Photonic Crystals with Alternate Arrays of Rods and Holes in a Low Dielectric-Index Material

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THE CITY UNIVERSITY OF NEW YORK
Abstract

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Adviser: Kai Shum

This thesis theoretically deals with the propagation of electromagnetic waves (light beams) in periodically modulated dielectric material structures based on Maxwell’s equations. We are interested in novel light propagation characteristics in these man-made dielectric material structures for practical applications, especially on optical communications and computations. Since the wavelength range of light is on the same order of magnitude as the modulation periods of dielectric materials, an analogy of the light propagation in dielectric-constant modulated structures with the electron transport in solid-state crystals is used throughout my thesis by using a term “photonic crystals (PhCs)” referring to these dielectric structures. I started my work on two-dimensional (2D) PhCs. A new type of PhCs is proposed which consists of alternate arrays of rods and holes (AARH), embedded in a low dielectric-constant material such as ultraviolet-curable polymer. By modeling them as 2D PhCs, it is discovered that this type of PhCs exhibits overlapped photonic band gaps (PBGs) for both transverse electric (TE) and transverse magnetic (TM) polarized light beams. This discovery is important for many practical applications related to light manipulation. It opens the door to more effective optical computing elements, as well as better
wave guides, LEDs and micro-lasers. It is also found that new AARH PhCs possess many interesting near-band-edge properties such as left-hand-material characteristics manifested by perfect reflection, negative refraction, and superlensing. I then extended my work to three dimensional (3D) counterparts of the discovered PhCs, which are called photonic crystal slabs (PCSs). I found that the overlapped TE and TM PBGs persist in these PCSs although they are restricted to a partial k-space. By manipulating certain structure parameters such as the thickness of PCS and its cladding, it is possible to achieve overlapping incomplete PBGs exactly in the frequency range predicted by 2D simulations. Hence, one can use fast and cheap 2D simulation instead of slow and expensive 3D and still engineer complex 3D photonic structures. The AARH PCSs also exhibit negative refraction and near zero effective refractive index. These effects allow for a strong control over the light propagation in PhCs. Additionally, the edge and surface modes of proposed PCSs are observed that effectively enlarge slabs’ PBGs.
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I would like also to thank my committee members for their valuable time to review my thesis.

Finally, I dedicate this thesis to my mother, who always wanted to see next to her Philosophy PhD title, a Natural Philosophy PhD title in the family.
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Abbreviations

TE – Transverse Electric

TM – Transverse Magnetic

PhC – Photonic Crystal

PCS – Photonic Crystal Slab

AARH – Alternate Arrays of Rods and Holes

PWE – Plane Wave Expansion

FDTD – Finite Difference Time Domain
Chapter 1 Introduction

1.1 Motivation

In the recent two decades, PhCs have captured the imagination of many researchers. The unusual properties of PhCs have promised many breakthroughs in the field of optical computing. In the near future, the electronics industry will inevitably hit the threshold of miniaturization, and the Moor Law will be breached. Many expect this to happen just in a few years. The alternatives are quantum or and optical computing. For optical computing, one needs elements that are analogous to electronic logic gates, transistors, etc. PhCs can play this role because they possess a crucial property – PBGs. PBGs are frequency regions where light is forbidden to propagate. Thus, they allow for controlling over the photons similar to the one over charge carriers in electronics. To be practical, PBGs should be active for both Transverse Electric (TE) and Transverse Magnetic (TM) polarizations at all angles of light incidence. 2D PhCs can exhibit a variety of such PBGs. However, idealized 2D PhCs are not realistic and are used only for computational modeling. 3D PhCs are realistic but very hard to be manufactured. PCS are a useful compromise between the 2D and 3D PhCs.

