with liquid crystal (LC). Structures (a) and (b) are large area addressable between top and bottom planes, while the third (c) is inter-digitally addressable in that the rows of different radii are individually biased or unbiased to enhance/deactivate the superlattice effect.

7.1 The E/O static superlattice tunable PC

Recently, Leonard et al. infiltrated a 3D PC with LC and observed that they could only achieve 60% of the full index change because of pinning of the LC molecules [48]. This would limit the tunability that was predicted by Park and Summers because the effectiveness of their superlattice structure relies upon the LC index contrast between adjacent rows of holes. In addition, LC response time is very slow (ms) in comparison to alternative electro-optic (EO) materials, such as lead lanthanum zirconate titanate (PLZT)(GHz) as was proposed by Scrymgeour et al. and Xiong et al. for use as the PC background medium [84, 102]. In
Figure 7.1: Three static superlattice configurations with dynamic tuning of the optical response through an externally applied bias: a) the infiltrated static superlattice (ISSL), b) the E/O static superlattice (ESSL), and c) the hybrid superlattice (HSL).
response to these two effects, we propose a solution for increasing the superlattice strength by building in a refractive index contrast directly into the PC lattice by alternating the radius of adjacent rows of holes between two values. This creates what we call a ‘static’ superlattice [55]. Using an EO material as the host for the static superlattice, Figure 7.1(a), reintroduces tunability to the superlattice PC and dynamic functionality.

7.1.1 The superlattice strength

In order to achieve tunable refraction effects in the superlattice PC structure, previous work focused on using EO or NL material in the holes of the structure, such as LC [70, 88, 66]. Here, we follow the concept of Scrymgeour et al. and Xiong et al. and pattern a static superlattice of air holes into an EO material such as lead lanthanum zirconate titanate (PLZT) which has an EO coefficient of $\sim 4 \times 10^{-16} \text{m}^2/\text{V}^2$. This translates to an index tunability of $\Delta n \approx 0.12$ [84, 102]. The difference in hole radii between rows $i$ and $j$ effectively creates a refractive index modulation between adjacent rows if we average the refractive index of a row $j$ hole over the area of a row $i$ hole. The additional area $A_\delta$ between rows $i$ and $j$ of holes has the refractive index of the background $n_b$, as shown in Figure 7.2. Therefore, this amount of additional material in a row $j$ hole should be averaged over the entire area of a row $i$ hole to find the effective index $n_{\text{eff}}$ of the row $j$ hole which is given by:

$$n_{\text{eff}} = \left[ \epsilon_b \left( 1 - \left( \frac{r_2}{r_1} \right)^2 \right)^2 + \epsilon_c \left( \frac{r_2}{r_1} \right)^2 \right]^{1/2}$$

(7.1)

which was defined previously in Equation 3.16. For example, a change in radius of $\Delta r = 0.15a$, from $r_1 = 0.35a$ to $r_2 = 0.2a$, is equivalent to a change in refractive index $\Delta n = 1.003$ between rows of holes for a background of unbiased PLZT, $n = 2.49$. Naturally, this is an oversimplification of the actual structure since it neglects the actual change in the dimensions of the dielectric/air interface for each hole. However, it is convenient because it allows a comparison of the magnitude of the modulation between rows of the static superlattice to the dynamic superlattice previously reported. From Equation 7.1, the magnitude of the index modulation between rows is directly related to the difference
Figure 7.2: Schematic defining the terms in Equation 7.1. The amount of area change in the structure when the radius is reduced can be used to calculate the effective index of a row $j$ hole.
between the hole radii. Consequently, we use the radius ratio \( r_2/r_1 \) to refer to the ‘strength’ of the superlattice.

### 7.1.2 Computational method

Computations were performed in 2D and 3D using the plane-wave expansion [31] (PWE) and finite difference time-domain (FDTD) methods [15, 96, 69], respectively. The 2D calculations served as approximations to the 2D-PC slab waveguide, which are the actual devices that are fabricated. Since the 2D PWE method offers increased speed and reduced computational load of the over 3D FDTD calculations, the majority of the calculations were performed using PWE. However, we are aware that real 2D-PC devices are of a finite thickness, requiring 3D calculations that account for effects such as the guided-mode condition of a slab waveguide. This effect relies on index confinement in the out-of-plane direction, and it is more accurately modeled using FDTD since FDTD will explicitly include the guiding conditions in the calculations[69]. One drawback of the FDTD method is the large computational load for a full 3D calculation, extending computation time greatly. Thus, the amount of 3D calculations done was limited only to confirm that the results observed in the PWE calculations are valid for a slab waveguide.

### 7.1.3 Results

Figures 7.3(a) and (b) present the band structures for a conventional and a static superlattice 2D PC made from PLZT, with an increase in superlattice strength from \( r_2/r_1 = 1.0 \) to 0.571, respectively. Note that in Figure 7.3(a), we assume an infinitesimal \( \Delta r \) so that a comparison to the regular triangular lattice PC band structure can be made. We observed that in this band structure both the photonic band gap and the other photonic bands do not change in character between conventional and SL band structures, as expected. However in Figure 7.3(b), the band structure is shown to be strongly affected by the modulation of the hole radii and several effects are observed. The most pronounced is on the full PBG which decreases by 80.2% for an unbiased slab and 79.6% for a biased slab when \( \Delta r_2 = 0.15a \). The decrease in width of the PBG with decrease in \( r_2 \) is expected because by reducing \( r_2 \) we are effectively increasing the overall effective index of the system.
Figure 7.3: Band structures for the ESSL (a) with an infinitesimal modulation in the hole radii, and (b) with a modulation of $\Delta r = 0.15$. In all figures in this section, the solid line represents the unbiased PLZT case ($\epsilon = 6.2$), while the dashed line represents the biased case ($\epsilon = 6.75$).
and decreasing the number of lattice elements that scatter the longer wavelength photons. With less scattering events, there is less probability of Bragg refraction occurring as light propagates in the SSL-PC. This is confirmed by the lack of movement of the dielectric band and the significant movement of the air band to lower frequencies.

Figure 7.4 shows the dispersion contours for the superlattice structure of Figure 7.3(b) for a normalized frequency range of 0.359 to 0.373. Again, the solid curves indicate the dispersion contours of the unbiased PC, while the dashed lines indicate the biased case. The modulation introduced by the different hole radii increases the curvature of the dispersion contour modes along the $Y - M$ and the $M - X$ directions in comparison to the superlattice of infinitesimal $\Delta r$. The result is a gap between modes along the $Y - M$ direction and beam refraction at normal incidence along the $\Gamma - M$ direction. As shown, the dispersion contours of the unbiased and biased cases are similar in shape, however, they are shifted due to the change in refractive index of the slab. This allows for a tunable refraction response of the PC controlled by an external bias that is applied to the slab as indicated by Figure 7.5 which plots the change in a beam’s refracted angle as a function of its incident angle at a normalized frequency of $\omega_n = 0.366$ for $r_2/r_1 = 0.571$.

Figure 7.5 was derived using $k$-vector diagrams on the dispersion contours of Figure 7.4 using the Russell et al. technique described in Chapter 6. The solid line indicates the refraction behavior of the unbiased ESSL, while the dashed line is the behavior of the biased ESSL. Here, we have defined a positive angle as counter-clockwise to the normal to the PC/air interface. Notice that at normal incidence, the beam experiences some refraction in both the biased and unbiased cases. Also the the refracted angle increases rapidly with a small change in incident angle. For example, at an incident angle of $14^\circ$ the refracted beam will refract by $\approx 55.2^\circ$ when the PC is unbiased. However, when the slab is biased, the shift of the dispersion contours decreases the magnitude of the refraction to $\approx 3.7^\circ$. Essentially, a refracted beam can continuously scan over a range of $> 55^\circ$ with a change in refractive index of $\Delta n = 0.108$ induced by an applied bias on the slab.
Figure 7.4: Dispersion contours for a PLZT ESSL of strength $r_2/r_1 = 0.571$ under two different biasing conditions: unbiased (solid lines) or biased (dashed lines).
Figure 7.5: Optical response of the PLZT static superlattice at a normalized frequency of 0.366.
7.1.4 Conclusion

The optical properties of PCs can be dynamically changed by incorporating NL or EO materials into the device structure so that the refractive index of these elements can be altered. Tuning the refraction behavior of a 2D-PC is attractive because of potential applications in beam steering and switching. Structures with these materials as the lattice elements or as the lattice background have been previously proposed and their optical responses reported. However, in these reports, large changes in the refractive index were necessary for an input beam to be refracted $5 - 10^\circ$. A solution was proposed by Park and Summers that involved creating a PC superlattice through modulation of the refractive index between adjacent rows of holes. In this section, a tunable 2D-PC design that is a modification of the dynamic superlattice was proposed. In this design, the background medium itself is composed of an EO material, such as PLZT, while the lattice structure consists of holes of two different radii arranged in such a way to create a superlattice structure. The PLZT host material allows modification of the optical properties of this structure so that an electrical bias changes the dielectric constant from 6.2 to 6.75. Numerical calculations show the band structure of the superlattice can be highly modified in comparison to the triangular lattice with the first full photonic band gap decreasing in size and band splitting occurring at high symmetry points of the lattice. Analysis of the dispersion contours using $k$-vector diagrams yielded the refraction angle as a function of the incident angle of an input beam. By changing the biasing conditions on the structure, the refracted beam can be tuned by $> 55^\circ$ at an incident angle of $14^\circ$ for a 0.55 change in the dielectric constant. This represents an increase of functionality over the regular triangular lattice infiltrated with LC which is tunable for a range of $5 - 10^\circ$ for a change in dielectric constant of 1.36 and an increase in performance over the PLZT triangular lattice of Scrymgeour et al. In addition to a large tunability of refraction, the proposed superlattice will also show large dispersive behavior, ideal for wavelength-division demultiplexing systems or any other system requiring a separation of an input signal into different wavelength signals. The impact of this effect will be explored in future work.
7.2 The Hybrid Infiltrated Superlattice

7.2.1 Introduction

Photonic crystals (PCs) possess a k-space dispersion surface, analogous to the Fermi surface, which is dramatically different from an isotropic material, opening up the possibility of giant refraction effects, huge dispersion (the superprism effect), and large modifications of the photon group velocity [21, 80, 49, 42, 61, 69]. In a typical PC, these light propagation effects are passive since they depend upon refractive index, lattice period, and feature size. However, the ability to dynamically alter propagation properties by actively changing one of these parameters while under excitation can lead to many new effects. For example, the refractive index of the structure can be modified through the use of electro-optic (EO) or nonlinear materials (NL) [69, 14, 48, 65, 84, 102, 110] or mechanical deformation can modify the lattice period [67, 109]. Experimentally, Leonard et al. found that infiltrating a 2D triangular lattice of air pores in silicon with a liquid crystal (LC) allowed temperature dependent tunability of the air band edge frequency. However, the maximum theoretical tuning of the air band edge was not achieved because pinning of the LC molecules limited the alignment of the director to an escaped-radial configuration, which reduced the E7 refractive index tuning to below the maximum $\Delta n$ of 0.2. To overcome this, Park and Summers proposed a superlattice PC configuration which is more sensitive to changes in refractive index [70]. However, the superlattice strength of this structure was also limited by the index tunability of the refractive index of the LC which in principle can range from $0 < \Delta n < 0.6$. In the current work, we present several new lattice structures with dynamic refractive index tuning that offer significant improvements over the triangular lattice and which allow greater control over the superlattice strength due to a superlattice periodicity formed by using holes of two different radii together with the use of EO or NL materials.

7.2.2 Tunable superlattice structures

Figure 7.1 illustrates the three tunable superlattice structures discussed in the current section. Common to all three structures is the additional lattice periodicity formed by modulating the hole radius in adjacent [1 0] rows of a triangular lattice [55]. In Figure
7.1(a), the air holes are patterned into an EO material such as lead lanthanum zirconium titanate (PLZT) [59], while the structures in Figure 7.1(b) and (c) are patterned in silicon and infiltrated with LC. Structures (a) and (b) are large area addressable between top and bottom planes, while the third (c) has an interdigital addressing scheme in that the rows of different radii can be individually biased, or unbiased, to enhance/deactivate the superlattice effect. In all three structures, a superlattice strength of \( \frac{r_2}{r_1} = 0.3a/0.35a = 0.857 \) was used, where \( a \) is the lattice constant of the triangular lattice [55, 59].

Calculations of the dispersion surface were performed using the 2D plane wave expansion method [31] on a k-space mesh of 125 x 125 points in the irreducible BZ. The refractive index of silicon was taken to be 3.464, for PLZT the index was varied between 2.475 to 2.598 [84, 102], and between 1.5 to 1.7 for the LC. The beam propagation direction inside the PC as a function of the incident angle was calculated using k-vector analysis as discussed by Russell, Kosaka, and others [80, 42, 5] for a beam traveling in the \( \Gamma - M \) direction. Results for TE polarization are presented, however a similar analysis can be made for the TM case.

The introduction of the hole modulated superlattice has been shown to decrease the photonic band gap (PBG) width, lift modal degeneracies of specific bands [55], and cause drastic modifications to the dispersion surface through BZ folding effects [70]. The decrease in the PBG is attributed to the decrease in hole radii and the subsequent addition of dielectric material to the structure. The lifting of modal degeneracies is a consequence of the BZ folding and the reduction of the symmetry of the lattice from six- to two-fold. Most importantly, the dispersion contours (constant frequency plots of the dispersion surface) become significantly different from the triangular lattice because of the interaction between the folded dispersion surfaces in the new rectangular BZ. For example, refraction from the curve radiating from the M point occurs even at normal incidence, (eg. light incident along the \( \Gamma - M \) direction) [55], in strong contrast to lattices with no superlattice periodicity (triangular or square) and bulk isotropic materials where refraction is symmetric across \( \theta_i = 0^\circ \).

Electro-optic or nonlinear elements in the PC structure allow an electrically or optically applied bias to increase or decrease the refractive index of the structural elements. Biasing
the LC infiltrated structures parallel to the hole axes aligns the LC director parallel to the hole walls. For TE polarization this is perpendicular to the $E$-field plane, thus decreasing the refractive index of the holes. This raises the frequency of the air bands accordingly and changes the shape of the dispersion contours, which in turn, tunes the propagation direction of the refracted beam inside the PC. A similar effect occurs in the EO large area addressed superlattice PC.

### 7.2.3 Numerical results and discussion

Figure 7.6(a) shows the biased (solid black lines) and unbiased (dashed red lines) band structures for the large area addressed infiltrated structure (Figure 7.1(b)) indicating the $3s$ and $3p$ bands that split from degenerate states of band 3 in the triangular lattice [55]. Figures 7.6(b) and (c) show the dispersion contours and refraction response of the $3p$ band of the large area addressed infiltrated superlattice structure (Figure 7.1(b)) under biased and unbiased conditions. The incident beam direction is measured relative to the $\Gamma - M$ direction, which is the normal direction of the air-PC interface. The gray lines parallel to $\Gamma - M$ in Figure 7.6(b) are the construction lines that indicate the conservation of the tangential wavevector component across the air-PC interface for the various incident angles, $\theta_i$, at the fixed normalized frequency, $\omega_n = 0.273$, of the excitation beam. As shown in Figure 7.6(c), the refraction angle, $\theta_r$, increases with increasing $\theta_i$, until $\theta_r$ reaches $60^\circ$, at which point the contour intersects the BZ boundary. Also with increasing $\theta_i$, the refraction response is positive, negative, then positive again. This refraction response is typical for all three structures for the $3p$ band, except for one biasing configuration of the interdigital scheme (Figure 7.1(c)) for which the refraction response is closer to that of a triangular lattice. This difference occurs because the interdigital biasing scheme enables independent control over the refractive indices of the holes in relation to the refractive index of the background. For example in case 1, the smaller holes are biased (lower index) and the larger holes are unbiased (higher index). Thus, the larger holes have a higher index and closely match the area-averaged-index of the smaller holes, thus minimizing the strength of the superlattice formed by the different hole sizes. This results in a refraction response closer to the triangular
Figure 7.6: (a) Band structures, (b) dispersion contours and (c) refraction response of the 3p band of the large area addressed infiltrated superlattice structure (Figure 7.1(b)) at a normalized frequency of $\omega_n = 0.273$. 
lattice, where the contours have a flatter shape across the Γ – M line; rather than the more curved dispersion contour of the superlattice. In case 2, the smaller holes are unbiased and the larger holes are biased so that the refractive index modulation strengthens the superlattice that is created by the different hole radii, thus the dispersion contours have a more rounded shape across the Γ – M line as in the other two structures, Figures 7.1(a) and (b). This effect is interesting since it can be used to switch between a non-refracting to a refracting regime at normal incidence, $\theta_i = 0^\circ$. However, the large area biased structures offer greater refraction tunability from the 3$p$ band than the interdigital structure.

As shown in Figure 7.6(c), a large tunability of refraction angle, $\Delta \theta_r > 55^\circ$, from the 3$p$ band can be achieved when the bias on the structure is switched and the appropriate incident angle is chosen for the excitation beam. However, because the dispersion contours of the 3$p$ band do not show a large change in curvature in the vicinity of the Γ–M line, the incident angle must be chosen so that the construction line intersects one of the dispersion contours near the BZ boundary where the change in curvature is large. For the large area addressed infiltrated superlattice, an incident beam angle of $\theta_i = 14.02^\circ$ and normalized frequency of $\omega_n = 0.273$ produces a maximum tunability of $\Delta \theta_r = 55.3^\circ$ when the bias is switched from $n_h = 1.5$ to 1.7 (see Figure 7.6(c)). This is also found in the EO structure at a value of $\theta_i = 9.97^\circ$ and $\omega_n = 0.394$ which produces $\Delta \theta_r = 53.4^\circ$ when the dielectric constant of the background, $\epsilon_b$, changes from 6.1256 to 6.75. For the interdigital biasing scheme, there are two possible biasing configurations as mentioned earlier. At the same incident angle and normalized frequency given above for the large area addressed infiltrated superlattice, a beam steering of $\Delta \theta_r = 47.74^\circ$ can be achieved when the structure is switched from a uniform bias to case 1 or a steering of $\Delta \theta_r = 54.34^\circ$ for a uniform bias to case 2.

Despite the large degree of beam steering presented above, certain complications arise when using the 3$p$ band in the manner described where the incident angle is chosen so that the construction line intersects one of the contours near the BZ boundary. In particular, when considering a finite excitation beam size, rather than an infinite plane wave source, the conservation condition holds for a range of $k$-values, rather than a single point on the contour. Thus, this introduces a narrow $k$-vector operating region on the dispersion contour.
Figure 7.7: Irreducible BZ dispersion contours and the corresponding refraction response as calculated by the $k$-vector method for (a) the EO superlattice, (b) the large area addressed infiltrated superlattice, and (c) the interdigital addressed superlattice. Case 1: larger holes unbiased ($\epsilon_{h1} = 2.89$), smaller holes biased ($\epsilon_{h2} = 2.25$). Case 2: the opposite configuration ($\epsilon_{h1} = 2.25, \epsilon_{h2} = 2.89$).
When the operation point is chosen to be near a BZ boundary, the range of $k$-values will spread over a region of the contour that exhibits an extremely large curvature. As reported by Baba and others, the large curvature will introduce a large dispersion to a finite beam, causing the excitation to spread rapidly and decay within the PC structure [5]. Thus, either a very wide beam or a different operating regime must be used to obtain the desired effect in the tunable superlattice structures. Example contours from the $3s$ band are shown in Figure 7.7(a). The contour radiating from the M point shows a considerably different shape across the $\Gamma$–M line than the $3p$ band in that the $3s$ band has two flat regions and an inflection point that now lies near the $\Gamma$–M line. Note that this corner is non-symmetric across $\Gamma$–M, with one flat region being longer than the other. This is key in the use of this contour for tunable refraction effects as discussed below.

The top row of Figure 7.7 shows the $3s$ band contours in the irreducible BZ for the three structures in their biased and unbiased states at the normalized frequencies $\omega_n = 0.380$, 0.273, and 0.273, for (a) the EO structure, (b) large area addressed infiltrated, and (c) the interdigital structures respectively. The results of wave vector analysis to calculate the beam refraction angle as a function of incident beam angle with respect to the $\Gamma$–M direction are presented in the bottom row under the corresponding contour plot. We assume the incident beam frequency is fixed and couples only to the $3s$ band contours that radiate from the M point. The refraction response is very different from the $3p$ band as can be seen in Figures 7.7(d-f). Again, the refraction angle cutoff due to the BZ boundary must be $-30^\circ$ on one side and $60^\circ$ on the other. However in the positive refraction angle regime of the $3s$ band, $\theta_r$ can exceed $60^\circ$ briefly because of the contour shape before it reaches the BZ boundary.