The motivation of this work is to find a useful photonic structure which exhibits large overlapping TE and TM PBGs. Simulations are focused on 2D PhCs and 3D PCSs. There are two main kinds of PhC structures: one kind of structures with high dielectric index pillars in air that tends to open TM PBGs, and another kind of structures with air holes in high dielectric background that tends to open TE PBGs. We make use of the general properties of these two kinds of PhC structures and propose a new kind of PhC structures with alternate arrays of rods and holes (AARH) that exhibits large overlapping TE and TM PBGs with a suitable set of material and structural parameters.
My thesis is organized as follows. After this chapter, chapter 2 covers the basics of photonic
theory based on Maxwell’s equations. The clear and unambiguous solutions can be obtained for
electromagnetic waves propagating through modulated media that show many unusual refractive
and reflective properties. Chapter 3 describes the numerical methods used in this thesis work. In
Chapter 4, we present the specific parameters that control light propagation in PhCs. Especially,
the symmetry breaking is discussed as a way to increase the usefulness of photonic structures. The
2D photonic crystals with alternate arrays of rod and holes are introduced in this chapter. The
structure of their supercells breaks certain symmetries, which leads to the emergence of PBGs for
both TE and TM polarizations. With the change of the structure/material parameters of AARH
PhCs, like dielectric constants and filling factors, TE and TM PBGs are shifting in frequency with
different rates. This allows for the overlapping of the PBGs for both polarizations. The results on
unusual refractive and reflective properties of AARH PhCs such as negative refraction,
superlensing, and zero effective refractive index are also discussed. In Chapter 5, we focus on the
incomplete PBGs of AARH PCSs with the same structure as their 2D counterparts discussed in
Chapter 4. Dispersions in k-space and associated transmissions in time domain are investigated by
varying structure and material parameters in effort to create similar results for both 2D and 3D
photonic structures. The surface and edge modes are also discussed. In Chapter 6, we present our
experimental work and future research. In the last chapter, a brief conclusion is given.

1.2 Photonic crystals: natural, early man-made and recent developments

Lord Rayleigh first studied the electromagnetic wave propagations in periodic media in
1888 when he observed unconventional reflective properties in a crystal.1 After several failed
explanations, he theorized that the mineral was built by many alternate layers with different
physical properties. Thus, he identified the first natural one-dimensional photonic crystal with a
very narrow band gap prohibiting the light from propagating in certain directions on certain
wavelengths. Incomplete gaps were observed in the form of iridescent colors on the wings of
certain butterflies\textsuperscript{2} as well as some natural opals and inverted opals.

In 1936, Smakura\textsuperscript{3} developed an antireflection coating device using the principle of the
emerging PhC theory. Later, in the seventies, Bykov\textsuperscript{4} proposed that spontaneous optical emission
could be inhibited in more than one dimension, by introducing two dimensional periodic photonic
structure.

The field of PhCs has been intensely studied throughout the 20\textsuperscript{th} century. The lack of tools
and practical technologies for their fabrication was a great obstacle to its further development until
the early 1980s. In 1987, Yablonovitch\textsuperscript{5} and S. John\textsuperscript{6} introduced the term of “photonic crystal”
and the idea of creating omnidirectional PBGs. These gaps could dramatically increase the
effectiveness of lasers and other optical devices suffering from random spontaneous emissions.
Additionally, PhCs could be used to store and localize light for numerous applications. In 1991,
Yablonovitch and his colleagues successfully created the first artificial PhC known now as
“Yablonovit” with a 3D PBG in the microwave range. They mechanically drilled millimeter holes
into a $\varepsilon = 3.6$ dielectric index material.

During the 1990s, the papers on PhCs grew exponentially, as researchers realized their
great potential as elements of optical computing and in many other fields. Unfortunately, most of
them remained theoretical, as experiments were limited to microwave and far infrared ranges. The
fast development of computation power in this period allowed for the development of series of
powerful software tools that could compute the light propagations in the computer-designed PhCs.
It was found that 2D PhCs exhibit several exotic properties like complete PBGs for TE and TM
polarizations, left-hand behavior, and super-collimation. The first experimental demonstration of
this kind of PhCs in optical wavelength was in 1996 by Thomas Krauss. The initial technique was
to etch a semiconductor wafer to form structures either with semiconductor rods surrounded by air
or air holes in semiconductor medium. This technique provided for high dielectric contrast
between the two media as the air has a dielectric constant of $\varepsilon = 1$ while semiconductors could
exhibit dielectric constants ranging from $\varepsilon = 6$ to $\varepsilon = 20$. As a practical application, these types
of PhCs have been used commercially since 1998 in the form of photonic crystal fibers that
exhibited enhanced properties in comparison to the conventional optical fibers.