This localized peak in the refraction angle in addition to the shallow, flat refraction response of the paired biased scheme allows a dramatic increase in the degree of tunability, $\Delta \theta_r$, that is achievable by the superlattice structure. For example, at a positive incident angle of $20^\circ$ in Figure 7.7(b), the construction line intersects the biased curve along the vertical portion of the contour, sending the incident beam in a negatively refracted direction, while the same line intersects the unbiased curve on the horizontal portion of the contour, sending the beam in a positively refracted direction. The optimum incident angle at a
Figure 7.8: Response of the refraction angle as a function of the refractive index of the LC infiltrate in the large area addressable superlattice structure for (a) band 3s and (b) band 3p at the various fixed incident angles and normalized frequencies indicated.
particular fixed $\omega_n$ for maximum beam steering was found by choosing $\theta_i$ at the peak $\theta_r$ as indicated by the vertical lines in Figure 7.7(d-f). In the large area addressed infiltrated structure, the optimum $\theta_i$ is $20.8^\circ$, where a tunability of $\Delta \theta_r = 96.9^\circ$ can be achieved. This is over $17^\circ$ higher than the EO or interdigital structures where $\Delta \theta_r$ is $79.4^\circ$, $75.6^\circ$ (case 1), or $79.0^\circ$ (case 2), respectively.

The sensitivity of the refraction dependence as a function of relative change in refractive index for the $3s$ and $3p$ bands of the large area addressed infiltrated superlattice are given in Figure 7.8(a) and (b) respectively. These values were calculated at a fixed normalized frequency of $\omega_n=0.264$ and $0.273$ for bands $3s$ and $3p$, respectively, and at the incident angles indicated next to each curve. The curves associated with the $3p$ band show a greater refraction angle sensitivity with a change in the refractive index of the infiltrate; however, recall that this large degree of tunability occurs in the narrow operating regime near the BZ boundary. The curves of band $3s$ show a slower rate of change in refraction angle as the infiltrate is tuned, but the total $\Delta \theta_r$ is almost twice that of band $3p$. Similar analyses were performed for the EO structure and the interdigital structure; however, their performance did not exceed the large area addressed infiltrated superlattice.

### 7.2.4 Conclusion

In the preceding section, we have investigated three dynamically tunable superlattice photonic crystal structures that offer improved performance over the standard triangular lattice configuration. An unprecedented degree of beam steering of $\Delta \theta_r > 96^\circ$ was predicted through a change in refractive index of $\Delta n = 0.2$ of the NL elements of the large area addressable infiltrated structure. While the EO slab structure offers the best performance for high switching speed applications ($\Delta \theta_r > 79^\circ$), the large area addressable infiltrated superlattice offers the highest sensitivity to the refractive index tuning, $\Delta n$. Because of their refraction behavior, these structures can be exploited as optical switches, tunable superprisms, and dynamic-ultra-short focal length lenses.
CHAPTER VIII

CONCLUSIONS

In this work, we have investigated the optical properties of a photonic crystal (PC) lattice that possesses multiple structural periodicities, forming a superlattice (SL). We have proven the hypothesis that the long-range periodicity in the geometry of the lattice produces unique optical phenomena quite different from the triangular lattice upon which the SL is based. The PC structure investigated consisted of a triangular lattice of air holes in which adjacent rows of holes have either one of two radii, $r_1$ or $r_2$, where $r_2 < r_1$. Having two hole sizes forming this configuration generated a new unit cell with a two “atom” basis, reshaping the triangular unit cell of the base lattice into a rectangle.

The SL theory was successfully applied to the new lattice, deriving the new reciprocal space representation of the SL structure which incorporated a structure factor that vanished when $r_1 = r_2$, and introducing the concept of the SL strength, $r_2/r_1$. The reciprocal lattice definition was shown to affect the dispersion relationship of the PC by “folding” the photonic bands of the triangular lattice into the new Brillouin zone (BZ) representation which was rectangular. In addition, the symmetry of the BZ was reduced from six-fold (hexagonal) to two-fold (rectangular). Numerical solutions of Maxwell’s equations showed that the combination of the new BZ and subsequent symmetry reduction greatly affected the dispersion surfaces of the PC which dictate the optical properties of the structure. In addition, increasing the SL strength modifies the distribution of EM energy within the PC structure, splitting modal degeneracies that existed in the triangular lattice, thereby creating new regions of the dispersion surface that were not present in the triangular lattice. For example, at the M-point, the first band above the bandgap splits into two states labeled $3s$ and $3p$ in this work. As the SL strength increases, the width of the frequency gap between these modes at the M-point increases as the $3s$ mode shifts to lower frequencies towards the dielectric band, and the $3p$ shifts to higher frequencies. Both of these effects were
attributed to the redistribution of EM energy in the PC to the dielectric areas as the SL strength increased, \textit{i.e.} as $r_2$ decreased and $r_1$ remained constant.

Experimentally, triangular and SL PC structures were successfully designed and fabricated on single crystal silicon-on-insulator wafers using electron-beam lithography and reactive-ion etching. The coupled resonant band technique was used to directly measure the dispersion relationship of the structures and showed remarkably strong correlations between the calculated and measured photonic band structures, thus confirming the theoretical analysis of the SL PC. In particular, the experimental results showed the same trends as the calculations when structural parameters, such as lattice constant, hole radii, and SL strength, were modified. In addition, first explicit measurements of the band folding effect in multidimensional PCs and the dispersion relation of the dielectric band of a PC were made. The former can lead to a large number of new devices with increased functionality, while the latter achievement can be applied as a technique for measuring the dielectric band of a non-SL PC, advancing the knowledge in the field and thereby providing a new tool for researchers to optimize their designs for applications.

From this basis, the “bulk” propagation properties of the SL PC were investigated via two avenues: wavevector diagrams and beam visualization calculations. Overall, both analysis methods showed that along the $\Gamma - M$ direction the SL structure exhibited giant refraction and superprism effects for frequencies lying within the $3s$ and $3p$ bands. In a structure where the incident beam width is large enough to be approximated by an infinite plane wave, wavevector analysis predicted beam steering over $100^\circ$ for small changes in the incident angle of the beam. The refraction was also strongly dependent upon the frequency of the incident beam, ideal for applications in wavelength-division demultiplexers or miniaturized spectrometers. It was shown that when the excitation beam is of comparable size to the PC lattice, finite beam size effects must be included in the investigations. Beam visualization calculations provided a means for investigating the bulk propagation behavior for finite-sized systems. These calculations revealed that the regions of the dispersion contours with large curvature caused beam spreading in the PC. Thus, a fairly flat curvature is desirable to maintain beam collimation. The $3s$ band, with its rectangular geometry,
provided large refraction (\(\approx 100^\circ\)) while maintaining beam collimation, whereas the \(3p\) band did not show a large change in beam propagation angle when collimation was maintained.

Finally, an investigation was made into the possibility of actively modifying the optical properties of the SL PC by introducing nonlinear or electro-optic materials into the structure. Through band structure and wavevector analysis, it was predicted that the SL offers an improvement over the traditional PC lattice for tunable refraction effects. An unprecedented degree of beam steering of \(\Delta \theta_r > 96^\circ\) was predicted through a change in refractive index of \(\Delta n = 0.2\) of the NL elements of the large area addressable infiltrated structure. While the EO slab structure offers the best performance for high switching speed applications (\(\Delta \theta_r > 79^\circ\)), the large area addressable infiltrated superlattice offers the highest sensitivity to the refractive index tuning, \(\Delta n\).

The field of PCs is continually growing and evolving with new discoveries in the physical interpretation of their optical properties and new devices and application concepts emerging constantly. It is our belief that the work presented in this dissertation will provide a platform for future studies of SL PC configurations as the concepts proposed are applicable to SLs with lattice bases other than triangular. Indeed, further characterization of the refraction properties of the SL should be pursued, quantifying and maximizing the coupling efficiency of the incident beam to structure and analyzing the refraction behavior at the exit side of a SL PC region. A continued pursuit of the SL is also recommended as a means to characterize the dielectric band of PC structures.
APPENDIX A

MPB CONTROL FILE

The following is the control file used for the dispersion surface calculations using the MPB code [33]. This file is read by the executable before the calculation begins, defining the parameters of the size of the computational domain, the geometry of the structure, and the dielectric constants of the different regions of the structure. Also, the size of the \( k \)-point mesh over the BZ is defined as well as the polarization state and number of bands for which the code will solve.

; File name: efcsuperLCholes.ctl
; 2D system: holes in a dielectric patterned to create a superlattice
; Code for doing dispersion surfaces
; written by C. Neff

; first, define the lattice vectors for a rectangular lattice:
(set! geometry-lattice (make lattice (size 1 (sqrt 3) no-size)))
(define-param kz 0) ; use non-zero kz to consider vertical propagation

; Define the BZ mesh that we will use to find the curves
; Default is 50 x 50
(define-param k-mesh 50)
(set! k-mesh (- k-mesh 2))

(define x 0) ; indexing term

; Use the symmetry directions that are parallel to one another to set up
; the mesh.
(define n1 (list (vector3 0 0 0) (vector3 0.5 0 0))) ; make the first segment
; that will be divided.
(define n2 (list (vector3 0 0.5 0) (vector3 0.5 0.5 0))) ; make the second seg.

(set! n1 (interpolate k-mesh n1)) ; make the divisions desired
(set! n2 (interpolate k-mesh n2))

; Now divide up the interior of the BZ and add them to the k-points list

(while (<= x (+ k-mesh 1))(set! k-points (append k-points
(interpolate k-mesh (list (list-ref n1 x))))
(define-param eps 12) ; the dielectric constant of the background
(define-param r1 0.35) ; the radius of hole#1
(define-param r2 0.35) ; the radius of hole#2
(define-param ehole1 1.0) ; the dielectric constant of the hole1
(define-param ehole2 1.0) ; the dielectric constant of hole2
(set! default-material (make dielectric (epsilon eps)))
(set! geometry (list (make cylinder (center 0)
                               (material (make dielectric (epsilon ehole1)))
                               (radius r1) (height infinity))
        (make cylinder (center 0.5 (/ (sqrt 3) 2))
                     (material (make dielectric (epsilon ehole2)))
                     (radius r2) (height infinity))))

(set-param! resolution 64)

; Solve for the number of bands--Default is 4
(set-param! num-bands 4)

(if (= kz 0)
  (begin
    (run-te
     )
  )
(run)); if kz != 0 there are no purely te and tm bands
APPENDIX B

FDTD BEAM VISUALIZATION INPUT FILE

The following is an example input file for the beam visualization calculations using the F2P code [76]. This file is read by the executable before the calculation begins, defining the parameters of the size of the computational domain, the geometry of the structure, and the dielectric constants of the different regions of the structure. Also, the number and size of the time steps are defined, as well as the excitation type and size and the boundary conditions.

Code:
```
########################################################################
# This is an example of the input file for F2P calculations.
# It demonstrates refraction in a PC with a superlattice
# of air holes that is oriented with the Gamma-M direction parallel
# to the x-axis.
#:::------------------------------------------------Prepared by C. Neff
########################################################################
########################################################################
#Calculate the TM or TE modes??
# ==0: TE modes
# ==1: TM modes
0
########################################################################
########################################################################
#Define the materials used in the calculations.
#:::------------------------------------------------
#The number of materials
3
#The dielectric constant, and conductivity of each material
#Index---dielectric constant---conductivity
1 1.0000 0.00E+0 #air
2 12.0000 0.00E+0 #Si (n=3.464)
3 1.00 0.00E+0 #air
#:::----------------------------------
#End of material definition.
#:::------------------------------------------------
#define the size of the computational domain
#:::----------------------------------
#--- lattice constant (For normalized purpose)
1.0
#---Sx------Sy------
70.0 200.0
```

```
#Background materials index
2

#Absorbing boundary condition (ABC)

#---ABC type----------------------------------------------------------
0

#---number of PML layers in X----in Y---------The exponent index for PML
12 12 2.0

#Define parameters for FDTD

#-----Dt_Coe---
0.95

#Number of total time steps
16500

#Output the z-field component in some time steps.
#For snapshot purpose.
#If interval is less than 1, no output.
#The current z-field distribution is always stored in "Fieldz_Bin.dat".
#---Start Time steps---------End Time steps------Interval--------------
5500 11000 -5500

#define the inclusions, could be waveguides, cylinders, ...

#Inclusion type:
# == 1: ellipse
# == 2: quadrilateral
# == 3: triangular

#The total number of inclusions
8

#Inclusion No. 1, r1 circles, layer down 1
#Inclusion Type ----Material index----
1 3
#-----Rx---------Ry---------Xc---------Yc--------Theta--
0.35 0.35 10.00 0.5 0.0
#-----Mx--------Lx--------My--------Ly------Alpha-----(For Repeat)
15 3.4641 100 2.00 0.0

#Inclusion No. 2, r2 circles, layer down 2
<table>
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<th>Inclusion No.</th>
<th>r1 circles, layer down</th>
<th>r2 circles, layer down</th>
</tr>
</thead>
</table>

### Inclusion Type ----Material index----

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#### Rx---------Ry---------Xc---------Yc--------Theta--

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#### Mx--------Lx--------My--------Ly------Alpha-----(For Repeat)

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### Examples of Triangular

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</thead>
<tbody>
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<td>3</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

#### X1------Y1------X2------Y2------X3------Y3---
# 10.5 0.0 24.5 3.964 16.0 9.964
#---Mx-----Lx-----My-----Ly----Alpha---(For Repeat)
# 1 0.00 1 0.00 0.0
########################################################################
#Source part
########################################################################
# For source type: ==1 point source
#
#==2 line source, direction, from P1 to P2, in P3
#
#==3 waveguide mode source
#:
#---Number of Sources---------
# 1
#:
#Source Examples
#---Source Type-----Source frequency (a/lambda)---Pulse Width (Delta_w)---
# 1 0.305 0.007
#---XS-----YS-------- (Point source position)
# 4.0 6.06218
#:
# Gaussian Line Source sample
#For line source, direction == +1(X); -1(-X); +2(+Y); -2(-Y);
#---Source Type-----Source frequency (a/lambda)---Pulse Width (Delta_w)---
# 2 0.25 0.1
#---direction---XS-----YS-----Beam Width---Material Type----Theta-------
# 1 9.00 6.06218 2.0 2 0.0
#:
# Waveguide Source sample
#For Waveguide source, direction == +1(X); -1(-X); +2(+Y); -2(-Y);
#---Source Type-----Source frequency (a/lambda)---Pulse Width (Delta_w)---
# 3 0.295 0.007
#---direction---XS-----YS-----Waveguide Width---Mode Number---------
# 1 1.00 6.06218 2.60 1
#---Material Up (Left)----Material Core----Material Down (Right)-----
# 1 2 1
#:
# Gaussian Line Source sample
#For line source, direction == +1(X); -1(-X); +2(+Y); -2(-Y);
#---Source Type-----Source frequency (a/lambda)---Pulse Width (Delta_w)---
# 2 0.310 -0.1
#---direction---XS-----YS-----Beam Width---Material Type----Theta-------
# 1 5.00 100.0 24.0 2 1.0
########################################################################
#detectors definition
########################################################################
# For detector type: ==1 point detector
#
#==2 line detector
#
#direction == +1(X); -1(-X); +2(+Y); -2(-Y);
#:
#FT frequency range and points in between
#-W_min---------W_max-------NF---
# 0.10 0.40 201
#:
#---Number of Detector---------
# 0
#:
# Line Detector Example

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### Detector Example

<table>
<thead>
<tr>
<th>Type</th>
<th>Starting Time Steps</th>
<th>Ending Time Steps</th>
</tr>
</thead>
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#### Direction

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<th>Yc</th>
<th>Length</th>
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<td>6.06218</td>
<td>4.00</td>
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</tbody>
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---

#### Point Detector Example

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<th>Ending Time Steps</th>
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</thead>
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#### Xc | Yc
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<th></th>
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<tbody>
<tr>
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<td>6.06218</td>
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---
APPENDIX C

FDTD SLAB WAVEGUIDE PC WITHOUT MIRROR SYMMETRY

C.1 An example input file

The following is an example input file for the SWG without mirror symmetry code which is read by the executable before the calculation begins, defining the parameters of the size of the computational domain, the geometry of the structure, the dielectric constants of the slab waveguide material, the bottom oxide layer, the substrate, the background medium, and the holes. Also, the number and size of the time steps are defined.

```
18   ixmax
15   bclayer
30   airlayer
15   slablayer
47   oxide
3    substrate
18   izmax
1.0  Q(1)
1.0  Q(2)
1.732 Q(3)
0.003 dt
0.37388 radius1
0.22151 radius2
0.0  radius_pit1
0.0  radius_pit2
0    pit_depth
12.6736 eps slab
2.09737 eps oxide
2.09737 eps substrate
1.0  cylind1
1.0  cylind2
0.0  akx
0.0  aky
0.0  akz
10   ikmax
32   n_block
2048  block_size
51   n_pts_store
1    n_segment
F    overlap
0.0  damping
```


C.2 The FDTD code

The following is the FDTD code used for calculating the band structure of the 2D SSL SWG PC structure that does not contain mirror symmetry. This code is based upon the ONYX code [96], however major modifications have been made to the dielectric function as well as other subroutines. This code is written in the FORTRAN 90 language and will compile with a variety of commercial and non-commercial FORTRAN 90 compilers.