In the early 21st century, a new method became popular for fabrication of PCS. It is known
as Photo-lithography and has many advantages as flexibility, fabrication in bulk and high
resolution. However, the attempts to fabricate 3D PhC with PBG for infrared and visible spectral
ranges faced serious technological difficulties. For a long time, the most widespread method for
fabrication of 3D PhC for the visible range has been the self-assembling growth of colloidal crystal.
Apart from natural Opals, one can produce artificial opals using amorphous silica particles.
Between the spherical particles of several hundred nanometers, there exist empty spaces that could
be filled with low refraction index liquid. The result is a periodic structure with properties of PhC
that extend into the visible range. Later, invert opals were synthesized in a similar way. However,
natural and artificial opals are known to suffer from a large number of lattice defects that till
recently represented an unsurmountable obstacle to fabrication of quality PhC.

Recently, a new method became popular allowing for the fabrication of defect-free PhCs
with almost arbitrary shapes. It is called laser 3D writing and is based on two-photon absorption
of UV curable polymer. In a way not dissimilar to photolithography, the light from a femtosecond
laser is focused on a photosensitive material and converts a semi-liquid polymer like SU-8 into
solid. The high resolution of this method can result in features less than 100 nm of arbitrary shape and below the diffraction limit.

### 1.3 A brief summary of PhC applications

There are various fields that enthusiastically incorporate PhCs for manipulating light propagation. Described below are some applications of PhCs.

PBGs are the most important feature of PhCs, and they are usually combined with an artificially introduced defect into the crystal. If one introduces a linear defect, it could play the role of a waveguide, as light is not allowed to propagate outside the waveguide.\(^{13-16}\) The defect may not even be linear and bend at random direction. As the loss increases with the sharpness of the bend, a new set of point defects could be added at appropriate places close to the bends. The quest, for greater efficiency of transmission through waveguides with complicated shapes, leads to increasingly complicated defect patterns.\(^ {17-19}\) Nano-cavities are point defects in PhCs that allow trapping light and releasing it later at a suitable time.\(^ {20,21}\) The combination of line and point defect could result in nano-scale optical circuits for low power applications.\(^ {22}\)

Close to the edge of PBGs, it is possible to limit light propagation in a small region, where it can form a standing wave. By pumping suitable optical energy, one can realize a highly efficient coherent laser.\(^ {23}\)

PBGs were also proved to be useful in designing highly efficient LEDs with high coherence in blue wavelength range.\(^ {24}\) LEDs could be combined with a Bragg mirror that reflects only selected wavelengths and then waveguides to lead the light to a suitable position.\(^ {25}\)
Other applications of PhCs incorporating defects are single photon light sources\textsuperscript{26}, large area coherent emission,\textsuperscript{27} and high-Q optical functions.\textsuperscript{28} PBGs can be modulated by doping PhCs with different sizes of radiuses of rods or air holes.

PhCs could play a significant role in future telecommunications by replacing common optical fibers. Contemporary fibers are limited in their information carrying ability by the chromatic dispersion, where light with a different wavelength propagates with different speeds in the glass fibers. In 1998, the so called holey fiber was introduced that is a lattice of air holes into a glass medium. Among its many advantages are the ability to transport larger amounts of information, low loss for wide range wavelengths, low diameter and the ability to limit its transmission to a very narrow single light mode.

PhCs exhibit a unique feature that is not found in nature and non-periodic materials. The index of refraction can become negative. This phenomenon leads to many interesting applications as the Snell Law is still valid, but the Pointing Vector is antiparallel to phase velocity. The result is that the light pulse is not propagating in the same direction as the phase. One possible application is ultra-small polarization splitters if only one of the light polarizations exhibits negative refraction.\textsuperscript{29}

The complicated dispersion relation between the wave vector $k$ and the frequency $\omega$ in PhCs can lead to several exotic effects. Supercollimation is an effect related to the left handed property of certain PhCs. Super-prism is a related effect that enhances hundreds of times the common prism effect where the angle of refraction is changed with change of frequency of the incoming light. Superlensing is one of most curious effects related to negative refraction. It is believed that it is possible to build an optical system with resolution below diffraction limit.
More proposed PhC applications are beam splitters, add/drop filters, switches, waveguide branches, transistors, limiters, modulators, amplifiers and optical delay lines. Many applications have been realized with good performance such as the drop filter, optical filter, polarization splitter, Y-splitter and Mach-Zehnder interferometer.

PhCs exhibit a wide range of useful properties. Also, there are many possible structures. It is good to characterize it first computationally before starting to manufacture a structure. Hence, it will be known on which frequency range one can find PBG, negative reflection or some other photonic effect. It means to solve Maxwell’s equations in space, time and frequency domain. The solutions would be in a form of transfer matrix that should show the energy flux that is reflected, refracted and scattered as loss inside PhCs. These are very complicated mathematical expressions because of the multiple scattering processes for each photonic element in the structure. Still, Maxwell’s equations possess exact solutions, and several approximations could be made without endangering the overall accuracy of characterizations that from now on will be referred to as “computational simulations”. The next chapter will present the simulation methods used in this thesis.
2.1 Maxwell's equations for light modes in photonic crystals

The basic problem of engineering PhCs with useful properties is in solving the time, space and frequency relations for the intensity of light and the strengths of electric and magnetic fields. The medium is periodically modified dielectric; therefore Maxwell equations will form the basics.

Light propagation in any linear, isotropic and macroscopic medium can be best described by Maxwell Equations for magnetic and electric fields.

\[
\begin{align*}
\nabla \cdot \mathbf{H} &= 0 \\
\nabla \cdot \mathbf{D} &= 4\pi \rho \\
\n\nabla \times \mathbf{E} &= -\frac{1}{\mu} \frac{\partial \mathbf{H}}{\partial t} \\
\n\nabla \times \mathbf{H} &= \frac{4\pi}{c} \mathbf{j} + \frac{1}{\mu} \frac{\partial \mathbf{D}}{\partial t} 
\end{align*}
\]

(2.1)

As the dealings are with nanostructures, the space inside the photonic crystal is not homogeneous and both the dielectric index and the refractive index are space dependent. Here \( E(r,t) \) and \( H(r,t) \) are the electric and magnetic fields respectively, while \( D(r,t) \) and \( B(r,t) \) are the electric flux density and magnetic flux density. \( D(r,t) \) is also called electric displacement equal to \( \varepsilon(r)E(r,t) \) with \( \varepsilon(r) \) dielectric index. The other quantities are density of charge \( \rho(r) \), magnetic permeability \( \mu(r,t) \) and current density \( J(r,t) \). The current density is directly dependent on electric conductivity \( \sigma(r) \) and is expressed as \( J(r,t) = \sigma(r)E(r,t) \). The physical effects of these relations are very complicated. They can include non-linearity, polarization, magnetization and even hysteresis behavior. There are several simplifications that can be assumed without losing any relevant physics. The periodic materials of interest are non-magnetic \( \mu = 1 \) and are not
metallic with negligible density of charge $\rho = 0$. Therefore the Maxwell equations are simplified to the form of:

$$
\begin{align*}
\nabla \cdot \mathbf{H} &= 0 \\
\nabla \cdot (\varepsilon \mathbf{E}) &= 0 \\
\nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t} \\
\nabla \times \mathbf{H} &= \frac{4\pi \sigma}{c} \mathbf{E} + \frac{\varepsilon}{c} \frac{\partial \mathbf{E}}{\partial t}
\end{align*}
$$

(2.2)

One important assumption is that $\varepsilon(r)$ is not a function of frequency, so the material dispersion is not taken into account. Magnetic and electric fields are dependent on both time and space. Since Maxwell’s equations are linear, they can be expressed by a combination of time and space. Expanding the fields into sets of harmonic modes the solutions become:

$$
\begin{align*}
\mathbf{E}(r,t) &= \mathbf{E}(r)e^{-i\omega t} \\
\mathbf{H}(r,t) &= \mathbf{H}(r)e^{-i\omega t}
\end{align*}
$$