```fortran
! super_band-nomirror_2.0.f90 Absoft 64FX & Lahey Fortran version.!
! Modifications from v1.0: added substrate to dielectric function
! (see square-slab-pits_1.2.f90) using no mirror BC in the code. Top & Bottom PML
! Code that has multiple layers (substrate, oxide, slab, airlayer)
! and pits in the oxide layer.
! Based on test-slab-nomirror-64fx3.f90 & super_bd-tri-even_64fx1.f90
! Code removes the mirror boundary condition in the slab
! I have added the ability to do cylinders of two different radii.
! This is the modified version of the Order N photonics code
!
! modifications by C.Neff (curtis.neff@mse.gatech.edu) & W. Park
! original (c) Andrew Ward, Imperial College, London. Dec 1997.
!
! $Revision: 2.0 $
! $Date: 27 June 2005 $
! $Source: $
! $Author: C Neff$
!
module interface1
interface
subroutine init_store_pts_band(store_pts,ix_cur,iy_cur,iz_cur,i_pol)
  implicit none
  integer,pointer :: store_pts(:,:)
  integer,intent(in) :: ix_cur,iy_cur,iz_cur,i_pol
end subroutine init_store_pts_band

subroutine initfields(g1,g2,g3,e,h,eps_hat,mu_hat,ix,iy,iz,i_pol)
  implicit none
  real,intent(in) :: g1(3),g2(3),g3(3)
  complex,pointer :: e(:,,:,:,:),h(:,,:,:,:)
  complex,pointer :: eps_hat(:,,:,:,:),mu_hat(:,,:,:,:)
  integer,intent(in) :: ix,iy,iz,i_pol
end subroutine initfields

subroutine defcell(eps,mu,sigma,sigma_m,u1,u2,u3)
  implicit none
  complex,pointer :: eps(:,:,:,:),mu(:,:,:)
  real,pointer :: sigma(:,:,:,:),sigma_m(:,:,:)
  real :: u1(3),u2(3),u3(3)
end subroutine defcell