(2.3)

Considering that the functions are harmonic one can substitute them into Maxwell equations and after few calculations find expressions that explicitly relate the two fields and the frequency.

$$
\begin{align*}
\nabla \times \mathbf{E}(r) &= i\omega \mu_0 \mathbf{H}(r) \\
\nabla \times \mathbf{H}(r) &= -i\omega \varepsilon(r) \varepsilon_0 \mathbf{E}(r)
\end{align*}
$$

(2.4)

There is no need for the solutions to describe both electric and magnetic fields. They can be presented as:

$$
\begin{align*}
\nabla \times (\nabla \times \mathbf{E}(r)) + (1 - \varepsilon(r)) \mathbf{E}(r) &= \frac{\omega^2}{c^2} \mathbf{E}(r) \\
\n\nabla \times \frac{1}{\varepsilon(r)} \nabla \times \mathbf{H}(r) &= \frac{\omega^2}{c^2} \mathbf{H}(r)
\end{align*}
$$

(2.5)
These equations are known as the master equations. They fully describe the electric and magnetic fields in the current problem. The eigenvalues \( \frac{\omega^2}{c^2} \) are real and are solutions to a Hermitian operator.

### 2.2 Bloch-Floquet Theorem

This theorem is called alternatively “Bloch’s” or “Floquet’s” theorem depending upon whether you drink beer or wine. It states that a photonic crystal by definition is a periodic dielectric material, represented by a periodic function \( \varepsilon(r) = \varepsilon(r + \vec{R}_i) \) for any primitive lattice vector \( \vec{R}_i (i = 1, 2, 3) \) in any of the three dimensions. The solutions to equation for periodic eigenstates become:

\[
\vec{E} = E_k(r)e^{i(k \cdot \vec{R} - \omega t)}
\]

\[
\vec{H} = H_k(r)e^{i(k \cdot \vec{R} - \omega t)}
\]

(2.6)

As a consequence of the theorem one can observe that the wavevector is a conserved quantity. Propagating light with fixed \( k \) cannot scatter. Substituting once again the eigenvalues and periodic function \( H(r,t) \) one reach the expression for a Hermitian Eigen problem in finite domain.

\[
\left( \nabla + i\vec{k} \right) \times \frac{1}{\varepsilon(r)} \left( \nabla + i\vec{k} \right) \times H_k(r) = \left( \frac{\omega(\vec{k})}{c} \right)^2 \tilde{H}_k(r)
\]

(2.7)

The PhC may have large number of regions with different materials as long as they form some repeating structure. The different materials having different dielectric constant present a real problem of finding appropriate solution. That’s why one can assign effective dielectric constant for the whole structure and respectively effective refractive index.
\[ n_{\text{eff}} = \sqrt{\varepsilon_{\text{eff}}} \]  

(2.8)

Periodicity of \( H(r,t) \) means that one needs to consider only a finite space domain called unit cell. Its eigenvalues \( \omega_n \left( \vec{k} \right) \) (n=1, 2, 3…) are discrete and countable set of continuous function of \( \vec{k} \). When eigenvalues are plotted as function of wavevector, the result is a map of all electromagnetic interaction in the dielectric. It is called dispersion diagram and it is formed by “frequency bands” that define the band structure of the photonic crystal.

As a consequence eigenvalues are also periodic functions of the wave vectors \( \vec{k} \). Therefore the solution at \( \vec{k} \) is identical to the solution at \( \vec{k} + \vec{G}_j \) where \( \vec{G}_j \) is the primitive vector of the reciprocal lattice defined by the expression \( \vec{R}_i \cdot \vec{G}_j = 2\pi \delta_{ij} \). Periodicity enables one to compute the eigenvalues for \( \vec{k} \) only within a region called First Brillouin Zone defined as a set of inequivalent vectors. In one dimensional case the first Brillouin zone is the range \( k = -\frac{\pi}{a}, ..., \frac{\pi}{a} \) where symbol \( a \) is some periodicity defined by \( R_i = a \) and \( G_i = \frac{2\pi}{a} \).

PhC may exhibit other symmetries that could make the first Brillouin zone redundant. This allows us to reduce even further the range of unique eigenvalues. This new region is called Irreducible Brillouin Zone and in the well-known one – dimensional case with time reversal symmetry it is just \( k = 0, ..., \frac{\pi}{a} \).
2.3 Origin of photonic band gaps

The PBG is a frequency region where the light is forbidden to propagate. It is often compared to the forbidden energy levels as electrons and holes are propagating through a semiconductor. The periodicity of the semiconductor crystals creates periodic potentials with their discrete eigenvalues. They have similar representation as photonic energy bands on a dispersion diagram.

PBGs can be complete with no propagating solutions for any wavevector k. However the PBG can be incomplete which means that solutions are prohibited only for certain wavevector k or certain polarization of light wave. They can be also omnidirectional or PBG only for certain direction depending on the specific topology of the PhC.

One can consider transparent dielectric material with periodic structure. The two simplest structures are hole – based: air holes drilled in high refractive index dielectric and rod – base: high refractive index pillars in air. When photons pass through such material, the sequence of high and low refractive index regions look exactly like periodic potential. If the dielectric index contrast is high enough then most of the light is going to be confined either to low refractive index regions or to high refractive index regions. Depending on the properties of the crystal the light would be forbidden to propagate at some wavelength and would be reflected, while at other wavelength the crystal will remain perfectly transparent.

There are two general properties of Hermitian that can explain the existence of PBG in PhC: First of all its harmonic modes must be orthogonal and its eigenvalues should be real and positive.
\[ \langle \vec{H}_i, \vec{H}_j \rangle = 0 \quad i \neq j \] (2.9)

Secondly according the electromagnetic vibrational theorem the lowest band minimizes the energy functional.

\[
\omega(k)^2 = \min \left[ \frac{\int dr \left( \nabla \times H_i(r) \right)^2}{\int dr \left| H_i(r) \right|^2} \right] \frac{c^2}{\varepsilon} \tag{2.10}
\]

The second band should satisfy the same variation rule but also should fulfil the orthogonality rule. This is true for all higher bands. There are two conditions needed to be satisfied in order to minimize the energy functional. First the variation of field should be sufficiently small and second the electric field should be concentrated in the region with high refractive index. The second band gap is trying to satisfy the same rule but it is orthogonal to the first and cannot concentrate into the high refractive region. Consequently the band should either move to the low refractive index region or stay in the high refractive index region but cancel its oscillation to zero the integral. The result is huge frequency increase that creates forbidden frequency region between the two photonic bands.

Figure 2.3.1 is an example of one dimensional photonic crystal and the emergence of a PBG. The reality is that any one dimensional stack with any non-zero dielectric contrast creates PBGs. Unfortunately this is not true for two and three dimensional PhC as well as for the photonic crystal slabs. In the latter cases the size of the gap depends directly on the dielectric contrast and there is also relatively pretty high minimal dielectric index contrast needed for opening up a gap.
Figure 2.3.1: (a) Two modes are discretized due to periodicity of a dielectric structure, (b) the result is a PBG for frequencies in between.

The PBG can exist only in direction where the dielectric constant is periodically modulated and is impossible for homogeneous material. Thus the only PhC possessing complete omnidirectional gap in reality are the 3D PhCs. One dimensional PhCs may possess a gap only for light falling perpendicular on its surface. The two dimensional crystals though are very complicated structures and deserve more thorough description in following chapters.

2.4 Plane wave expansion simulation method

The most common frequency domain analysis method is the Plane-Wave Expansion (PWE) method. It is a decomposition of the photonic modes, with infinite periodicity in all direction. This method can handle point like defects in the cell but is not good enough for extended defects. Our computational tool CrystalWave band solver can calculate:
1. 2D band calculations for 2D lattices

2. 3D band calculations for 2D lattices – far more realistic tool but with much greater use of computer resources.