subroutine renorm(eps,mu,sigma,sigma_m,eps_inv,mu_inv,eps_hat,mu_hat,g,omega)
end subroutine renorm
```

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!

module interface1

interface

subroutine renorm
imPLICIT none
COMPLEX, pointer :: eps(:,:,,:), mu(:,:,,:)
COMPLEX, pointer :: eps_inv(:,:,,:,:), mu_inv(:,:,,:,:)
COMPLEX, pointer :: eps_hat(:,:,,:,:), mu_hat(:,:,,:,:)
REAL, pointer :: sigma(:,:,,:), sigma_m(:,:,,:)
REAL, INTENT(IN) :: g(3,3), omega
end subroutine renorm

subroutine driver(e,h,eps_inv,mu_inv,eps_hat,mu_hat,sigma,sigma_m, &
& fft_data,store_pts,iky)
imPLICIT none
COMPLEX, pointer :: e(:,:,,:)
COMPLEX, pointer :: h(:,:,,:)
COMPLEX, pointer :: eps_inv(:,:,,:,:), mu_inv(:,:,,:,:)
COMPLEX, pointer :: eps_hat(:,:,,:,:), mu_hat(:,:,,:,:)
COMPLEX, pointer :: fft_data(:,:,,:)
REAL, pointer :: sigma(:,:,,:), sigma_m(:,:,,:)
INTEGER, pointer :: store_pts(:,:,)
INTEGER :: iky
end subroutine driver

subroutine postproc_band(fft_data,spectrum,iki,b_cnt)
imPLICIT none
COMPLEX, pointer :: fft_data(:,:,,:)
REAL, pointer :: spectrum(:)
INTEGER :: iki,b_cnt
end subroutine postproc_band

end interface
end module interface1

! ----------------------------------------------------------------------------
module interface2

interface

subroutine int(e_cur,h_cur,e_prev,h_prev,eps_inv,mu_inv,sigma,sigma_m, &
& n_tsteps,iblock,fft_data,store_pts,intcurle,intcurlh,wy)
imPLICIT none
INTEGER, INTENT(IN) :: n_tsteps,iblock
COMPLEX, pointer :: e_cur(:,:,,:), e_prev(:,:,,:), h_cur(:,:,,:), h_prev(:,:,,:)
COMPLEX, pointer :: eps_inv(:,:,,:,:), mu_inv(:,:,,:,:)
COMPLEX, pointer :: fft_data(:,:,,:)
REAL, pointer :: sigma(:,:,,:), sigma_m(:,:,,:)
INTEGER, INTENT(IN) :: store_pts(:,:,)
COMPLEX, pointer :: intcurle(:,:,,:), intcurlh(:,:,,:)
REAL, pointer :: wy(:)
end subroutine int

end interface
end module interface2

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module interface3
interface

subroutine calc_div_B(h,mu_hat,div_B)
imPLICIT none
complex,pointer :: h(:,:,:,:)
complex,pointer :: mu_hat(:,:,:,:,:)
complex,pointer :: div_B(:,:,:)
end subroutine calc_div_B

subroutine calc_div_D(e,eps_hat,div_D)
imPLICIT none
complex,pointer :: e(:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:,:)
complex,pointer :: div_D(:,:,:)
end subroutine calc_div_D

subroutine calc_energy_density(E_cur,E_prev,H_prev,rho,eps_hat,mu_hat)
imPLICIT none
complex,pointer :: E_cur(:,:,:,:)
complex,pointer :: E_prev(:,:,:,:)
complex,pointer :: H_prev(:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:,:)
complex,pointer :: mu_hat(:,:,:,:,:)
real,pointer :: rho(:,:,:)
end subroutine calc_energy_density

subroutine calc_current(J,e_cur,h_cur,h_prev,ix,iy,iz)
imPLICIT none
complex,intent(out) :: J(3)
complex,pointer :: e_cur(:,:,:,:),h_cur(:,:,:,:)
complex,pointer :: h_prev(:,:,:,:)
integer,intent(in) :: ix,iy,iz
end subroutine calc_current

end interface
end module interface3

module interface4
interface

subroutine power_spec(f,spectrum)
imPLICIT none
complex,pointer :: f(:,:)
real,pointer :: spectrum(:)
end subroutine power_spec

end interface
end module interface4

module interface5
interface

subroutine bc_xmin_bloch(e,h)
imPLICIT none

end subroutine bc_xmin_bloch
end interface
end module interface5
complex, pointer :: e(:,:,:,:) 
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmin_bloch

subroutine bc_xmax_bloch(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmax_bloch

subroutine bc_ymin_bloch(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymin_bloch

subroutine bc_ymax_bloch(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymax_bloch

subroutine bc_zmin_bloch(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmin_bloch

subroutine bc_zmax_bloch(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmax_bloch

subroutine bc_xmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmin_metal

subroutine bc_xmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmax_metal

subroutine bc_ymin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymin_metal

subroutine bc_ymax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymax_metal

subroutine bc_zmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmin_metal

subroutine bc_zmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmax_metal

subroutine bc_xmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmin_metal

subroutine bc_xmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmax_metal

subroutine bc_ymin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymin_metal

subroutine bc_ymax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymax_metal

subroutine bc_zmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmin_metal

subroutine bc_zmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmax_metal

subroutine bc_xmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmin_metal

subroutine bc_xmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmax_metal

subroutine bc_ymin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymin_metal

subroutine bc_ymax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymax_metal

subroutine bc_zmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmin_metal

subroutine bc_zmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmax_metal

subroutine bc_xmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmin_metal

subroutine bc_xmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmax_metal

subroutine bc_ymin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymin_metal

subroutine bc_ymax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymax_metal

subroutine bc_zmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmin_metal

subroutine bc_zmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmax_metal

subroutine bc_xmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmin_metal

subroutine bc_xmax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_xmax_metal

subroutine bc_ymin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymin_metal

subroutine bc_ymax_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_ymax_metal

subroutine bc_zmin_metal(e,h)
implicit none
complex, pointer :: e(:,:,:,:)
complex, pointer :: h(:,:,:,:)
end subroutine bc_zmin_metal

subroutine bc_zmax_metal(e,h)
implicit none
complex,pointer :: e(:,:,:,:)
complex,pointer :: h(:,:,:,:)
end subroutine bc_zmin_metal

subroutine bc_zmax_metal(e,h)
implicit none
complex,pointer :: e(:,:,:,:)
complex,pointer :: h(:,:,:,:)
end subroutine bc_zmax_metal

subroutine PML_e(e_cur,e_prev,h_prev,intcurlh,wy,eps_inv)
implicit none
complex,pointer :: e_cur(:,:,:,:),e_prev(:,:,:,:),h_prev(:,:,:,:)
complex,pointer :: intcurlh(:,:,:)
complex,pointer :: eps_inv(:,:,:,:)
real,intent(in) :: wy(:)
end subroutine PML_e

subroutine PML_h(e_cur,h_cur,h_prev,intcurle,wy,mu_inv)
implicit none
complex,pointer :: e_cur(:,:,:,:),h_cur(:,:,:,:),h_prev(:,:,:,:)
complex,pointer :: intcurle(:,:,:)
complex,pointer :: mu_inv(:,:,:,:)
real,intent(in) :: wy(:)
end subroutine PML_h

subroutine bc_ymin_mirror_even(e,h)
complex,pointer :: e(:,:,:,:)
complex,pointer :: h(:,:,:,:)
end subroutine bc_ymin_mirror_even

subroutine bc_ymax_mirror_even(e,h)
complex,pointer :: e(:,:,:,:)
complex,pointer :: h(:,:,:,:)
end subroutine bc_ymax_mirror_even

end interface
end module interface5

!----------------------------------------------------------------------------
module interface6
interface
subroutine FFT(f,isign)
implicit none
integer,intent(in) :: isign
complex,pointer :: f(:,:)
end subroutine FFT

subroutine FT(f,isign)
implicit none
integer,intent(in) :: isign
complex,pointer :: f(:,:)
end subroutine FT

end interface
end module interface6
module matrices
interface

function matinv3(A,emach,fail)
imPLICIT none
complex,dimension(3,3) :: matinv3
complex,intent(in) :: A(3,3)
real,intent(in) :: emach
logical,intent(out) :: fail
end function matinv3

function cross_prod(a,b)
imPLICIT none
real,dimension(3) :: cross_prod
real,intent(in) :: a(3),b(3)
end function cross_prod

end interface
end module matrices

module physconsts
!
! Use Atomic units
! c0=Speed of light
! pi=3.1415...
! emach=Machine accuracy
real,parameter :: pi=3.14159265358979323846
real,parameter :: c0=137.0360
real,parameter :: eps0=1.0/(4.0*pi)
real,parameter :: mu0=1.0/(eps0*c0**2)
real,parameter :: abohr=5.291772e-11
real :: x
real,parameter :: emach=epsilon(x)
complex,parameter :: ci=(0.0,1.0)
end module physconsts

module files
!
! Set the unit numbers for the files we want to access
integer,parameter :: logfile=10,infile=11,outfile=12,fields=13
end module files

module parameters
!
! Define the run-time parameter list. These will be read in from a file
! ixmax, iymax, izmax define the number of mesh points in each of the
! principle directions
! itmax and dt are the number and size of timesteps respectively
! akx, aky, akz are the components of the k-vector expressed on the reciprocal
! lattice. They are normalised by the mesh spacing in the relevent direction
! ie. akx = (Q1*ixmax)*kx
! ikmax = No. of k-points
! Q(3) is the matrix holding the mesh spacing in each direction
! n_block : Break down itmax into ‘n_block’ blocks each of ‘block_size’ time
! steps. Fields can be written out, div’s calculated etc at the end of each block
! itmax=n_block*block_size
! n_pts_store : The number of real space points at which we store the fields
! For the FFT the itmax timesteps can be split up into segments which can be
either overlapping or not. For details see Numerical Receipes pg 425ff.
If overlap=.true. then itmax=fft_size*(n_segment+1)
If overlap=.false. then itmax=fft_size*(2*n_segment)
In both cases fft_size is the size the segment which is fourier transformed
so must be a power of 2.

integer :: ixmax,iymax,izmax,itmax,ikmax,n_block,block_size,n_pts_store
real :: Q0,Q(3),dt,akx,aky,akz
real (8) :: radius1,radius2,radius_pit1, radius_pit2
real (8) :: epsslab,epsox,epssub,epsil_h1,epsil_h2
integer :: n_segment,fft_size
integer :: bclayer,airlayer,slablayer,oxide,substrate,pit_depth
logical :: overlap
real :: damping
end module parameters

! ------------------end parameters-------------------------------------

program onyx
use interface1
use parameters
use physconsts
use files
implicit none

! Define necessary variables
integer :: ios,ik,ik2,ik3,iki,iky,ix_cur,iy_cur,iz_cur,i_pol,b_cnt
integer,pointer :: store_pts(:,:)
complex,pointer :: e(:,:,:,:)
complex,pointer :: h(:,:,:,:)
complex,pointer :: eps(:,:,:),mu(:,:,:)
complex,pointer :: eps_inv(:,:,:,:,:),mu_inv(:,:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:,:),mu_hat(:,:,:,:,:)
complex,pointer :: fft_data(:,:)
real,pointer :: sigma(:,:,:),sigma_m(:,:,:),spectrum(:)
real :: u1(3),u2(3),u3(3)
real :: g1(3),g2(3),g3(3)
real :: g(3,3),omega
character (len=10) :: date,zone
character (len=50) :: logname,outname,fieldsname,inname
character (len=256) :: LINE,EXE,wdir
character (len=30) :: time
integer :: dt1(8),dt2

! Read simulation number
call getarg(1,LINE)
call getarg(0,EXE)
call getcwd(wdir)
logname = "log.sl.band-multi.dat"
outname = "out.sl.band-multi.dat"
fieldsname = "fields.sl.band-multi.dat"
inname = "infile.sl.band-multi.dat"

!Attach simulation number to the file names
if (len_trim(LINE)>0) then
  logname = "log.sl.band-multi" // trim(LINE) // ".dat"
  outname = "out.sl.band-multi" // trim(LINE) // ".dat"
  fieldsname = "fields.sl.band-multi" // trim(LINE) // ".dat"
endif
inname = "infile.sl.band-multi" // trim(LINE) // ".dat"
end if

! Open the neccessary files
open(unit=logfile,file=trim(logname),status='replace',action='write')
open(unit=outfile,file=trim(outname),status='replace',action='write')
open(unit=fields,file=trim(fieldsname),status='replace',action='write')
open(unit=infile,file=trim(inname),status='old',action='read',iostat=ios)
if (ios.ne.0) call err(1)

! Read system clock
call date_and_time(date,time,zone,dt1)
write(logfile,'(A11,1X,I4,A1,I2,A1,I2,I5,A1,I2,A1,I2)') 'Time stamp:', &
& dt1(1),'/',dt1(2),'/',dt1(3), dt1(5),':',dt1(6),':',dt1(7)
dt2=dt1(7)+60*dt1(6)+60*60*dt1(5)+24*60*60*dt1(3)
write(logfile,*) 'Simulation ran with program: ',trim(EXE)
write(logfile,*) 'Command line argument: ', trim(LINE)

! Set the run time parameters
call setparam()

! Allocate arrays for fields
allocate (e(3,0:ixmax+1,0:iymax+1,0:izmax+1))
allocate (h(3,0:ixmax+1,0:iymax+1,0:izmax+1))
allocate (fft_data(n_pts_store,itmax))
allocate(spectrum(fft_size))
allocate(store_pts(n_pts_store,4))
spectrum=0.0
fft_data=0.0

! Define the unit vectors for the co-ordinate system

! Default
u1=/(1.0,0,0,0,0,0/)
u2=/(0.0,1.0,0,0,0,0/)
u3=/(0.0,0,0,1,0,0/)
call defmetric(u1,u2,u3,g1,g2,g3,g,omega)

! Initialise position dependent eps & mu
allocate (eps(ixmax,iymax,izmax),mu(ixmax,iymax,izmax))
allocate (sigma(ixmax,iymax,izmax),sigma_m(ixmax,iymax,izmax))
call defcell(eps,mu,sigma,sigma_m,u1,u2,u3)
close(unit=fields)
print *, 'Definition of dielectric function done'

! Define the effective eps**-1, mu**-1 for the generalised co-ordinates
allocate (eps_inv(3,3,ixmax,iymax,izmax),mu_inv(3,3,ixmax,iymax,izmax))
allocate (eps_hat(3,3,ixmax,iymax,izmax),mu_hat(3,3,ixmax,iymax,izmax))
call renorm(eps,mu,sigma,sigma_m,eps_inv,mu_inv,eps_hat,mu_hat,g,omega)

! counter for output
b_cnt=0
! added inner loop for complete band calculation
k_seg: do iki = 0,4

! Loop required for test band structure calculation
k_loop: do ik=0,ikmax-1,1

! Set the value for akx, aky, akz. akx=kx*(Q1*ixmax) etc.
if (iki==0) then
  ! Definitions of akx, akz for test band structure calculation: Gamma - M
  if (ikmax>1) akx=pi*ik/real(ikmax)
  if (ikmax>1) akz=pi*ik/real(ikmax)
elseif (iki==1) then
  ! Definitions of akx, akz for test band structure calculation: M - Y
  if (ikmax>1) akx=pi-pi*ik/real(ikmax)
  if (ikmax>1) akz=pi
elseif (iki==2) then
  ! Definitions of akx, akz for test band structure calculation: Y - Gamma
  if (ikmax>1) akx=0
  if (ikmax>1) akz=pi-pi*ik/real(ikmax)
elseif (iki==3) then
  ! Definitions of akx, akz for test band structure calculation: Gamma - X
  if (ikmax>1) akx=pi*ik/real(ikmax)
  if (ikmax>1) akz=0
else
  ! Definitions of akx, akz for test band structure calculation: X - M
  if (ikmax>1) akx=pi
  if (ikmax>1) akz=pi*ik/real(ikmax)
endif

iz_cur=2
iy_cur=1
ix_cur=2
i_pol=1

! Initialise store_pts which hold the locations of the points
! at which we store the fields
! For the band structure
call init_store_pts_band(store_pts,ix_cur,iy_cur,iz_cur,i_pol)

! Initialise fields
! For the band structure
call initfields(g1,g2,g3,e,h,eps_hat,mu_hat,ix_cur,iy_cur,iz_cur,i_pol)

! Transfer control to central driver
write(logfile,*) 'Begin main calculation'
iki=iki+1
iky=iki*ikmax+ik+1
call driver(e,h,eps_inv,mu_inv,eps_hat,mu_hat,sigma,sigma_m, k &
  & fft_data,store_pts,iky)
write(logfile,*) 'End main calculation'
! Postprocess if necessary

! For the band structure
call postproc_band(fft_data, spectrum, iki, b_cnt)
b_cnt=b_cnt+1

! End of loops over k
enddo k_loop
enddo k_seg

! Final postprocessing if necessary

! Tidy up!
write(logfile,*) 'Execution terminated normally'

! call system clock again

call date_and_time(date, time, zone, dt1)
dt2=dt1(7)+60*dt1(6)+60*60*dt1(5)+24*60*60*dt1(3)-dt2

dt1(7)=mod(dt2,60)
dt2=dt2/60

dt1(6)=mod(dt2,60)
dt2=dt2/60

dt1(5)=mod(dt2,24)
dt2=dt2/24

write(logfile,'(A24,I2,A6,I2,A5,I2,A5,I2,A4)')&
& 'Total simulation time = ', &
& dt2,' days ',dt1(5),' hrs ',dt1(6),' min ',dt1(7),' sec'

close(unit=logfile)
close(unit=outfile)
close(unit=infile)

deallocate (e,h,eps,mu,sigma,sigma_m,eps_inv,mu_inv,eps_hat,mu_hat)
deallocate (spectrum,fft_data)
deallocate(store_pts)

stop
end program onyx

! Subroutine driver
! Heart of the calculation. This subroutine actually does the time integration
! loop. Should be made to be as flexible as possible
! -----------------------------------------------------------------------------
subroutine driver(e_cur,h_cur,eps_inv,mu_inv,eps_hat,mu_hat,sigma,sigma_m, &
& fft_data,store_pts,iky)
use interface2
use interface3
use interface5
use interface6
use parameters
use files
use physconsts
implicit none

complex,pointer :: e_cur(:,:,:,,:)
complex,pointer :: h_cur(:,:,:,,:)
complex,pointer :: eps_inv(:,:,:,,:)

allocate(e_prev(3,0:ixmax+1,0:iymax+1,0:izmax+1))
allocate(h_prev(3,0:ixmax+1,0:iymax+1,0:izmax+1))
allocate(wy(iymax))
allocate(intcurle(ixmax,iymax,izmax))
allocate(intcurlh(ixmax,iymax,izmax))

! Initialize 2nd set of fields

e_prev=(0.0,0.0)
h_prev=(0.0,0.0)

intcurle=(0.0,0.0)
intcurlh=(0.0,0.0)

! Initialize the absorbing boundary layer PML
write(logfile,*) 'Define the absorbing boundary layer'
w=0.0
do i=1,bclayer
   w(i)=120.0*((bclayer-i)**2/(real(bclayer-1)**2)
   write(logfile,*) 'wy', i, w(i)
enddo

do i=iymax-bclayer+1,iymax
   w(i)=w(iymax+1-i)
   write(logfile,*) 'wy',i,w(i)
enddo

dt_dum=0
maintime: do iblock=1,n_block

! Various tests on the fields can be performed here...

! Update the remain boundaries prior to calculating divs

call bc_xmax_bloch(e_cur,h_cur)
call bc_ymax_metal(e_cur,h_cur)
call bc_zmax_bloch(e_cur,h_cur)

! Write out the fields to a file
!write(fields,*) e_cur

enddo maintime

dallocate(e_prev,h_prev)
dallocate(wy)
dallocate(intcurle,intcurlh)
return
end subroutine driver

! Subroutine int
! Do the time integration for nt time steps
! -----------------------------------------------------------------------------
subroutine int(e_cur,h_cur,e_prev,h_prev,eps_inv,mu_inv,sigma,sigma_m, &
& nt,iblock,fft_data,store_pts,intcurle,intcurlh,wy)
  use interface5
  use interface6
  use physconsts
  use parameters
  implicit none

  integer,intent(in) :: nt,iblock
  complex,pointer :: e_cur(:,:,:,:)
  complex,pointer :: e_prev(:,:,:,:)
  complex,pointer :: h_cur(:,:,:,:)
  complex,pointer :: h_prev(:,:,:,:)
  complex,pointer :: eps_inv(:,:,:,:,:)
  complex,pointer :: mu_inv(:,:,:,:,:)
  complex,pointer :: fft_data(:,:)
  real,pointer :: sigma(:,:,:),sigma_m(:,:,:)
  integer,intent(in) :: store_pts(:,:)
  complex,pointer :: intcurle(:,:,:),intcurlh(:,:,:)
  real,pointer :: wy(:)

  integer :: ix,iy,iz,it,i_pts
  complex :: curl(3)
  real :: dtcq2
  complex,pointer :: temp(:,:,:,:)

  dtcq2=(dt*c0/Q0)**2

  time: do it=1,nt

    ! Current fields become previous fields
    temp=>e_cur
    e_cur=>e_prev
    e_prev=>temp

    temp=>h_cur
    h_cur=>h_prev
    h_prev=>temp

    ! First the E-fields
    do iz=1,izmax
      do iy=bclayer+1,iymax
        ! do something with iz and iy
      enddo
    enddo

    ! do something with time
  enddo

end subroutine int
do ix=1,ixmax
  ! Define Curl H
  curl(1)=h_prev(3,ix,iy,iz)-h_prev(3,ix,iy-1,iz) &
  & -h_prev(2,ix,iy,iz)+h_prev(2,ix,iy,iz-1) &
  & -h_prev(1,ix,iy,iz)+h_prev(1,ix,iy-1,iz) &
  curl(2)=h_prev(1,ix,iy,iz)-h_prev(1,ix,iy,iz-1) &
  & -h_prev(3,ix,iy,iz)+h_prev(3,ix-1,iy,iz) &
  & -h_prev(1,ix,iy,iz)+h_prev(1,ix,iy-1,iz) &
  curl(3)=h_prev(2,ix,iy,iz)-h_prev(2,ix-1,iy,iz) &
  & -h_prev(1,ix,iy,iz)+h_prev(1,ix,iy-1,iz) &

  ! Integrate fields in time
  e_cur(1,ix,iy,iz)=(1.0-sigma(ix,iy,iz))*e_prev(1,ix,iy,iz)+ &
  & (eps_inv(1,1,ix,iy,iz)*curl(1) &
  & +eps_inv(1,2,ix,iy,iz)*curl(2) &
  & +eps_inv(1,3,ix,iy,iz)*curl(3)) &
  e_cur(2,ix,iy,iz)=(1.0-sigma(ix,iy,iz))*e_prev(2,ix,iy,iz)+ &
  & (eps_inv(2,1,ix,iy,iz)*curl(1) &
  & +eps_inv(2,2,ix,iy,iz)*curl(2) &
  & +eps_inv(2,3,ix,iy,iz)*curl(3)) &
  e_cur(3,ix,iy,iz)=(1.0-sigma(ix,iy,iz))*e_prev(3,ix,iy,iz)+ &
  & (eps_inv(3,1,ix,iy,iz)*curl(1) &
  & +eps_inv(3,2,ix,iy,iz)*curl(2) &
  & +eps_inv(3,3,ix,iy,iz)*curl(3)) &
endo
endo
endo

! Update Berenger type PML equations for the E-field
! (Absorbing boundary layer)
call PML_e(e_cur,e_prev,h_prev,intcurlh,wy,eps_inv)

! Update the boundary conditions needed for the E-fields
call bc_xmax_bloch(e_cur,h_cur)
call bc_ymax_metal(e_cur,h_cur)
call bc_zmax_bloch(e_cur,h_cur)

! Then the H-fields
do iz=1,izmax
  do iy=bclayer+1,iymax
    do ix=1,ixmax
      ! Define Curl E
      curl(1)=e_cur(3,ix,iy+1,iz)-e_cur(3,ix,iy,iz) &
      & -e_cur(2,ix,iy,iz+1)+e_cur(2,ix,iy,iz) &
      & -e_cur(1,ix+1,iy,iz)+e_cur(1,ix,iy,iz) &
      curl(2)=e_cur(1,ix,iy,iz+1)-e_cur(1,ix,iy,iz) &
      & -e_cur(3,ix+1,iy,iz)+e_cur(3,ix,iy,iz) &
      & -e_cur(1,ix+1,iy,iz)+e_cur(1,ix,iy,iz) &
      curl(3)=e_cur(2,ix+1,iy,iz)-e_cur(2,ix,iy,iz) &
      & -e_cur(1,ix,iy+1,iz)+e_cur(1,ix,iy,iz) &
      & -e_cur(1,ix,iy+1,iz)+e_cur(1,ix,iy,iz)

      ! Integrate the fields in time
\begin{verbatim}

h_cur(1,ix,iy,iz)=1.0/(1.0+sigma_m(ix,iy,iz))* &
  (h_prev(1,ix,iy,iz)-dtcq2* &
  (mu_inv(1,1,ix,iy,iz)*curl(1) &
  +mu_inv(1,2,ix,iy,iz)*curl(2) &
  +mu_inv(1,3,ix,iy,iz)*curl(3)))

h_cur(2,ix,iy,iz)=1.0/(1.0+sigma_m(ix,iy,iz))* &
  (h_prev(2,ix,iy,iz)-dtcq2* &
  (mu_inv(2,1,ix,iy,iz)*curl(1) &
  +mu_inv(2,2,ix,iy,iz)*curl(2) &
  +mu_inv(2,3,ix,iy,iz)*curl(3)))

h_cur(3,ix,iy,iz)=1.0/(1.0+sigma_m(ix,iy,iz))* &
  (h_prev(3,ix,iy,iz)-dtcq2* &
  (mu_inv(3,1,ix,iy,iz)*curl(1) &
  +mu_inv(3,2,ix,iy,iz)*curl(2) &
  +mu_inv(3,3,ix,iy,iz)*curl(3)))

enddo
enddo
enddo

! Update Berenger type PML equations for the H-field (Absorbing boundary layer)
call PML_h(e_cur,h_cur,h_prev,intcurle,wy,mu_inv)

! Update the boundary conditions needed for the H-fields
call bc_xmin_bloch(e_cur,h_cur)
call bc_zmin_bloch(e_cur,h_cur)
call bc_ymin_metal(e_cur,h_cur)

! Store points for Fourier transform later
do i_pts=1,n_pts_store
  if (store_pts(i_pts,1)<4) then
    fft_data(i_pts,it+(iblock-1)*nt)=e_cur(store_pts(i_pts,1), &
    store_pts(i_pts,2),store_pts(i_pts,3),store_pts(i_pts,4))
    else
    fft_data(i_pts,it+(iblock-1)*nt)=h_prev(store_pts(i_pts,1)-3, &
    store_pts(i_pts,2),store_pts(i_pts,3),store_pts(i_pts,4))
  endif
endo
do time
return
end subroutine int
\end{verbatim}
integer :: nbits, set_bits, i

write(logfile,*) 'Read in parameters'

read(infile,*) ixmax
if (ixmax<1) call err(2)
write(logfile, '(A1,A12,I10)') '#', 'ixmax=', ixmax
write(outfile, '(A1,A12,I10)') '#', 'ixmax=', ixmax
print *, 'ixmax=', ixmax

read(infile,*) bclayer
if (bclayer<1) call err(2)
write(logfile, '(A1,A12,I10)') '#', 'bclayer=', bclayer
write(outfile, '(A1,A12,I10)') '#', 'bclayer=', bclayer
print *, 'bclayer=', bclayer

read(infile,*) airlayer
if (airlayer<1) call err(2)
write(logfile, '(A1,A12,I10)') '#', 'airlayer=', airlayer
write(outfile, '(A1,A12,I10)') '#', 'airlayer=', airlayer
print *, 'airlayer=', airlayer

read(infile,*) slablayer
if (slablayer<1) call err(2)
write(logfile, '(A1,A12,I10)') '#', 'slablayer=', slablayer
write(outfile, '(A1,A12,I10)') '#', 'slablayer=', slablayer
print *, 'slablayer=', slablayer

print *, 'slab thickness=', float(slablayer)*2/float(ixmax), 'a'

read(infile,*) oxide
if (oxide<1) call err(2)
write(logfile, '(A1,A12,I10)') '#', 'oxide=', oxide
write(outfile, '(A1,A12,I10)') '#', 'oxide=', oxide
print *, 'oxide layer=', oxide
print *, 'oxide thickness=', float(oxide)/float(ixmax), 'a'

read(infile,*) substrate
if (substrate<1) call err(2)
write(logfile, '(A1,A12,I10)') '#', 'substrate=', substrate
write(outfile, '(A1,A12,I10)') '#', 'substrate=', substrate
print *, 'substrate layer=', substrate

iymax = 2*bclayer + substrate + oxide + slablayer + airlayer
write(logfile, '(A1,A12,I10)') '#', 'iymax=', iymax
write(outfile, '(A1,A12,I10)') '#', 'iymax=', iymax
print *, 'iymax=', iymax

read(infile,*) izmax
if (izmax<1) call err(2)
write(logfile, '(A1,A12,I10)') '#', 'izmax=', izmax
write(outfile, '(A1,A12,I10)') '#', 'izmax=', izmax
print *, 'izmax=', izmax

read(infile,*) Q(1)
if (Q(1)<=0.0) call err(2)
write(logfile, '(A1,A12,F15.5)') '#', 'Q(1)=', Q(1)
write(outfile, '(A1,A12,F15.5)') '#', 'Q(1)=', Q(1)

read(infile,*) Q(2)
if (Q(2)<=0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','Q(2)=',Q(2)
write(outfile,'(A1,A12,F15.5)') '#','Q(2)=',Q(2)

read(infile,*) Q(3)
if (Q(3)<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','Q(3)=',Q(3)
write(outfile,'(A1,A12,F15.5)') '#','Q(3)=',Q(3)

read(infile,*) dt
if (dt<=0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','dt=',dt
write(outfile,'(A1,A12,F15.5)') '#','dt=',dt
print *, 'dt=',dt

read(infile,*) radius1
if (radius1<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','radius1=',radius1
write(outfile,'(A1,A12,F15.5)') '#','radius1=',radius1
print *, 'radius1=',radius1

read(infile,*) radius2
if (radius2<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','radius2=',radius2
write(outfile,'(A1,A12,F15.5)') '#','radius2=',radius2
print *, 'radius2=',radius2

read(infile,*) radius_pit1
if (radius_pit1<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','radius_pit1=',radius_pit1
write(outfile,'(A1,A12,F15.5)') '#','radius_pit1=',radius_pit1
print *, 'radius_pit1=',radius_pit1

read(infile,*) radius_pit2
if (radius_pit2<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','radius_pit2=',radius_pit2
write(outfile,'(A1,A12,F15.5)') '#','radius_pit2=',radius_pit2
print *, 'radius_pit2=',radius_pit2

read(infile,*) pit_depth
if (pit_depth<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','pit_depth=',pit_depth
write(outfile,'(A1,A12,F15.5)') '#','pit_depth=',pit_depth
print *, 'pit_depth=',pit_depth

read(infile,*) epsslab
if (epsslab<=0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','eps slab=',epsslab
write(outfile,'(A1,A12,F15.5)') '#','eps slab=',epsslab
print *, 'Slab layer eps=',epsslab

read(infile,*) epsox
!if (dt<=0.0) call err(2)
write(logfile,'(A1,A12,F10.7,F10.7)') '#','epsox=',epsox
write(outfile,'(A1,A12,F10.7,F10.7)') '#','epsox=',epsox
print *, 'oxide layer eps=',epsox

read(infile,*) epssub
!if (dt<=0.0) call err(2)
write(logfile,'(A1,A12,F10.7,F10.7)') '#', 'epssub=', epssub
write(outfile,'(A1,A12,F10.7,F10.7)') '#', 'epssub=', epssub
print *, 'substrate epsilon=', epssub

read(infile,*) epsil_h1
if (epsil_h1<=0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#', 'epsilon_h1=', epsil_h1
write(outfile,'(A1,A12,F15.5)') '#', 'epsilon_h1=', epsil_h1
print *, 'Cylinder 1 epsilon=', epsil_h1

read(infile,*) epsil_h2
if (epsil_h2<=0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#', 'epsilon_h2=', epsil_h2
write(outfile,'(A1,A12,F15.5)') '#', 'epsilon_h2=', epsil_h2
print *, 'Cylinder 2 epsilon=', epsil_h2

read(infile,*) akx
if (akx<0.0.or.akx>pi) call err(2)
write(logfile,'(A1,A12,F10.5)') '#', 'akx=', akx
write(outfile,'(A1,A12,F10.5)') '#', 'akx=', akx

read(infile,*) aky
if (aky<0.0.or.aky>pi) call err(2)
write(logfile,'(A1,A12,F10.5)') '#', 'aky=', aky
write(outfile,'(A1,A12,F10.5)') '#', 'aky=', aky

read(infile,*) akz
if (akz<0.0.or.akz>pi) call err(2)
write(logfile,'(A1,A12,F10.5)') '#', 'akz=', akz
write(outfile,'(A1,A12,F10.5)') '#', 'akz=', akz

read(infile,*) ikmax
if (ikmax<0) call err(2)
write(logfile,'(A1,A12,I10)') '#', 'ikmax=', ikmax
write(outfile,'(A1,A12,I10)') '#', 'ikmax=', ikmax
print *, 'ikmax=', ikmax

read(infile,*) n_block
if (n_block<1) call err(2)
write(logfile,'(A1,A12,I10)') '#', 'n_block=', n_block
write(outfile,'(A1,A12,I10)') '#', 'n_block=', n_block
print *, 'n_block=', n_block

read(infile,*) block_size
if (block_size<1) call err(2)
write(logfile,'(A1,A12,I10)') '#', 'block_size=', block_size
write(outfile,'(A1,A12,I10)') '#', 'block_size=', block_size
print *, 'block_size=', block_size

itmax=n_block*block_size
write(logfile,'(A1,A12,I10)') '#', 'itmax=', itmax
write(outfile,'(A1,A12,I10)') '#', 'itmax=', itmax
print *, 'itmax=', itmax

read(infile,*) n_pts_store
if (n_pts_store<0) call err(2)
write(logfile,'(A1,A12,I10)') '#', 'n_pts_store=', n_pts_store
write(outfile,'(A1,A12,I10)') '#', 'n_pts_store=', n_pts_store
print *, 'n_pts_store=', n_pts_store
read(infile,*) n_segment
if (n_segment<1) call err(2)
write(logfile,'(A1,A12,I10)') '#','n_segment=',n_segment
write(outfile,'(A1,A12,I10)') '#','n_segment=',n_segment

read(infile,*) overlap
write(logfile,'(A1,A12,L5)') '#','overlap=',overlap
write(outfile,'(A1,A12,L5)') '#','overlap=',overlap

if (overlap) then
   fft_size=itmax/(n_segment+1)
else
   fft_size=itmax/(2*n_segment)
endif
if (fft_size<1) call err(2)

nbits=bit_size(fft_size)
set_bits=0
i=0
do
   if (i==nbits.or.set_bits>1) exit
   if (btest(fft_size,i)) set_bits=set_bits+1
   i=i+1
endo
do if (set_bits>1) call err(2)

read(infile,*) damping
write(logfile,'(A1,A12,F10.5)') '#','damping=',damping
write(outfile,'(A1,A12,F10.5)') '#','damping=',damping
if (damping<0.0) call err(2)
return
end subroutine setparam

!----------------------------------------------------------------------
! Subroutine initfields
! Set up the initial values of the E & H fields
! Should be able to read fields in from a file
! or set them to some appropriate analytic form
!----------------------------------------------------------------------
subroutine initfields(g1,g2,g3,e,h,eps_hat,mu_hat,ix_cur,iy_cur,iz_cur,i_pol)
use interface3
use interface5
use matrices
use files
use parameters
use physconsts
implicit none

real,intent(in) :: g1(3),g2(3),g3(3)
complex,pointer :: e(:,:,:,:),h(:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:),mu_hat(:,:,:,:)
integer,intent(in) :: ix_cur,iy_cur,iz_cur,i_pol

integer :: ix,iy,iz,jx,jy,jz,i
real :: G(3),k(3),v(3),k_plus_G(3)
complex :: vec(3), h0(3), expo
complex, pointer :: div(:, :, :)
real :: dtcq2

write(logfile,*) 'Initialize fields in initfields'

dtcq2=(dt*c0/Q0)**2
e=(0.0,0.0)
h=(0.0,0.0)

! Set up initial fields

! Initial fields following Chan, Yu and Ho's Order N paper
! Can be used for Band structure

v=(/1.0,1.0,1.0/)

! Loops over jx, jy, jz loop over the required reciprocal lattice vectors

do jz=-5,5
  do jy=-5,5
    do jx=-5,5
      G=2.0*pi*(g1*(jx)/real(ixmax)+g2*(jy)/real(iymax)+g3*(jz)/real(izmax))
      k=(akx/real(ixmax))*g1+(aky/real(iymax))*g2+(akz/real(izmax))*g3
      k_plus_G=k+G
      vec(1)=exp(ci*(k_plus_G(1)))-1.0
      vec(2)=exp(ci*(k_plus_G(2)))-1.0
      vec(3)=exp(ci*(k_plus_G(3)))-1.0
      h0(1)=v(2)*vec(3)-v(3)*vec(2)
      h0(2)=v(3)*vec(1)-v(1)*vec(3)
      h0(3)=v(1)*vec(2)-v(2)*vec(1)

    do iz=1,izmax
      do iy=1,iymax
        do ix=1,ixmax
          expo=exp(ci*(k_plus_G(1)*ix+k_plus_G(2)*iy+k_plus_G(3)*iz))
          do i=1,3
            h(i,ix,iy,iz)=h(i,ix,iy,iz)+h0(i)*expo
          enddo
        enddo
      enddo
    enddo
  enddo
enddo

! Gaussian field profile

!!$ do ix=1,ixmax+1
!!$ do iy=1,iymax+1
!!$ do iz=1,izmax+1
!!$  e(1,ix,iy,iz)=-dt*(0.0,1.0)*exp(-(((ix-ixmax/2)**2)/0.0001) &
!!$    *exp(-((iy-iymax/2)**2)/0.0001) &
!!$    *exp(-((iz-izmax/2)**2)/0.0001)
!!$1  e(1,ix,iy,iz)=(1.0,0.0)*exp(-((iz-2)**2)/1.0)
!!$!  h(1,ix,iy,iz)=(dt*c0/(Q(3)))*e(1,ix,iy,iz)
!!$enddo
!!$enddo
!!$enddo
!!$endif

! Delta function
! Needed for DOS, can be used for band structure

!!$if (i_pol<4) then
!!$  e(i_pol,ix_cur,iy_cur,iz_cur)=-dt*(0.0,1.0)*Q(i_pol)
!!$else
!!$  h(i_pol-3,ix_cur,iy_cur,iz_cur)=dt*(0.0,1.0)*Q(i_pol-3)
!!$endif

! Initialise the boundaries

!!$call bc_xmax_metal(e,h)
!!$call bc_ymax_metal(e,h)
!!$call bc_zmax_metal(e,h)
!!$
!!$call bc_xmin_metal(e,h)
!!$call bc_ymin_metal(e,h)
!!$call bc_zmin_metal(e,h)

! Optional: Test that the fields are divergence free here?

!allocate(div(ixmax,iymax,izmax))
!call calc_div_B(h,mu_hat,div)
!write(logfile,*) 'Sum div B',sum(abs(div))
!if (maxval(abs(div))>10.0e+3*emach) call err(6)
!call calc_div_D(e,eps_hat,div)
!write(logfile,*) 'sum div D',sum(abs(div))
!if (maxval(abs(div))>10.0e+3*emach) call err(5)
!deallocate(div)

return
end subroutine initfields
real :: u1(3), u2(3), u3(3)
complex :: epsset1, epsset2, eps_s, eps_h1, eps_h2
integer :: ix, iy, iz, i, j, l, m, isub, iatom
real :: asub, test, r(3), g(3, 3), vol, xhalf, zhalf
real :: r1, r2, r3, atom(3, 5)

write(logfile,*) 'Define unit cell'

! Set up the default parameters for the unit cell

! radius = ratio of the radius of cylinder to the unit cell
! eps_h1, h2 = dielectric constant for cylinder
! eps_s = dielectric constant for background medium
! isub = number of sub-divisions in average over each lattice point

eps=(1.0, 0.0, 0.0)
mu=(1.0, 0.0, 0.0)
sigma=(0.0, 0.0, 0.0)
sigma_m=(0.0, 0.0, 0.0)

! Position the holes

atom(1, 1)=0.0
atom(2, 1)=0.0
atom(3, 1)=0.0

atom(1, 2)=1.0
atom(2, 2)=0.0
atom(3, 2)=0.0

atom(1, 3)=0.0
atom(2, 3)=0.0
atom(3, 3)=1.0

atom(1, 4)=1.0
atom(2, 4)=0.0
atom(3, 4)=1.0

atom(1, 5)=0.5
atom(2, 5)=0.0
atom(3, 5)=0.5

! Setup air (top) and substrate (bottom) regions

do ix=1, ixmax
   do iz=1, izmax
      do iy=1, bclayer+substrate
         eps(ix, iy, iz)=epssub
enddo

do iy=bclayer+substrate+oxide+slablayer+1,iymax
  eps(ix,iy,iz)=(1.0,0.0)
endo
enddo

doiy=bclayer+substrate+oxide+slablayer+1,iymax
eps(ix,iy,iz)=(1.0,0.0)
endo
enddo
enddo

! Setup oxide region
eps_s=cmplx(epsox)
eps_h1=cmplx(epsil_h1)
eps_h2=cmplx(epsil_h2)
r1=radius_pit1**2
r2=radius_pit2**2
isub=10

vol=0.0
do ix=1,ixmax
do iz=1,izmax
  asub=1.0/float(isub)
test=0.0
epsset1=0.0
epsset2=0.0
do l=1,isub
do m=1,isub
  do iatom=1,4
    r(1)=Q(1)*((ix-1+(l-1)*asub)/float(ixmax)-atom(1,iatom))
    r(2)=0.0
    r(3)=Q(3)*((iz-1+(m-1)*asub)/float(izmax)-atom(3,iatom))
    r3=0.0
    do i=1,3
do j=1,3
      r3=r3+(g(i,j)*r(i)*r(j))
  enddo
endo
endo
if (r3.lt.r1) epsset1=epsset1+1.0
if (r3.lt.r1) test=test+1.0
endo
r(1)=Q(1)*((ix-1+(l-1)*asub)/float(ixmax)-atom(1,5))
  r(2)=0.0
  r(3)=Q(3)*((iz-1+(m-1)*asub)/float(izmax)-atom(3,5))
  r3=0.0
  do i=1,3
do j=1,3
    r3=r3+(g(i,j)*r(i)*r(j))
  enddo
endo
endo
if (r3.lt.r1) epsset2=epsset2+1.0
if (r3.lt.r1) test=test+1.0
endo
endo
epsset1=epsset1/float(isub**2)
epsset2=epsset2/float(isub**2)
test=test/float(isub**2)

! Write the dielectric function Oxide region
! Bottom oxide with no pits
do iy=bclayer+substrate+1,bclayer+substrate+oxide-pit_depth
  eps(ix,iy,iz)=epsox
endo
Oxide pit region

\[
\text{do } iy=bclayer+substrate+oxide-pit_depth+1, bclayer+substrate+oxide
\]

\[
\text{eps}(ix,iy,iz)=epsset1*\varepsilon_1+epsset2*\varepsilon_2+(1-epsset1-epsset2)*\varepsilon_s
\]

\text{enddo}

\[
\text{vol} = \text{vol} + \text{test}
\]

\text{enddo}

\text{enddo}

Setup Slab region

\[
\text{eps}_s=\text{cmplx}(\varepsilon_{sslab})
\]

\[
\text{eps}_h1=\text{cmplx}(\varepsilon_{slab})
\]

\[
\text{eps}_h2=\text{cmplx}(\varepsilon_{ilab})
\]

\[
\text{r}_1=\text{radius}_1^{**2}
\]

\[
\text{r}_2=\text{radius}_2^{**2}
\]

\[
\text{isub}=10
\]

\[
\text{vol}=0.0
\]

\[
\text{do } ix=1,ixmax
\]

\[
\text{do } iz=1,izmax
\]

\[
\text{asub}=1.0/\text{float}(\text{isub})
\]

\[
\text{test}=0.0
\]

\[
\text{epsset1}=0.0
\]

\[
\text{epsset2}=0.0
\]

\[
\text{do } l=1,\text{isub}
\]

\[
\text{do } m=1,\text{isub}
\]

\[
\text{do } iatom=1,4
\]

\[
\text{r}(1)=Q(1)*((ix-1+(l-1)*asub)/\text{float}(ixmax)-\text{atom}(1,iatom))
\]

\[
\text{r}(2)=0.0
\]

\[
\text{r}(3)=Q(3)*((iz-1+(m-1)*asub)/\text{float}(izmax)-\text{atom}(3,iatom))
\]

\[
\text{r}_3=0.0
\]

\[
\text{do } i=1,3
\]

\[
\text{do } j=1,3
\]

\[
\text{r}_3=\text{r}_3+(g(i,j)*r(i)*r(j))
\]

\text{enddo}

\text{enddo}

\[
\text{if } (\text{r}_3.\text{lt}.\text{r}_1) \text{ epsset1}=\text{epsset1}+1.0
\]

\[
\text{if } (\text{r}_3.\text{lt}.\text{r}_1) \text{ test}=\text{test}+1.0
\]

\text{enddo}

\[
\text{r}(1)=Q(1)*((ix-1+(l-1)*asub)/\text{float}(ixmax)-\text{atom}(1,5))
\]

\[
\text{r}(2)=0.0
\]

\[
\text{r}(3)=Q(3)*((iz-1+(m-1)*asub)/\text{float}(izmax)-\text{atom}(3,5))
\]

\[
\text{r}_3=0.0
\]

\[
\text{do } i=1,3
\]

\[
\text{do } j=1,3
\]

\[
\text{r}_3=\text{r}_3+(g(i,j)*r(i)*r(j))
\]

\text{enddo}

\text{enddo}

\[
\text{if } (\text{r}_3.\text{lt}.\text{r}_2) \text{ epsset2}=\text{epsset2}+1.0
\]

\[
\text{if } (\text{r}_3.\text{lt}.\text{r}_2) \text{ test}=\text{test}+1.0
\]

\text{enddo}

\text{enddo}

\[
\text{epsset1}=\text{epsset1}/\text{float}(\text{isub}^{**2})
\]

\[
\text{epsset2}=\text{epsset2}/\text{float}(\text{isub}^{**2})
\]

\[
\text{test}=\text{test}/\text{float}(\text{isub}^{**2})
\]

Write the dielectric function slab region
do iy=bclayer+substrate+oxide+1,bclayer+substrate+oxide+slablayer
   eps(ix,iy,iz)=epsset1*eps_h1+epsset2*eps_h2+(1.0-epsset1-epsset2)*eps_s
endo

vol=vol+test
endo
endo

write(logfile,*) vol/(ixmax*izmax),2*pi*((radius1+radius2)/2)**2/sqrt(3.0)
do ix=1,ixmax
   do iz=1,izmax
      write(fields,*) (real(eps(ix,iy,iz)), iy=bclayer+1,iymax-bclayer)
   enddo
endo

doit,’Data dimensions’,ixmax, ’x’, izmax, ’x’, iymax-2*bclayer
write(logfile,*) ’Data dimensions’,ixmax, ’x’, izmax, ’x’, iymax-2*bclayer
return
end subroutine defcell

! Subroutine init_store_pts_band
! Initialize the random points for storing the fields for the FFT
! For the band structure store fields at random set of points
! -----------------------------------------------------------------------------
subroutine init_store_pts_band(store_pts,ix_cur,iy_cur,iz_cur,i_pol)
use files
use parameters
implicit none

integer,pointer :: store_pts(:,1)
integer,intent(in) :: ix_cur,iy_cur,iz_cur,i_pol
integer :: i,j
real :: x

write(logfile,*) ’Initialize store_pts in init_store_pts_band’
do i=1,n_pts_store
   call random_number(x)
   store_pts(i,1)=floor(3.0*x+4.0)
   call random_number(x)
   store_pts(i,2)=floor(ixmax*x+1.0)
   call random_number(x)
   store_pts(i,3)=floor(2*(slablayer)*x+1.0+bclayer+airlayer)
   if (store_pts(i,3)>(bclayer+airlayer+2*slablayer)) call err(8)
   call random_number(x)
   store_pts(i,4)=floor(izmax*x+1.0)
   if (store_pts(i,1)<1.or.store_pts(i,1)>6 &
     .or.store_pts(i,2)<1.or.store_pts(i,2)>ixmax &
     .or.store_pts(i,3)<=bclayer.or.store_pts(i,3)>izmax &
     .or.store_pts(i,4)<1.or.store_pts(i,4)>izmax) call err(8)
   write(logfile,*) ’store point #’, i, (store_pts(i,j), j=1,4)
endo

return
end subroutine init_store_pts_band
! Subroutine postproc_band
! Post-process the stored time dependent fields to extract the bands at
! that k-point
! -----------------------------------------------------------------------------
subroutine postproc_band(fft_data,spectrum,iki,b_cnt)
  use files
  use physconsts
  use parameters
  use interface4
  implicit none

  complex,pointer :: fft_data(:,:)
  real,pointer :: spectrum(:)
  integer :: i,iki,b_cnt
  real :: tmp

write(logfile,*) 'Postprocessing in postproc_band'

! Call FFT routine to calculate the power spectrum
! For the Band Structure

spectrum=0
  call power_spec(fft_data,spectrum)

if (ikmax==1) then
  ! Write out the spectrum
  do i=1,fft_size
    write(outfile,*) i,(spectrum(i))
  enddo
else
  ! Write out the Band structure
    do i=1,fft_size
      tmp=((i/(dt*2.0*fft_size))*(Q(1)*ixmax)/c0)
      if (tmp <= 0.8) then
        write(outfile,*) akx,akz,b_cnt,tmp,spectrum(i)
      endif
    enddo
endif

return
end subroutine postproc_band

! -----------------------------------------------------------------------------
! Subroutine defmetric
! Define the metric and various other factors needed for
! generalised co-ordinate systems
! -----------------------------------------------------------------------------
subroutine defmetric(u1,u2,u3,g1,g2,g3,g,omega)
  use parameters
use matrices
use files
implicit none

real,intent(in) :: u1(3),u2(3),u3(3)
real,intent(out) :: g1(3),g2(3),g3(3)
real,intent(out) :: g(3,3),omega

real :: tmp(3)

write(logfile,*) 'Define the metric'

! g is the metric. (g**-1)ij = ui.uj
! ui's are the real space lattice vectors while
! the gi's are the reciprocal lattice vectors
! (apart from the 2*pi/Qi factor!)

! omega=|u1.u2xu3|

tmp=cross_prod(u2,u3)
omega=dot_product(u1,tmp)

! Define the reciprocal vectors

g1=tmp/omega


g2=cross_prod(u3,u1)/omega


g3=cross_prod(u1,u2)/omega

! Define the metric g

\[
g(1,1) = \text{dot} \_	ext{product}(g1,g1) \\
g(1,2) = \text{dot} \_	ext{product}(g1,g2) \\
g(1,3) = \text{dot} \_	ext{product}(g1,g3) \\
g(2,1) = \text{dot} \_	ext{product}(g2,g1) \\
g(2,2) = \text{dot} \_	ext{product}(g2,g2) \\
g(2,3) = \text{dot} \_	ext{product}(g2,g3) \\
g(3,1) = \text{dot} \_	ext{product}(g3,g1) \\
g(3,2) = \text{dot} \_	ext{product}(g3,g2) \\
g(3,3) = \text{dot} \_	ext{product}(g3,g3)
\]

! Q0 is scale factor equal to a typical length

Q0=Q(1)

return
end subroutine defmetric

!--------------------------------------------------------------------------

! Subroutine renorm
! Sets up eps_hat, mu_hat, eps_inv, mu_inv, sigma and sigma_m
! based on the metric for our co-ordinate system

subroutine renorm(eps,mu,sigma,sigma_m,eps_inv,mu_inv,eps_hat,mu_hat,g &
& omega)
use matrices
use parameters
use physconsts
use files
implicit none
complex, pointer :: eps(:,:,:,:), mu(:,:,:,:)
complex, pointer :: eps_inv(:,:,:,:,:)
complex, pointer :: mu_inv(:,:,:,:,:)
complex, pointer :: eps_hat(:,:,:,:,:)
complex, pointer :: mu_hat(:,:,:,:,:)
real, pointer :: sigma(:,:,:), sigma_m(:,:,:)
real, intent(in) :: g(3,3), omega
complex, dimension(3,3) :: eps_tmp, mu_tmp
integer :: i, j, ix, iy, iz
logical :: fail

write(logfile,*) 'Define eps_inv, mu_inv for general co-ordinates'
do ix=1, ixmax
  do iy=1, iymax
    do iz=1, izmax
! Define effective eps & mu for the generalised co-ordinates
      do i=1,3
        do j=1,3
          eps_tmp(i,j)=eps(ix,iy,iz)*g(i,j)*omega*Q(1)*Q(2)*Q(3)/(Q(i)*Q(j)*Q0)
          mu_tmp(i,j)=mu(ix,iy,iz)*g(i,j)*omega*Q(1)*Q(2)*Q(3)/(Q(i)*Q(j)*Q0)
        enddo
      enddo
! Invert effective eps & mu
      eps_inv(1:3,1:3,ix,iy,iz)=matinv3(eps_tmp, emach, fail)
      if (fail) call err(3)
      mu_inv(1:3,1:3,ix,iy,iz)=matinv3(mu_tmp, emach, fail)
      if (fail) call err(3)
! Store the non-inverted eps & mu (used in calculating the div's)
      eps_hat(1:3,1:3,ix,iy,iz)=eps_tmp
      mu_hat(1:3,1:3,ix,iy,iz)=mu_tmp
! Define the effective conductivity
      sigma(ix,iy,iz)=sigma(ix,iy,iz)*dt/(eps0*eps(ix,iy,iz))
      sigma_m(ix,iy,iz)=sigma_m(ix,iy,iz)*dt/(mu0*mu(ix,iy,iz))
    enddo
  enddo
enddo
return
end subroutine renorm

!----------------------------------------------------------------------------
! Subroutine bc_xmin_bloch
! Set the boundary conditions at ix=1
!----------------------------------------------------------------------------
subroutine bc_xmin_bloch(e, h)
  use physconsts
  use parameters
  implicit none
! Set the Bloch phase shift
fxm1=exp(-ci*akx)
!
! Loop over the surface at ix=1

do iy=1,iymax
   do iz=1,izmax
      do i=1,3
         e(i,0,iy,iz)=fxm1*e(i,ixmax,iy,iz)
         h(i,0,iy,iz)=fxm1*h(i,ixmax,iy,iz)
      enddo
   enddo
enddo

to return
end subroutine bc_xmin_bloch

! Subroutine bc_xmax_bloch
! Set the boundary conditions at ix=ixmax
! Subroutine bc_xmax_bloch(e,h)
use physconsts
use parameters
implicit none

complex,pointer :: e(:,:,:,:)
complex,pointer :: h(:,:,:,:)
integer :: iy,iz,i
complex :: fxp1

! Set the Bloch phase shift
fxp1=exp(ci*akx)
!
! Loop over the surface at ix=ixmax

do iy=1,iymax
   do iz=1,izmax
      do i=1,3
         e(i,ixmax+1,iy,iz)=fxp1*e(i,1,iy,iz)
         h(i,ixmax+1,iy,iz)=fxp1*h(i,1,iy,iz)
      enddo
   enddo
enddo

to return
end subroutine bc_xmax_bloch
! Subroutine bc_ymin_bloch
! Set the boundary conditions at iy=1
!---------------------------------------------------------------------------------
subroutine bc_ymin_bloch(e,h)
use physconsts
use parameters
implicit none

complex,pointer :: e(:,:,,:)
complex,pointer :: h(:,:,,:)

integer :: ix,iz,i
complex :: fym1

! Set the Bloch phase shift
fym1=exp(-ci*aky)

! Loop over the surface at iy=1
do ix=1,ixmax
  do iz=1,izmax
    do i=1,3
      e(i,ix,0,iz)=fym1*e(i,ix,iymax,iz)
h(i,ix,0,iz)=fym1*h(i,ix,iymax,iz)
    enddo
  enddo
enddo
return
end subroutine bc_ymin_bloch

!---------------------------------------------------------------------------------
! Subroutine bc_ymax_bloch
! Set the boundary conditions at iy=iymax
!---------------------------------------------------------------------------------
subroutine bc_ymax_bloch(e,h)
use physconsts
use parameters
implicit none

complex,pointer :: e(:,:,,:)
complex,pointer :: h(:,:,,:)

integer :: ix,iz,i
complex :: fyp1

! Set the Bloch phase shift
fyp1=exp(ci*aky)

! Loop over the surface at iy=iymax
do ix=1,ixmax
  do iz=1,izmax
    do i=1,3
      e(i,ix,iymax+1,iz)=fyp1*e(i,ix,1,iz)
h(i,ix,iymax+1,iz)=fyp1*h(i,ix,1,iz)
    enddo
  enddo
enddo
! Subroutine bc_zmin_bloch
! Set the boundary conditions at iz=1
! -----------------------------------------------
subroutine bc_zmin_bloch(e,h)
use physconsts
use parameters
implicit none

complex,pointer :: e(:,:,,:),
complex,pointer :: h(:,:,,:)

integer :: ix,iy,i
complex :: fz1

! Set the Bloch phase shift
fz1=exp(-ci*akz)

! Loop over the surface at iz=1
do ix=1,ixmax
  do iy=1,iymax
    do i=1,3
      e(i,ix,iy,0)=fz1*e(i,ix,iy,izmax)
      h(i,ix,iy,0)=fz1*h(i,ix,iy,izmax)
    enddo
  enddo
enddo
return
end subroutine bc_zmin_bloch

! Subroutine bc_zmax_bloch
! Set the boundary conditions at iz=izmax
! -----------------------------------------------
subroutine bc_zmax_bloch(e,h)
use physconsts
use parameters
implicit none

complex,pointer :: e(:,:,,:),
complex,pointer :: h(:,:,,:)

integer :: ix,iy,i
complex :: fz1

! Set the Bloch phase shift
fz1=exp(ci*akz)
! Loop over the surface at iz=izmax

do ix=1,ixmax
  do iy=1,iymax
    do i=1,3
      e(i,ix,iy,izmax+1)=fzp1*e(i,ix,iy,1)
      h(i,ix,iy,izmax+1)=fzp1*h(i,ix,iy,1)
    enddo
  enddo
enddo

return
end subroutine bc_zmax_bloch

! ----------------------------------------------------------------------------
! Subroutine bc_xmin_metal
! Set the boundary conditions at ix=1
! ----------------------------------------------------------------------------
subroutine bc_xmin_metal(e,h)
  use parameters
  implicit none
  complex,pointer :: e(:,:,:,:)
  complex,pointer :: h(:,:,:,:)
  integer :: iy,iz,i

  ! Loop over the surface at ix=1
  do iy=1,iymax
    do iz=1,izmax
      do i=1,3
        e(i,0,iy,iz)=(0.0,0.0)
        h(i,0,iy,iz)=(0.0,0.0)
      enddo
    enddo
  enddo

  return
end subroutine bc_xmin_metal

! ----------------------------------------------------------------------------
! Subroutine bc_xmax_metal
! Set the boundary conditions at ix=ixmax
! ----------------------------------------------------------------------------
subroutine bc_xmax_metal(e,h)
  use parameters
  implicit none
  complex,pointer :: e(:,:,:,:)
  complex,pointer :: h(:,:,:,:)
  integer :: iy,iz,i

  ! Loop over the surface at ix=ixmax
  do iy=1,iymax
    do iz=1,izmax
      do i=1,3
        e(i,ix,iy,iz)=(0.0,0.0)
        h(i,ix,iy,iz)=(0.0,0.0)
      enddo
    enddo
  enddo

  return
end subroutine bc_xmax_metal

232
enddo
enddo
enddo
return
end subroutine bc xmax metal

! Subroutine bc ymin metal
! Set the boundary conditions at iy=1
! -----------------------------------------------------------------------------
subroutine bc ymin metal(e,h)
use parameters
implicit none
complex,pointer :: e(:,,:,:)
complex,pointer :: h(:,,:,:)
integer :: ix,iz,i

! Loop over the surface at iy=1
do ix=1,imax
  do iz=1,izmax
    do i=1,3
      e(i,ix,0,iz)=(0.0,0.0)
      h(i,ix,0,iz)=(0.0,0.0)
    enddo
  enddo
enddo
return
end subroutine bc ymin metal

! Subroutine bc ymax metal
! Set the boundary conditions at iy=iymax
! -----------------------------------------------------------------------------
subroutine bc ymax metal(e,h)
use parameters
implicit none
complex,pointer :: e(:,,:,:)
complex,pointer :: h(:,,:,:)
integer :: ix,iz,i

! Loop over the surface at iy=iymax
do ix=1,imax
  do iz=1,izmax
    do i=1,3
      e(i,ix,imax+1,iz)=(0.0,0.0)
      h(i,ix,imax+1,iz)=(0.0,0.0)
    enddo
  enddo
enddo
return
end subroutine bc_ymax_metal

! Subroutine bc_zmin_metal
! Set the boundary conditions at iz=1
! Subroutine bc_zmin_metal(e,h)
use parameters
implicit none

complex,pointer :: e(:,:,,:)
complex,pointer :: h(:,:,,:)
integer :: ix,iy,i

! Loop over the surface at iz=1

do ix=1,ixmax
do iy=1,iymax
do i=1,3
e(i,ix,iy,0)=(0.0,0.0)
h(i,ix,iy,0)=(0.0,0.0)
enddo
enddo
enddo
return
end subroutine bc_zmin_metal

! Subroutine bc_zmax_metal
! Set the boundary conditions at iz=izmax
! Subroutine bc_zmax_metal(e,h)
use parameters
implicit none

complex,pointer :: e(:,:,,:)
complex,pointer :: h(:,:,,:)
integer :: ix,iy,i

! Loop over the surface at iz=izmax

do ix=1,ixmax
do iy=1,iymax
do i=1,3
e(i,ix,iy,izmax+1)=(0.0,0.0)
h(i,ix,iy,izmax+1)=(0.0,0.0)
enddo
enddo
enddo
return
end subroutine bc_zmax_metal
Subroutine PML_e
Update for the Berenger type PML

subroutine PML_e(e_cur,e_prev,h_prev,intcurlh,wy,eps_inv)
use parameters
implicit none

complex,pointer :: e_cur(:,:,:,:),e_prev(:,:,:,:),h_prev(:,:,:,:)
complex,pointer :: intcurlh(:,:,:)
complex,pointer :: eps_inv(:,:,:,:,:)
real,intent(in) :: wy(:)
integer :: ix,iy,iz
complex :: curl(3)

! Update equations for the Berenger type PML

! Update the face at iy=1

do iy=1,bclayer
  do iz=1,izmax
    do ix=1,ixmax
      ! Define Curl H
      curl(1)=h_prev(3,ix,iy,iz)-h_prev(3,ix,iy-1,iz) &
      & -h_prev(2,ix,iy,iz)+h_prev(2,ix,iy,iz-1)
      curl(2)=h_prev(1,ix,iy,iz)-h_prev(1,ix,iy,iz-1) &
      & -h_prev(3,ix,iy,iz)+h_prev(3,ix-1,iy,iz)
      curl(3)=h_prev(2,ix,iy,iz)-h_prev(2,ix-1,iy,iz) &
      & -h_prev(1,ix,iy,iz)+h_prev(1,ix,iy-1,iz)
      ! Update integral of z-component of curl H
      intcurlh(ix,iy,iz)=intcurlh(ix,iy,iz)+curl(2)
      ! Integrate fields in time
      e_cur(1,ix,iy,iz)=(e_prev(1,ix,iy,iz) &
      & +curl(1)*eps_inv(1,1,ix,iy,iz)+curl(3)*eps_inv(1,3,ix,iy,iz))&
      & /(1.0+wy(iy)*dt)
      e_cur(3,ix,iy,iz)=(e_prev(3,ix,iy,iz) &
      & +curl(3)*eps_inv(3,3,ix,iy,iz)+curl(1)*eps_inv(3,1,ix,iy,iz))&
      & /(1.0+wy(iy)*dt)
      e_cur(2,ix,iy,iz)=e_prev(2,ix,iy,iz) &
      & +(curl(2)+wy(iy)*dt*intcurlh(ix,iy,iz))*eps_inv(2,2,ix,iy,iz)
    enddo
  enddo
enddo

! Update the face at iy=iymax

do iy=iymax-bclayer,iymax
  do iz=1,izmax
    do ix=1,ixmax
      ! Define Curl H
      curl(1)=h_prev(3,ix,iy,iz)-h_prev(3,ix,iy-1,iz) &
      & -h_prev(2,ix,iy,iz)+h_prev(2,ix,iy,iz-1)
      curl(2)=h_prev(1,ix,iy,iz)-h_prev(1,ix,iy,iz-1) &
      & -h_prev(3,ix,iy,iz)+h_prev(3,ix-1,iy,iz)
      curl(3)=h_prev(2,ix,iy,iz)-h_prev(2,ix-1,iy,iz) &
      & -h_prev(1,ix,iy,iz)+h_prev(1,ix,iy-1,iz)
      ! Update integral of z-component of curl H
      intcurlh(ix,iy,iz)=intcurlh(ix,iy,iz)+curl(2)
      ! Integrate fields in time
      e_cur(1,ix,iy,iz)=(e_prev(1,ix,iy,iz) &
      & +curl(1)*eps_inv(1,1,ix,iy,iz)+curl(3)*eps_inv(1,3,ix,iy,iz))&
      & /(1.0+wy(iy)*dt)
      e_cur(3,ix,iy,iz)=(e_prev(3,ix,iy,iz) &
      & +curl(3)*eps_inv(3,3,ix,iy,iz)+curl(1)*eps_inv(3,1,ix,iy,iz))&
      & /(1.0+wy(iy)*dt)
      e_cur(2,ix,iy,iz)=e_prev(2,ix,iy,iz) &
      & +(curl(2)+wy(iy)*dt*intcurlh(ix,iy,iz))*eps_inv(2,2,ix,iy,iz)
    enddo
  enddo
enddo
! Define Curl H

curl(1)=h_prev(3,ix,iy,iz)-h_prev(3,ix,iy-1,iz) 
& -h_prev(2,ix,iy,iz)+h_prev(2,ix,iy,iz-1) 
curl(2)=h_prev(1,ix,iy,iz)-h_prev(1,ix,iy,iz-1) 
& -h_prev(3,ix,iy,iz)+h_prev(3,ix-1,iy,iz) 
curl(3)=h_prev(2,ix,iy,iz)-h_prev(2,ix-1,iy,iz) 
& -h_prev(1,ix,iy,iz)+h_prev(1,ix,iy-1,iz)

! Update integral of z-component of curl H

intcurlh(ix,iy,iz)=intcurlh(ix,iy,iz)+curl(2)

! Integrate fields in time

e_cur(1,ix,iy,iz)=(e_prev(1,ix,iy,iz) 
& +curl(1)*eps_inv(1,1,ix,iy,iz)+curl(3)*eps_inv(1,3,ix,iy,iz))& 
& /(1.0+wy(iy)*dt)
e_cur(3,ix,iy,iz)=(e_prev(3,ix,iy,iz) 
& +curl(3)*eps_inv(3,3,ix,iy,iz)+curl(1)*eps_inv(3,1,ix,iy,iz))& 
& /(1.0+wy(iy)*dt)
e_cur(2,ix,iy,iz)=e_prev(2,ix,iy,iz) &
& +(curl(2)+wy(iy)*dt*intcurlh(ix,iy,iz))*eps_inv(2,2,ix,iy,iz)

enddo
dendo
dendo

return
end subroutine PML_e

! ----------------------------------------------------------------------------
! Subroutine PML_h
! Update for the Berenger type PML
! ----------------------------------------------------------------------------
subroutine PML_h(e_cur,h_cur,h_prev,intcurle,wy,mu_inv)
  use parameters
  use physconsts
  implicit none

  complex,pointer :: e_cur(:,:,:,:),h_cur(:,:,:,:),h_prev(:,:,:,:)
  complex,pointer :: intcurle(:,:,:)
  complex,pointer :: mu_inv(:,:,:,:,:)
  real,intent(in) :: wy(:)
  integer :: ix,iy,iz
dtcq2=(dt*c0/Q0)**2

  ! Update equations for the Berenger type PML
  ! Update the face at iy=1
  do iy=1,bclayer
dz=1,izmax

enddo
do ix=1,ixmax

! Define Curl E

curl(1)=e_cur(3,ix,iy+1,iz)-e_cur(3,ix,iy,iz) &
   & -e_cur(2,ix,iy,iz+1)+e_cur(2,ix,iy,iz)
curl(2)=e_cur(1,ix,iy,iz+1)-e_cur(1,ix,iy,iz) &
   & -e_cur(3,ix+1,iy,iz)+e_cur(3,ix,iy,iz)
curl(3)=e_cur(2,ix+1,iy,iz)-e_cur(2,ix,iy,iz) &
   & -e_cur(1,ix,iy+1,iz)+e_cur(1,ix,iy,iz)

! Update the integral of z-component of curl E

intcurle(ix,iy,iz)=intcurle(ix,iy,iz)+curl(2)

! Integrate the fields in time

h_cur(1,ix,iy,iz)=1.0/(1.0+wy(iy)*dt)* &
   & (h_prev(1,ix,iy,iz)-dtcq2*curl(1)*mu_inv(1,1,ix,iy,iz)&
   & -dtcq2*curl(3)*mu_inv(1,3,ix,iy,iz))

h_cur(3,ix,iy,iz)=1.0/(1.0+wy(iy)*dt)* &
   & (h_prev(3,ix,iy,iz)-dtcq2*curl(3)*mu_inv(3,3,ix,iy,iz)&
   & -dtcq2*curl(1)*mu_inv(3,1,ix,iy,iz))

h_cur(2,ix,iy,iz)=h_prev(2,ix,iy,iz)-dtcq2* &
   & (curl(2)+wy(iy)*dt*intcurle(ix,iy,iz))*mu_inv(2,2,ix,iy,iz)

enddo
enddo
endo

! Update the face at iy=iymax

do iy=iymax-bclayer,iymax
   do iz=1,izmax
      do ix=1,ixmax

! Define Curl E

curl(1)=e_cur(3,ix,iy+1,iz)-e_cur(3,ix,iy,iz) &
   & -e_cur(2,ix,iy,iz+1)+e_cur(2,ix,iy,iz)
curl(2)=e_cur(1,ix,iy,iz+1)-e_cur(1,ix,iy,iz) &
   & -e_cur(3,ix+1,iy,iz)+e_cur(3,ix,iy,iz)
curl(3)=e_cur(2,ix+1,iy,iz)-e_cur(2,ix,iy,iz) &
   & -e_cur(1,ix,iy+1,iz)+e_cur(1,ix,iy,iz)

! Update the integral of z-component of curl E

intcurle(ix,iy,iz)=intcurle(ix,iy,iz)+curl(2)

! Integrate the fields in time

h_cur(1,ix,iy,iz)=1.0/(1.0+wy(iy)*dt)* &
   & (h_prev(1,ix,iy,iz)-dtcq2*curl(1)*mu_inv(1,1,ix,iy,iz)&
   & -dtcq2*curl(3)*mu_inv(1,3,ix,iy,iz))

h_cur(3,ix,iy,iz)=1.0/(1.0+wy(iy)*dt)* &
   & (h_prev(3,ix,iy,iz)-dtcq2*curl(3)*mu_inv(3,3,ix,iy,iz)&
   & -dtcq2*curl(1)*mu_inv(3,1,ix,iy,iz))

enddo
enddo
endo

! Update the face at iy=iymax
\begin{verbatim}
h_cur(2,ix,iy,iz)=h_prev(2,ix,iy,iz)-dtcq2* &   (curl(2)+wy(iy)*dt*intcurle(ix,iy,iz))*mu_inv(2,2,ix,iy,iz)
enddo
enddo
enddo
return
end subroutine PML_h

! Subroutine calc_div_D
! Calculates the divergence of D integrated over each mesh cell
! ---------------------------------------------------------------------------
subroutine calc_div_D(e,eps_hat,div_D)
use parameters
use files
implicit none
complex,pointer :: e(:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:,:)
complex,pointer :: div_D(:,:,:)
integer :: ix,iy,iz,ixm1,iym1,izm1,i
write(logfile,*) 'Calculate div D'
! We actually calculate (div D)/Q0 here
div_D=0.0
do iz=1,izmax
  do iy=1,iymax
    do ix=1,ixmax
      ! Boundary conditions for eps. Assumes periodic but this will also
      ! work for metal BC's as the field will be zero anyway.
      ixm1=ix-1
      iym1=iy-1
      izm1=iz-1
      if (ix==1) ixm1=ixmax
      if (iy==1) iym1=iymax
      if (iz==1) izm1=izmax
      ! Calculate the divergence
      div_D(ix,iy,iz)=(0.0,0.0)
      do i=1,3
        div_D(ix,iy,iz)=div_D(ix,iy,iz) &
        +eps_hat(1,i,ix,iy,iz)*e(i,ix,iy,iz) &
        -eps_hat(1,i,ixm1,iy,iz)*e(i,ix-1,iy,iz) &
        +eps_hat(2,i,ix,iy,iz)*e(i,ix,iy,iz) &
        -eps_hat(2,i,ix,iym1,iz)*e(i,ix,iy-1,iz) &
        +eps_hat(3,i,ix,iy,iz)*e(i,ix,iy,iz) &
        -eps_hat(3,i,ix,iy,izm1)*e(i,ix,iy,iz-1)
      enddo
    enddo
  enddo
enddo
end subroutine calc_div_D
\end{verbatim}
enddo

return
end subroutine calc_div_D

! Subroutine calc_div_B
! Calculates the divergence of B integrated over each mesh cell
! -----------------------------------------------------------------------------
subroutine calc_div_B(h,mu_hat,div_B)
use parameters
use files
implicit none
complex,pointer :: h(:,:,:,:)
complex,pointer :: mu_hat(:,:,:,:,:)
complex,pointer :: div_B(:,:,:)
integer :: ix,iy,iz,ixp1,iyp1,izp1,i

write(logfile,*) 'Calculate div B'
! We actually calculate (div B)/Q0 here
div_B=0.0

do iz=1,izmax
  do iy=1,iymax
    do ix=1,ixmax
      ! Boundary conditions for mu. Assumes periodic but this will also
      ! work for metal BC's as the field will be zero anyway.
      ixp1=ix+1
      iyp1=iy+1
      izp1=iz+1
      if (ix==ixmax) ixp1=1
      if (iy==iymax) iyp1=1
      if (iz==izmax) izp1=1

      ! Calculate the divergence
      div_B(ix,iy,iz)=(0.0,0.0)
      do i=1,3
        div_B(ix,iy,iz)=div_B(ix,iy,iz) &
        +mu_hat(1,i,ixp1,iy,iz)*h(i,ix+1,iy,iz) &
        -mu_hat(1,i,ix,iy,iz)*h(i,ix,iy,iz) &
        +mu_hat(2,i,ix,iyp1,iz)*h(i,ix,iy+1,iz) &
        -mu_hat(2,i,ix,iy,iz)*h(i,ix,iy,iz) &
        +mu_hat(3,i,ix,iy,izp1)*h(i,ix,iy,iz+1) &
        -mu_hat(3,i,ix,iy,iz)*h(i,ix,iy,iz)
      enddo
    enddo
  enddo
enddo

return
end subroutine calc_div_B
! Subroutine calc_energy_density
! Calculates the stored energy integrated over one mesh cell
! *--------------------------------------------------------------------------

subroutine calc_energy_density(e_cur,e_prev,h_prev,rho,eps_hat,mu_hat)
use physconsts
use parameters
use files
implicit none

complex,pointer :: e_cur(:,:,:,:)
complex,pointer :: e_prev(:,:,:,:)
complex,pointer :: h_prev(:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:,:)
complex,pointer :: mu_hat(:,:,:,:,:)
real,pointer :: rho(:,:,:)
integer :: ix,iy,iz
integer :: i,j
real :: dtcq2

write(logfile,*) 'Calculate the energy density'

! Calculate the energy stored (rho) in the mesh cell at ix,iy,iz
! Actually calc rho/((Q0*eps0)/(2*Q1*Q2*Q3*|u1.u2xu3|))
! but the constant doesn't matter

dtcq2=(dt*c0/Q0)**2

do iz=1,izmax
  do iy=1,iymax
    do ix=1,ixmax

      rho(ix,iy,iz)=(0.0,0.0)
      do i=1,3
        do j=1,3
          rho(ix,iy,iz)=rho(ix,iy,iz)+real(eps_hat(i,j,ix,iy,iz) &
          *conjg(E_cur(i,ix,iy,iz))*E_prev(j,ix,iy,iz)) &
          +real(mu_hat(i,j,ix,iy,iz) &
          *conjg(H_prev(i,ix,iy,iz))*H_prev(j,ix,iy,iz))/dtcq2
        enddo
      enddo

    enddo
  enddo
enddo

return
end subroutine calc_energy_density

! *--------------------------------------------------------------------------
! Subroutine calc_current
! Calculates the three components of the current flowing away from the point
! at ix,iy,iz
! *--------------------------------------------------------------------------

subroutine calc_current(J,e_cur,h_cur,h_prev,ix,iy,iz)
implicit none

integer :: ix,iy,iz
integer :: i,j
real :: dtcq2

write(logfile,*) 'Calculate the energy density'

! Calculate the energy stored (rho) in the mesh cell at ix,iy,iz
! Actually calc rho/((Q0*eps0)/(2*Q1*Q2*Q3*|u1.u2xu3|))
! but the constant doesn't matter

dtcq2=(dt*c0/Q0)**2

do iz=1,izmax
  do iy=1,iymax
    do ix=1,ixmax

      rho(ix,iy,iz)=(0.0,0.0)
      do i=1,3
        do j=1,3
          rho(ix,iy,iz)=rho(ix,iy,iz)+real(eps_hat(i,j,ix,iy,iz) &
          *conjg(E_cur(i,ix,iy,iz))*E_prev(j,ix,iy,iz)) &
          +real(mu_hat(i,j,ix,iy,iz) &
          *conjg(H_prev(i,ix,iy,iz))*H_prev(j,ix,iy,iz))/dtcq2
        enddo
      enddo

    enddo
  enddo
enddo

return
end subroutine calc_current
complex, intent(out) :: J(3)
complex, pointer :: e_cur(:,,:,:,:), h_cur(:,,:,:,:), h_prev(:,,:,:,:)
integer, intent(in) :: ix, iy, iz

J(1) = -(e_cur(3, ix+1, iy, iz)*conjg(h_cur(2, ix, iy, iz)) &
& - e_cur(2, ix+1, iy, iz)*conjg(h_cur(3, ix, iy, iz)) &
& + conjg(e_cur(3, ix+1, iy, iz))*h_prev(2, ix, iy, iz) &
& - conjg(e_cur(2, ix+1, iy, iz))*h_prev(3, ix, iy, iz))

J(2) = -(e_cur(1, ix, iy+1, iz)*conjg(h_cur(3, ix, iy, iz)) &
& - e_cur(3, ix, iy+1, iz)*conjg(h_cur(1, ix, iy, iz)) &
& + conjg(e_cur(1, ix, iy+1, iz))*h_prev(3, ix, iy, iz) &
& - conjg(e_cur(3, ix, iy+1, iz))*h_prev(1, ix, iy, iz))

J(3) = -(e_cur(2, ix, iy, iz+1)*conjg(h_cur(1, ix, iy, iz)) &
& - e_cur(1, ix, iy, iz+1)*conjg(h_cur(2, ix, iy, iz)) &
& + conjg(e_cur(2, ix, iy, iz+1))*h_prev(1, ix, iy, iz) &
& - conjg(e_cur(1, ix, iy, iz+1))*h_prev(2, ix, iy, iz))

return
end subroutine calc_current

! Subroutine err
! Error trap. Write error message to log file and stop
! -----------------------------------------------------------------------------
subroutine err(ierr)
use files
implicit none

integer, intent(in) :: ierr

error: select case(ierr)
case(1)
write(logfile,*) 'Non-existent input file'
case(2)
write(logfile,*) 'Invalid input file'
case(3)
write(logfile,*) 'Attempt to invert a matrix with zero determinant'
case(4)
write(logfile,*) 'Failure in energy conservation'
case(5)
write(logfile,*) 'Failure in div D'
case(6)
write(logfile,*) 'Failure in div B'
case(7)
write(logfile,*) 'Error in Fast-Fourier transform - not a power of 2'
case(8)
write(logfile,*) 'Error in random numbers'
case default
write(logfile,*) 'Unknown error'
end select error

stop
end subroutine err

! Function matinv3
! Inverts a 3x3 matrix
! -----------------------------------------------------------------------------
function matinv3(A,emach,fail)
implicit none

complex,dimension(3,3) :: matinv3
complex,intent(in) :: A(3,3)
real,intent(in) :: emach
logical,intent(out) :: fail

complex :: det,B(3,3)

fail=.false.
det=A(1,1)*A(2,2)*A(3,3)-A(1,1)*A(3,2)*A(2,3) &
  & -A(1,2)*A(2,1)*A(3,3)+A(1,2)*A(3,1)*A(2,3) &
  & +A(1,3)*A(2,1)*A(3,2)-A(1,3)*A(3,1)*A(2,2)

if (abs(det)<emach) then
    fail=.true.
else
    B(1,1)=A(2,2)*A(3,3)-A(3,2)*A(2,3)
    B(1,2)=A(1,3)*A(3,2)-A(1,2)*A(3,3)
    B(1,3)=A(1,2)*A(2,3)-A(1,3)*A(2,2)
    B(2,1)=A(3,1)*A(2,3)-A(2,1)*A(3,3)
    B(2,2)=A(1,1)*A(3,3)-A(3,1)*A(1,3)
    B(2,3)=A(2,1)*A(1,3)-A(1,1)*A(2,3)
    B(3,1)=A(2,1)*A(3,2)-A(3,1)*A(2,2)
    B(3,2)=A(3,1)*A(1,2)-A(1,1)*A(3,2)
    B(3,3)=A(1,1)*A(2,2)-A(2,1)*A(1,2)

    B=B/det
endif

! Test Patch
!!$write(*,*) 'A*A^(-1)',matmul(A,B)
! End Patch

matinv3=B
derm function matinv3

! -----------------------------------------------------------------------------
! Function cross_prod
! Calculate axb where a & b are real 3-vectors
! -----------------------------------------------------------------------------
function cross_prod(a,b)
implicit none

real,dimension(3) :: cross_prod
real,intent(in) :: a(3),b(3)

cross_prod(1)=a(2)*b(3)-a(3)*b(2)
cross_prod(2)=a(3)*b(1)-a(1)*b(3)
cross_prod(3)=a(1)*b(2)-a(2)*b(1)

derm function cross_prod

! -----------------------------------------------------------------------------
! Subroutine power_spec
! Calculates the power spectrum for a given data set f and returns the
! result in spectrum
! Follows Numerical Recipes pg 425ff and has a choice of three possible
! window functions and an option for data overlapping
! -----------------------------------------------------------------------------
subroutine power_spec(f,spectrum)
use parameters
use physconsts
use interface6
implicit none
complex,pointer :: f(:,:)
real,pointer :: spectrum(:)
integer :: j,k,mm,m2,offset
real :: den,facm,facp,sumw
real :: window
complex,pointer :: w1(:,:),w2(:,:)
!
!window(j)=(1.0-abs(((j-1)-facm)*facp)) ! Parzen window function
!window(j)=1.0 ! Square window function
!window(j)=(1.0-((j-1)-facm)*facp)**2) ! Welch window function
!
offset=0
mm=2*fft_size
m2=mm+2
den=0.0
facm=fft_size-0.5
facp=1.0/(fft_size+0.5)
sumw=0.0
allocate(w1(n_pts_store,mm),w2(n_pts_store,fft_size))
do j=1,mm
sumw=sumw+window(j)**2
endo
do j=1,mm
sumw=sumw+window(j)**2
endo
if (overlap) then
do j=1,fft_size
w2(:,j)=f(:,j+offset)
dono
do j=1,fft_size
w1(:,j)=w2(:,j)
dono
offset=offset+fft_size
endif
outloop: do k=1,n_segment
!
if (overlap) then
do j=1,fft_size
w1(:,j)=w2(:,j)
dono
do j=1,fft_size
w2(:,j)=f(:,j+offset)
dono
offset=offset+fft_size
endo
else
endif
do j=1,mm
    w1(:,j)=f(:,j+offset)
enddo
offset=offset+mm
endif

do j=1,mm
    w1(:,j)=w1(:,j)*window(j)
enddo
call FFT(w1,1)
!
! Calculate the power spectrum (for band structures etc.)
!
spectrum(1)=spectrum(1)+sum(abs(w1(:,1))**2)
do j=2,fft_size
    spectrum(j)=spectrum(j)+sum(abs(w1(:,j))**2) &
      & +sum(abs(w1(:,m2-j))**2)
endo
den=den+sumw
endo outloop
den=mm*den
do j=1,fft_size
    spectrum(j)=spectrum(j)/den
endo
deallocate(w1,w2)
return
end subroutine power_spec

! Subroutine FFT
! Calculates the fourier transform of the set of n complex arrays each of
! size nmax: f(n,1:nmax)
! If isign=1 calculates the transform, isign=-1 calculates inverse transform
! On exit isign=0 indicates failure
! nmax must be an integer power of two
! -----------------------------------------------------------------------------
subroutine FFT(f,isign)
  use physconsts
  implicit none
  integer,intent(in) :: isign
  complex,pointer :: f(:,:)
  complex :: tmp,w,wp
  real :: theta
  integer :: n,nmax,nbits,set_bits
  integer :: i,j,k,m,mmax,istep

  ! First check that nmax is a power of 2

  n=size(f,1)
nmax=size(f,2)
nbits=bit_size(nmax)
set_bits=0
i=0

do
  if (i>nbits.or.set_bits>1) exit
  if (btest(nmax,i)) set_bits=set_bits+1
  i=i+1
endo

if (set_bits>1) then
  call err(7)
endif

! Bit reversal loop

do k=1,n
  j=1
  do i=1,nmax
    if (i>j) then
      tmp=f(k,j)
      f(k,j)=f(k,i)
      f(k,i)=tmp
    endif
    m=nmax/2
    do while ((m>=2).and.(j>m))
      j=j-m
      m=m/2
    enddo
    j=j+m
  enddo
endo

! Now transform part

do k=1,n
  mmax=1
  do while (nmax>mmax)
    istep=mmax*2
    theta=2.0*pi/(isign*istep)
    wp=exp(ci*theta)
    w=(1.0,0.0)
    do m=1,mmax
      do i=m,nmax,istep
        j=i+mmax
        tmp=w*f(k,j)
        f(k,j)=f(k,i)-tmp
        f(k,i)=f(k,i)+tmp
      enddo
      w=w*wp
    enddo
    mmax=istep
  enddo
endo

! Half time-step offset correction

do i=1,nmax/2
  w=2.0*pi*(i-1)/real(nmax)
  f(1,i)=f(1,i)*cexp(+isign*ci*w*0.50)
endo
return
end subroutine FFT

! Subroutine FT
! Calculates the slow fourier transform of the set of n complex arrays each of
! size nmax: f(n,1:nmax)
! If isign=1 calculates the transform, isign=-1 calculates inverse transform
! On exit isign=0 indicates failure
! -----------------------------------------------------------------------------
subroutine FT(f,isign)
use physconsts
implicit none

integer,intent(in) :: isign
complex,pointer :: f(:,:)
complex,pointer :: ft_f(:)
complex :: tmp
real :: w
integer :: n,nmax
integer :: iw,i,it

n=size(f,1)
nmax=size(f,2)
allocate(ft_f(nmax))

do iw=1,nmax/2
  w=2.0*pi*(iw-1)/real(nmax)
tmp=(0.0,0.0)
do it=1,nmax
  tmp=tmp+f(1,it)*cexp(isign*ci*w*(it))
dendo
ft_f(iw)=tmp
dendo

f(1,:)=ft_f(:)
deallocate(ft_f)

! Half time-step offset correction

do iw=1,nmax/2
  w=2.0*pi*(iw-1)/real(nmax)
f(1,iw)=f(1,iw)*cexp(-isign*ci*w*0.50)
dendo

return
end subroutine FT
APPENDIX D

FDTD SLAB WAVEGUIDE PC WITH MIRROR SYMMETRY

D.1 An example input file

The following is an example input file for the SWG with mirror symmetry code which is read by the executable before the calculation begins, defining the parameters of the size of the computational domain, the geometry of the structure, the dielectric constants of the slab waveguide material, the background medium, and the holes. Also, the number and size of the time steps are defined.

```
20 ixmax
14 bclayer
16 airlayer
8 slablayer
20 izmax
1.0 Q(1)
1.0 Q(2)
1.732 Q(3)
0.003 dt
0.3 radius1
0.19 radius2
12.0 epsilon
1.0 cylind1
1.0 cylind2
0.0 akx
0.0 aky
0.0 akz
12 ikmax
32 n_block
1024 block_size
51 n_pts_store
1 n_segment
F overlap
0.0 damping
```

D.2 The FDTD code

The following presents excerpts of the FDTD code used for calculating the band structure of the 2D SSL SWG PC structure with mirror symmetry. Since this code is closely related
to the code in Appendix C, only the major differences between the codes is presented.
Where applicable, line numbers are included to show the location of the modified lines of
code. This code is based upon the ONYX code [96], however major modifications have been
made to the dielectric function as well as other subroutines. This code is written in the
FORTRAN 90 language and will compile with a variety of commercial and non-commercial
FORTRAN 90 compilers.

!----------------------------------------------------------------------------
! super_bd-tri-even_64fx2.f90 Absoft 64FX Fortran version.
! universal input file format
! Modified version of the triangular lattice code from April of 2003.
! I have added the ability to do cylinders of two different radii (superlattices).
! This is the modified version of the Order N photonics code
! Modifications done by W. Park (wpark@colorado.edu)
! Additional modifications by C. Neff (curtis.neff@mse.gatech.edu)
! original (c) Andrew Ward, Imperial College, London. Dec 1997. a.j.ward@ic.ac.uk
!----------------------------------------------------------------------------
module parameters
! Define the run-time parameter list. These will be read in from a file
! ixmax, iymax, izmax define the number of mesh points in each of the
! principle directions
! itmax and dt are the number and size of timesteps respectively
! akx, aky, akz are the components of the k-vector expressed on the reciprocal
! lattice. They are normalised by the mesh spacing in the relevant direction
! ie. akx = (Q1*ixmax)*kx
! imax = No. of k-points
! Q(3) is the matrix holding the mesh spacing in each direction
! n_block : Break down itmax into 'n_block' blocks each of 'block_size' time
! steps. Fields can be written out, div's calculated etc at the end of each block
! npts_store : The number of real space points at which we store the fields
! For the FFT the itmax timesteps can be split up into segments which can be
! either overlapping or not. For details see Numerical Recipes pg 425ff.
! If overlap=.true. then itmax=fft_size*(n_segment+1)
! If overlap=.false. then itmax=fft_size*(2*n_segment)
! In both cases fft_size is the size the segment which is fourier transformed
! so must be a power of 2.
integer :: ixmax,iymax,izmax,itmax,ikmax,n_block,block_size,n_pts_store
real :: Q0,Q(3),dt,akx,aky,akz,radius1,radius2,epsil,epsil_h1,epsil_h2
integer :: n_segment,fft_size,bclayer,airlayer,slablayer
logical :: overlap
real :: damping
end module parameters
!----------------------------------------------------------------------------
logname = "log.super.bd-tri-even.dat"
outname = "out.super.bd-tri-even.dat"
fieldsname = "fields.super.bd-tri-even.dat"
inname = "inFILE.super.band.dat"

! Attach simulation number to the file names
if (len_trim(LINE)>0) then
    logname = "log.super.bd-tri-even" // trim(LINE) // ".dat"
    outname = "out.super.bd-tri-even" // trim(LINE) // ".dat"
    fieldsname = "fields.super.bd-tri-even" // trim(LINE) // ".dat"
    inname = "infile.super.band" // trim(LINE) // ".dat"
end if
!
! Subroutine driver
!
! Heart of the calculation. This subroutine actually does the time integration
!
! Loop. Should be made to be as flexible as possible
!
subroutine driver(e_cur,h_cur,eps_inv,mu_inv,eps_hat,mu_hat,\
    sigma,sigma_m, fft_data,store_pts,iky)
use interface2
use interface3
use interface5
use interface6
use parameters
use files
use physconsts
implicit none
complex,pointer :: e_cur(:,:,:,:)
complex,pointer :: h_cur(:,:,:,:)
complex,pointer :: eps_inv(:,:,:,:,:)
complex,pointer :: mu_inv(:,:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:,:)
complex,pointer :: mu_hat(:,:,:,:,:)
complex,pointer :: fft_data(:,:)
real,pointer :: sigma(:,:,:),sigma_m(:,:,:)
integer,pointer :: store_pts(:,:)
integer :: iky
complex,pointer :: intcurle(:,:,:),intcurlh(:,:,:)
real,pointer :: wy(:)
complex,pointer :: e_prev(:,:,:,:)
complex,pointer :: h_prev(:,:,:,:)
complex,pointer :: div(:,:,:)
real,pointer :: rho(:,:,:)
integer :: i,iblock,dt_dum
allocate(e_prev(3,0:ixmax+1,0:iymax+1,0:izmax+1))
allocate(h_prev(3,0:ixmax+1,0:iymax+1,0:izmax+1))
allocate(wy(bclayer))
allocate(intcurle(ixmax,bclayer,izmax))
allocate(intcurlh(ixmax,bclayer,izmax))
!
! Initialize 2nd set of fields

   e_prev=(0.0,0.0)
   h_prev=(0.0,0.0)
   intcurle=(0.0,0.0)
   intcurlh=(0.0,0.0)
!
! Initialize the absorbing boundary layer PML
write(logfile,*) 'Define the absorbing boundary layer'
w
= 0

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do i=1,bclayer
    wy(i)=120.0*((bclayer-i)**2/(real(bclayer-1)**2)
enddo

dt_dum=0
maintime: do iblock=1,n_block
    call int(e_cur,h_cur,e_prev,h_prev,eps_inv,mu_inv,sigma,sigma_m, &
    & block_size,iblock,fft_data,store_pts,intcurle,intcurlh,wy)
    ! Various tests on the fields can be performed here...
    ! Update the remain boundaries prior to calculating divs
    call bc_xmax_bloch(e_cur,h_cur)
call bc_ymax_mirror_even(e_cur,h_cur)
call bc_zmax_bloch(e_cur,h_cur)
endo maintime

dallocate(e_prev,h_prev)
dallocate(wy)
dallocate(intcurle,intcurlh)
return
end subroutine driver

! Subroutine int
! Do the time integration for nt time steps
! Subroutine int(e_cur,h_cur,e_prev,h_prev,eps_inv,mu_inv,sigma,sigma_m, &
! nt,iblock,fft_data,store_pts,intcurle,intcurlh,wy)
use interface5
use interface6
use physconsts
use parameters
implicit none

integer,intent(in) :: nt,iblock
complex,pointer :: e_cur(:,:,:,:)
complex,pointer :: e_prev(:,:,:,:)
complex,pointer :: h_cur(:,:,:,:)
complex,pointer :: h_prev(:,:,:,:)
complex,pointer :: eps_inv(:,:,:,:,:)
complex,pointer :: mu_inv(:,:,:,:,:)
complex,pointer :: fft_data(:,:)
real,pointer :: sigma(:,:,:),sigma_m(:,:,:)
integer,intent(in) :: store_pts(:,:)
complex,pointer :: intcurle(:,:,:),intcurlh(:,:,:)
real,pointer :: wy(:)

integer :: ix,iy,iz,it,i_pts
complex :: curl(3)
real :: dtcq2

dtcq2=(dt*c0/Q0)**2

time: do it=1,nt
! Current fields become previous fields

temp => e_cur
e_cur => e_prev
e_prev => temp

temp => h_cur
h_cur => h_prev
h_prev => temp

! First the E-fields

do iz = 1, izmax
  do iy = bclayer + 1, iymax
    do ix = 1, ixmax

! Define Curl H

curl(1) = h_prev(3, ix, iy, iz) - h_prev(3, ix, iy-1, iz) &
& - h_prev(2, ix, iy, iz) + h_prev(2, ix, iy, iz-1)
curl(2) = h_prev(1, ix, iy, iz) - h_prev(1, ix, iy, iz-1) &
& - h_prev(3, ix, iy, iz) + h_prev(3, ix-1, iy, iz)
curl(3) = h_prev(2, ix, iy, iz) - h_prev(2, ix-1, iy, iz) &
& - h_prev(1, ix, iy, iz) + h_prev(1, ix, iy-1, iz)

! Integrate fields in time

e_cur(1, ix, iy, iz) = (1.0 - sigma(ix, iy, iz)) * e_prev(1, ix, iy, iz) + &
& (eps_inv(1, 1, ix, iy, iz) * curl(1) &
& + eps_inv(1, 2, ix, iy, iz) * curl(2) &
& + eps_inv(1, 3, ix, iy, iz) * curl(3))
e_cur(2, ix, iy, iz) = (1.0 - sigma(ix, iy, iz)) * e_prev(2, ix, iy, iz) + &
& (eps_inv(2, 1, ix, iy, iz) * curl(1) &
& + eps_inv(2, 2, ix, iy, iz) * curl(2) &
& + eps_inv(2, 3, ix, iy, iz) * curl(3))
e_cur(3, ix, iy, iz) = (1.0 - sigma(ix, iy, iz)) * e_prev(3, ix, iy, iz) + &
& (eps_inv(3, 1, ix, iy, iz) * curl(1) &
& + eps_inv(3, 2, ix, iy, iz) * curl(2) &
& + eps_inv(3, 3, ix, iy, iz) * curl(3))

endo
dndo
donddo

! Update Berenger type PML equations for the E-field (Absorbing boundary layer)
call PML_e(e_cur, e_prev, h_prev, intcurlh, wy, eps_inv)

! Update the boundary conditions needed for the E-fields
call bc_xmax_bloch(e_cur, h_cur)
call bc_ymax_mirror_even(e_cur, h_cur)
call bc_zmax_bloch(e_cur, h_cur)

! Then the H-fields
do iz=1,izmax
    do iy=bclayer+1,iymax
        do ix=1,ixmax
            ! Define Curl E
            curl(1)=e_cur(3,ix,iy+1,iz)-e_cur(3,ix,iy,iz) &
                -e_cur(2,ix,iy,iz+1)+e_cur(2,ix,iy,iz)
            curl(2)=e_cur(1,ix,iy,iz+1)-e_cur(1,ix,iy,iz) &
                -e_cur(3,ix+1,iy,iz)+e_cur(3,ix,iy,iz)
            curl(3)=e_cur(2,ix+1,iy,iz)-e_cur(2,ix,iy,iz) &
                -e_cur(1,ix,iy+1,iz)+e_cur(1,ix,iy,iz)

            ! Integrate the fields in time
            h_cur(1,ix,iy,iz)=1.0/(1.0+sigma_m(ix,iy,iz))* &
                (h_prev(1,ix,iy,iz)-dtcq2* &
                    (mu_inv(1,1,ix,iy,iz)*curl(1) &
                    +mu_inv(1,2,ix,iy,iz)*curl(2) &
                    +mu_inv(1,3,ix,iy,iz)*curl(3)))
            h_cur(2,ix,iy,iz)=1.0/(1.0+sigma_m(ix,iy,iz))* &
                (h_prev(2,ix,iy,iz)-dtcq2* &
                    (mu_inv(2,1,ix,iy,iz)*curl(1) &
                    +mu_inv(2,2,ix,iy,iz)*curl(2) &
                    +mu_inv(2,3,ix,iy,iz)*curl(3)))
            h_cur(3,ix,iy,iz)=1.0/(1.0+sigma_m(ix,iy,iz))* &
                (h_prev(3,ix,iy,iz)-dtcq2* &
                    (mu_inv(3,1,ix,iy,iz)*curl(1) &
                    +mu_inv(3,2,ix,iy,iz)*curl(2) &
                    +mu_inv(3,3,ix,iy,iz)*curl(3)))
        enddo
    enddo
enddo

! Update Berenger type PML equations for the H-field (Absorbing boundary layer)
call PML_h(e_cur,h_cur,h_prev,intcurle,wy,mu_inv)
! Update the boundary conditions needed for the H-fields
call bc_xmin_bloch(e_cur,h_cur)
call bc_zmin_bloch(e_cur,h_cur)
call bc_ymin_mirror_even(e_cur,h_cur)
! Store points for Fourier transform later
do i_pts=1,n_pts_store
    if (store_pts(i_pts,1)<4) then
        fft_data(i_pts,it+(iblock-1)*nt)=e_cur(store_pts(i_pts,1), &
            store_pts(i_pts,2),store_pts(i_pts,3),store_pts(i_pts,4))
    else
        fft_data(i_pts,it+(iblock-1)*nt)=h_prev(store_pts(i_pts,1)-3, &
            store_pts(i_pts,2),store_pts(i_pts,3),store_pts(i_pts,4))
    endif
enddo
enddo time

return
end subroutine int

! Subroutine setparam
! Set the key parameters from a config file
! -----------------------------------------------
subroutine setparam()
use parameters
use physconsts
use files
implicit none
integer :: nbits, set_bits, i

write(logfile,*) 'Read in parameters'

read(infile,*) ixmax
if (ixmax<1) call err(2)
write(logfile, '(A1,A12,I10)') '#','ixmax=',ixmax
write(outfile, '(A1,A12,I10)') '#','ixmax=',ixmax
write(fields, '(A1,A12,I10)') '#','ixmax=',ixmax

read(infile,*) bclayer
if (bclayer<1) call err(2)
write(logfile, '(A1,A12,I10)') '#','bclayer=',bclayer
write(outfile, '(A1,A12,I10)') '#','bclayer=',bclayer
write(fields, '(A1,A12,I10)') '#','bclayer=',bclayer

read(infile,*) airlayer
if (airlayer<1) call err(2)
write(logfile, '(A1,A12,I10)') '#','airlayer=',airlayer
write(outfile, '(A1,A12,I10)') '#','airlayer=',airlayer
write(fields, '(A1,A12,I10)') '#','airlayer=',airlayer

read(infile,*) slablayer
if (slablayer<1) call err(2)
write(logfile, '(A1,A12,I10)') '#','slablayer=',slablayer
write(outfile, '(A1,A12,I10)') '#','slablayer=',slablayer
write(fields, '(A1,A12,I10)') '#','slablayer=',slablayer

iymax=bclayer+airlayer+slablayer
read(infile,*) izmax
if (izmax<1) call err(2)
write(logfile, '(A1,A12,I10)') '#','izmax=',izmax
write(outfile, '(A1,A12,I10)') '#','izmax=',izmax
write(fields, '(A1,A12,I10)') '#','izmax=',izmax

read(infile,*) Q(1)
if (Q(1)<=0.0) call err(2)
write(logfile, '(A1,A12,F15.5)') '#','Q(1)=',Q(1)
write(outfile, '(A1,A12,F15.5)') '#','Q(1)=',Q(1)
write(fields, '(A1,A12,F15.5)') '#','Q(1)=',Q(1)

read(infile,*) Q(2)
if (Q(2)<=0.0) call err(2)
write(logfile, '(A1,A12,F15.5)') '#','Q(2)=',Q(2)
write(outfile, '(A1,A12,F15.5)') '#','Q(2)=',Q(2)
write(fields,'(A1,A12,F15.5)') '#','Q(2)=',Q(2)

read(infile,*) Q(3)
if (Q(3)<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','Q(3)=',Q(3)
write(outfile,'(A1,A12,F15.5)') '#','Q(3)=',Q(3)
write(fields,'(A1,A12,F15.5)') '#','Q(3)=',Q(3)

read(infile,*) dt
if (dt<=0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','dt=',dt
write(outfile,'(A1,A12,F15.5)') '#','dt=',dt
write(fields,'(A1,A12,F15.5)') '#','dt=',dt

read(infile,*) radius1
if (radius1<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','radius1=',radius1
write(outfile,'(A1,A12,F15.5)') '#','radius1=',radius1
write(fields,'(A1,A12,F15.5)') '#','radius1=',radius1

read(infile,*) radius2
if (radius2<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','radius2=',radius2
write(outfile,'(A1,A12,F15.5)') '#','radius2=',radius2
write(fields,'(A1,A12,F15.5)') '#','radius2=',radius2

read(infile,*) epsil
if (epsil<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','epsilon=',epsil
write(outfile,'(A1,A12,F15.5)') '#','epsilon=',epsil
write(fields,'(A1,A12,F15.5)') '#','epsilon=',epsil

read(infile,*) epsil_h1
if (epsil_h1<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','epsilon_h1=',epsil_h1
write(outfile,'(A1,A12,F15.5)') '#','epsilon_h1=',epsil_h1
write(fields,'(A1,A12,F15.5)') '#','epsilon_h1=',epsil_h1

read(infile,*) epsil_h2
if (epsil_h2<0.0) call err(2)
write(logfile,'(A1,A12,F15.5)') '#','epsilon_h2=',epsil_h2
write(outfile,'(A1,A12,F15.5)') '#','epsilon_h2=',epsil_h2
write(fields,'(A1,A12,F15.5)') '#','epsilon_h2=',epsil_h2

read(infile,*) akx
if (akx<0.0.or.akx>pi) call err(2)
write(logfile,'(A1,A12,F10.5)') '#','akx=',akx
write(outfile,'(A1,A12,F10.5)') '#','akx=',akx
write(fields,'(A1,A12,F10.5)') '#','akx=',akx

read(infile,*) aky
if (aky<0.0.or.aky>pi) call err(2)
write(logfile,'(A1,A12,F10.5)') '#','aky=',aky
write(outfile,'(A1,A12,F10.5)') '#','aky=',aky
write(fields,'(A1,A12,F10.5)') '#','aky=',aky

read(infile,*) akz
if (akz<0.0.or.akz>pi) call err(2)
write(logfile,'(A1,A12,F10.5)') '#','akz=',akz
write(outfile,'(A1,A12,F10.5)') '#','akz=',akz
write(fields,'(A1,A12,F10.5)') '#','akz=',akz
write(outfile,'(A1,A12,F10.5)') '#','akz=',akz
write(fields,'(A1,A12,F10.5)') '#','akz=',akz

read(infile,*) ikmax
if (ikmax<0) call err(2)
write(logfile,'(A1,A12,I10)') '#','ikmax=',ikmax
write(outfile,'(A1,A12,I10)') '#','ikmax=',ikmax
write(fields,'(A1,A12,I10)') '#','ikmax=',ikmax

read(infile,*) n_block
if (n_block<1) call err(2)
write(logfile,'(A1,A12,I10)') '#','n_block=',n_block
write(outfile,'(A1,A12,I10)') '#','n_block=',n_block
write(fields,'(A1,A12,I10)') '#','n_block=',n_block

read(infile,*) block_size
if (block_size<1) call err(2)
write(logfile,'(A1,A12,I10)') '#','block_size=',block_size
write(outfile,'(A1,A12,I10)') '#','block_size=',block_size
write(fields,'(A1,A12,I10)') '#','block_size=',block_size

itmax=n_block*block_size
write(logfile,'(A1,A12,I10)') '#','itmax=',itmax
write(outfile,'(A1,A12,I10)') '#','itmax=',itmax
write(fields,'(A1,A12,I10)') '#','itmax=',itmax

read(infile,*) n_pts_store
if (n_pts_store<0) call err(2)
write(logfile,'(A1,A12,I10)') '#','n_pts_store=',n_pts_store
write(outfile,'(A1,A12,I10)') '#','n_pts_store=',n_pts_store
write(fields,'(A1,A12,I10)') '#','n_pts_store=',n_pts_store

read(infile,*) n_segment
if (n_segment<1) call err(2)
write(logfile,'(A1,A12,I10)') '#','n_segment=',n_segment
write(outfile,'(A1,A12,I10)') '#','n_segment=',n_segment
write(fields,'(A1,A12,I10)') '#','n_segment=',n_segment

read(infile,*) overlap
write(logfile,'(A1,A12,L5)') '#','overlap=',overlap
write(outfile,'(A1,A12,L5)') '#','overlap=',overlap
write(fields,'(A1,A12,L5)') '#','overlap=',overlap

if (overlap) then
    fft_size=itmax/(n_segment+1)
else
    fft_size=itmax/(2*n_segment)
endif

if (fft_size<1) call err(2)
nbits=bit_size(fft_size)
set_bits=0
i=0
do
    if (i==nbits.or.set_bits>1) exit
    if (btest(fft_size,i)) set_bits=set_bits+1
    i=i+1
endo
if (set_bits>1) call err(2)

read(infile,*) damping
write(logfile,'(A1,A12,F10.5)') '#','damping=',damping
write(outfile,'(A1,A12,F10.5)') '#','damping=',damping
write(fields,'(A1,A12,F10.5)') '#','damping=',damping
if (damping<0.0) call err(2)
return
end subroutine setparam

! Subroutine initfields
! Set up the initial values of the E & H fields
! Should be able to read fields in from a file
! or set them to some appropriate analytic form
! ---------------------------------------------------------------------
subroutine initfields(g1,g2,g3,e,h,eps_hat,mu_hat,ix_cur,iy_cur,iz_cur,i_pol)
use interface3
use interface5
use matrices
use files
use parameters
use physconsts
implicit none
real,intent(in) :: g1(3),g2(3),g3(3)
complex,pointer :: e(:,:,:,:),h(:,:,:,:)
complex,pointer :: eps_hat(:,:,:,:,:,:),mu_hat(:,:,:,:,:,:)
integer,intent(in) :: ix_cur,iy_cur,iz_cur,i_pol
integer :: ix,iy,iz,jx,jy,jz,i
real :: G(3),k(3),v(3),k_plus_G(3)
complex :: vec(3),h0(3),expo
complex,pointer :: div(:,:,:)
real :: dtcq2
write(logfile,*) 'Initialize fields in initfields'
dtcq2=(dt*c0/Q0)**2
e=(0.0,0.0)
h=(0.0,0.0)
! Set up initial fields
!
! Initial fields following Chan, Yu and Ho's Order N paper
! Can be used for Band structure
v=(/1.0,1.0,1.0/)
!
! Loops over jx,jy,jz loop over the required reciprocal lattice vectors
do jz=-5,5
  do jy=-5,5
    do jx=-5,5
      G=2.0*pi*(g1*(jx)/real(ixmax)+g2*(jy)/real(iymax)+g3*(jz)/real(izmax))
k=(akx/real(ixmax))*g1+(aky/real(iymax))*g2+(akz/real(izmax))*g3
    end do
  end do
end do
\[ k_{\text{plus}}G = k + G \]
\[ \text{vec}(1) = \exp(i(\text{vec}(1)G)) - 1.0 \]
\[ \text{vec}(2) = \exp(i(\text{vec}(2)G)) - 1.0 \]
\[ \text{vec}(3) = \exp(i(\text{vec}(3)G)) - 1.0 \]
\[ h_0(2) = v(3) \text{vec}(1) - v(1) \text{vec}(3) \]
\[ h_0(1) = 0 \]
\[ h_0(3) = 0 \]

\[
\text{do } iz=1,izmax \\
\text{do } iy=1,iymax \\
\text{do } ix=1,ixmax \\
\text{expo} = \exp(i(\text{vec}(1)Gix + \text{vec}(2)Giy + \text{vec}(3)Giz)) \\
\text{do } i=1,3 \\
\quad h(i,ix,iy,iz) = h(i,ix,iy,iz) + h_0(i) \text{expo} \\
\text{enddo} \\
\text{enddo} \\
\text{enddo} \\
\text{enddo} \\
\text{enddo} \\
\text{call bcxmax_bloch(e,h)} \\
\text{call bcymax_mirror_even(e,h)} \\
\text{call bczmax_bloch(e,h)} \\
\text{call bcxmin_bloch(e,h)} \\
\text{call bcymirror_even(e,h)} \\
\text{call bczmin_bloch(e,h)} \\
\text{return} \\
\text{end subroutine initfields} \]

! --------------------------------------------------------------------------
! Subroutine defcell 
! Define the eps, mu, sigma and sigma_m for our unit cell 
! Either analytically or from a file 
! Defines the dielectric cylinder for the test calculation 
! --------------------------------------------------------------------------
subroutine defcell(eps,mu,sigma,sigma_m,u1,u2,u3)
use files 
use parameters 
use physconsts 
implicit none 
complex,pointer :: eps(:,,:),mu(:,,:) 
real,pointer :: sigma(:,,:),sigma_m(:,,:) 
real :: u1(3),u2(3),u3(3) 
complex :: epsset1,epsset2,eps_s,eps_h1,eps_h2 
integer :: ix,iy,iz,i,j,l,m,isub,iatom 
real :: asub,test,r(3),g(3,3),vol,xhalf,zhalf 
real :: r1,r2,r3,atom(3,5) 
write(logfile,*) 'Define unit cell'
\[ g(1,1) = u_1(1)u_1(1) + u_1(2)u_1(2) + u_1(3)u_1(3) \]

\[ g(1,2) = u_1(1)u_2(1) + u_1(2)u_2(2) + u_1(3)u_2(3) \]

\[ g(1,3) = u_1(1)u_3(1) + u_1(2)u_3(2) + u_1(3)u_3(3) \]

\[ g(2,1) = u_2(1)u_1(1) + u_2(2)u_1(2) + u_2(3)u_1(3) \]

\[ g(2,2) = u_2(1)u_2(1) + u_2(2)u_2(2) + u_2(3)u_2(3) \]

\[ g(2,3) = u_2(1)u_3(1) + u_2(2)u_3(2) + u_2(3)u_3(3) \]

\[ g(3,1) = u_3(1)u_1(1) + u_3(2)u_1(2) + u_3(3)u_1(3) \]

\[ g(3,2) = u_3(1)u_2(1) + u_3(2)u_2(2) + u_3(3)u_2(3) \]

\[ g(3,3) = u_3(1)u_3(1) + u_3(2)u_3(2) + u_3(3)u_3(3) \]

! Set up the default parameters for the unit cell

! radius = ratio of the radius of cylinder to the unit cell
! \( \epsilon_{h1,h2} \) = dielectric constant for cylinder
! \( \epsilon_s \) = dielectric constant for background medium
! \( isub \) = number of sub-divisions in average over each lattice point

\[ \mu = (1.0, 0.0) \]
\[ \sigma = (0.0, 0.0) \]
\[ \sigma_m = (0.0, 0.0) \]

\[ \epsilon_s = \text{cmplx}(\text{epsil}) \]
\[ \epsilon_{h1} = \text{cmplx}(\text{epsil}_{h1}) \]
\[ \epsilon_{h2} = \text{cmplx}(\text{epsil}_{h2}) \]

\[ r1 = \text{radius1}**2 \]
\[ r2 = \text{radius2}**2 \]

\[ isub = 10 \]

\[ \text{atom}(1,1) = 0.0 \]
\[ \text{atom}(2,1) = 0.0 \]
\[ \text{atom}(3,1) = 0.0 \]

\[ \text{atom}(1,2) = 1.0 \]
\[ \text{atom}(2,2) = 0.0 \]
\[ \text{atom}(3,2) = 0.0 \]

\[ \text{atom}(1,3) = 0.0 \]
\[ \text{atom}(2,3) = 0.0 \]
\[ \text{atom}(3,3) = 1.0 \]

\[ \text{atom}(1,4) = 1.0 \]
\[ \text{atom}(2,4) = 0.0 \]
\[ \text{atom}(3,4) = 1.0 \]

\[ \text{atom}(1,5) = 0.5 \]
\[ \text{atom}(2,5) = 0.0 \]
\[ \text{atom}(3,5) = 0.5 \]

\[ \text{vol} = 0.0 \]

\[ \text{xhalf} = \text{float}(\text{ixmax})/2.0 \]

\[ \text{zhalf} = \text{float}(\text{izmax})/2.0 \]

\[ \text{do} \text{ ix}=1,\text{ixmax} \]
\[ \text{do} \text{ iz}=1,\text{izmax} \]

\[ \quad \text{asub} = 1.0/\text{float}(\text{isub}) \]
\[ \quad \text{test} = 0.0 \]
\[ \quad \text{epsset1} = 0.0 \]
\[ \quad \text{epsset2} = 0.0 \]
\[ \quad \text{do} \text{ l}=1,\text{isub} \]
\[ \quad \text{do} \text{ m}=1,\text{isub} \]
do iatom=1,4
    r(1)=Q(1)*((ix-1+(l-1)*asub)/float(ixmax)-atom(1,iatom))
    r(2)=0.0
    r(3)=Q(3)*((iz-1+(m-1)*asub)/float(izmax)-atom(3,iatom))
    r3=0.0
    do i=1,3
        do j=1,3
            r3=r3+(g(i,j)*r(i)*r(j))
        enddo
    enddo
    if (r3.lt.r1) epsset1=epsset1+1.0
    if (r3.lt.r1) test=test+1.0
enddo

r(1)=Q(1)*((ix-1+(l-1)*asub)/float(ixmax)-atom(1,5))
    r(2)=0.0
    r(3)=Q(3)*((iz-1+(m-1)*asub)/float(izmax)-atom(3,5))
    r3=0.0
    do i=1,3
        do j=1,3
            r3=r3+(g(i,j)*r(i)*r(j))
        enddo
    enddo
    if (r3.lt.r2) epsset2=epsset2+1.0
    if (r3.lt.r2) test=test+1.0
enddo

epsset1=epsset1/float(isub**2)
epsset2=epsset2/float(isub**2)
test=test/float(isub**2)

eps(ix,iy,iz)=(1.0,0.0)

eps(ix,iy,iz)=epsset1*eps_h1+epsset2*eps_h2+(1.0-epsset1-epsset2)*eps_s

vol=vol+test

write(logfile,*) vol/(ixmax*izmax),2*pi*((radius1+radius2)/2)**2/sqrt(3.0)

return
end subroutine defcell

! -----------------------------------------------------------------------------
! Subroutine init_store_pts_band
! Initialize the random points for storing the fields for the FFT
! For the band structure store fields at random set of points
! ----------------------------------------------------------------------------
subroutine init_store_pts_band(store_pts,ix_cur,iy_cur,iz_cur,i_pol)
  use files
  use parameters
  implicit none

  integer,pointer :: store_pts(:,:)
  integer,intent(in) :: ix_cur,iy_cur,iz_cur,i_pol
  integer :: i
  real :: x

  do iy=1,bclayer+airlayer
    eps(ix,iy,iz)=(1.0,0.0)
  enddo
  do iy=bclayer+airlayer+1,iymax
    eps(ix,iy,iz)=epsset1*eps_h1+epsset2*eps_h2+(1.0-epsset1-epsset2)*eps_s
  enddo
  vol=vol+test
enddo

write(logfile,*) vol/(ixmax*izmax),2*pi*((radius1+radius2)/2)**2/sqrt(3.0)

return
end subroutine init_store_pts_band

write(logfile,*) 'Initialize store_pts in init_store_pts_band'

do i=1,n_pts_store
   call random_number(x)
   store_pts(i,1)=floor(3.0*x+4.0)
   call random_number(x)
   store_pts(i,2)=floor(ixmax*x+1.0)
   call random_number(x)
   store_pts(i,3)=floor(2*(iymax-bclayer-airlayer)*x+1.0+bclayer+airlayer)
   if (store_pts(i,3)>iymax) store_pts(i,3)=2*iymax-store_pts(i,3)+1
   call random_number(x)
   store_pts(i,4)=floor(iymax*x+1.0)
   if (store_pts(i,1)<1.or.store_pts(i,1)>6 &
      .or.store_pts(i,2)<1.or.store_pts(i,2)>ixmax &
      .or.store_pts(i,3)<=bclayer.or.store_pts(i,3)>iymax &
      .or.store_pts(i,4)<1.or.store_pts(i,4)>izmax) call err(8)
endo

return
end subroutine init_store_pts_band

! Subroutine bc_ymin_mirror_even
! Set the mirror plane at iy=1
! -----------------------------------------------------------------------------
subroutine bc_ymin_mirror_even(e,h)
  use physconsts
  use parameters
  implicit none
  complex,pointer :: e(:,:,:,:)
  complex,pointer :: h(:,:,:,:)
  integer :: ix,iz,i,iy
  complex :: fym1

  ! Set the Bloch phase shift
  fym1=exp(-ci*aky)

  ! Loop over the surface at iy=1
  do ix=1,ixmax
     do iz=1,izmax
        e(1,ix,0,iz)=fym1*e(1,ix,1,iz)
        h(2,ix,0,iz)=fym1*h(2,ix,1,iz)
        e(3,ix,0,iz)=fym1*e(3,ix,1,iz)
        h(1,ix,0,iz)=(0.0,0.0)
        e(2,ix,0,iz)=(0.0,0.0)
        h(3,ix,0,iz)=(0.0,0.0)
     enddo
  enddo

  return
end subroutine bc_ymin_mirror_even

! Subroutine bc_ymax_mirror_even
! Set the boundary conditions at iy=iymax
!----------------------------------------------------------------------------
subroutine bc_ymax_mirror_even(e,h)
use phsysconsts
use parameters
implicit none

complex,pointer :: e(:,:,,:,:)
complex,pointer :: h(:,:,,:,:)

integer :: ix,iz,i,iy
!complex :: fyp1

! Set the Bloch phase shift

fyp1=exp(ci*aky)

! Loop over the surface at iy=iymax

d0 ix=1,ixmax
  d0 iz=1,izmax
    e(1,ix,iz,iy+1)=e(1,ix,iz,iy)
    h(2,ix,iz,iy+1)=h(2,ix,iz,iy)
    e(3,ix,iz,iy+1)=e(3,ix,iz,iy)
    h(1,ix,iz,iy+1)=-h(1,ix,iz,iy-1)
    e(2,ix,iz,iy+1)=-e(2,ix,iz,iy-1)
    h(3,ix,iz,iy+1)=-h(3,ix,iz,iy-1)
  enddo
enddo

return
end subroutine bc_ymax_mirror_even
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