3. 3D band calculations for 3D lattices – outside current research

These calculations generate band diagrams that show TM and TE bands and also their band gaps. Information about effective index, group velocity, dispersion and loss could be calculated for each point of the diagram. The output of a PWE analysis is the band structure or band diagram that is the plot of the normalized frequency, \( a/\lambda \) or \( \omega a/2\pi \) where “\( a \)” is the lattice constant and \( \lambda \) is the free space wavelength of the guided modes versus the wave vector.

PWE is adapted from solid state physics where translational symmetry of atomic lattice expanding the fields as Bloch vectors. The space function of periodic dielectric constant is Fourier transformed into reciprocal lattice vectors. A disadvantage of this method lay in the fact that dielectric function should be real, so it is not possible to simulate metals and other metamaterials.

Assuming that there is no periodicity in z direction, then the wave vector does not depend on z and its derivative is zero. The Maxwell equations could be written as:

\[
-\frac{1}{\varepsilon(r)} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \vec{E}_z(r) = \frac{\omega^2}{c^2} \vec{E}_z(r)
\]

\[
\left( \frac{\partial}{\partial x} \frac{1}{\varepsilon(r)} \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \frac{1}{\varepsilon(r)} \frac{\partial}{\partial y} \right) \vec{H}_z(r) = \frac{\omega^2}{c^2} \vec{H}_z(r)
\]

(2.11)
Here $\vec{r} = x\hat{a}_x + y\hat{a}_y$ and $r$ is a periodical for $\varepsilon(r)$. Every periodical function can be Fourier expanded as well as its inverse function. Therefore one can express the inverse of dielectric function as:

$$\frac{1}{\varepsilon(r)} = \sum_G k_G e^{j\vec{G} \cdot \vec{r}}$$

$$k_G = \frac{1}{A} \int_S \frac{1}{\varepsilon(r)} e^{-j\vec{G} \cdot \vec{r}} dS$$

(A is the area of the unit cell, $S$ is its contour. $G$ is the reciprocal unit vector that is normalized as:

$$e^{j\vec{G} \cdot \vec{a}} = 1$$

According the Bloch theorem electric and magnetic field can be expanded into sum of infinite number of plane waves:

$$\tilde{H}_z(\vec{r}) = e^{j\omega t} h_k(\vec{r})$$
$$E_z(\vec{r}) = e^{j\omega t} e_k(\vec{r})$$

$$h_k(\vec{r}) = h_k(\vec{r} + \vec{a})$$
$$e_k(\vec{r}) = e_k(\vec{r} + \vec{a})$$

These are the Bloch modes consisting of plane wave multiplied by a periodic function depending on their wave vector. The final solution requires to obtain the eigenvalues of magnetic and electric fields. They are the eigenvalues of the dispersion diagram:

$$-\sum_{\vec{G}} k_G \left( \vec{G} - \vec{G}' \right) \left( \vec{k} + \vec{G}' \right) \times \left[ \left( \vec{k} + \vec{G}' \right) \times \tilde{E}_{z_k} \left( \vec{G}' \right) \right] = \frac{\alpha_x^2}{c^2} \tilde{E}_{z_k} \left( \vec{G}' \right)$$

$$-\sum_{\vec{G}} k_G \left( \vec{G} - \vec{G}' \right) \left( \vec{k} - \vec{G}' \right) \times \left[ \left( \vec{k} + \vec{G}' \right) \times \tilde{H}_{z_k} \left( \vec{G}' \right) \right] = \frac{\alpha_y^2}{c^2} \tilde{H}_{z_k} \left( \vec{G}' \right)$$

(2.15)
The wave vector is restricted only along irreducible Brillouin zone. The contours for classic 2D PhCs and the AARH PhC are given on Figure 3.4.1 and Figure 3.4.2.

2.5 Finite difference time domain simulation method

The CrystalWave simulation tool uses Yee cell algorithm for FDTD calculations which solves Maxwell equations for both space and time domain.\textsuperscript{50} The grids for magnetic and electric fields in this case are staggered. In the special domain the electric fields are defined at the center of 6 cube faces and the magnetic field is defined at the center of 12 cube edges. The four magnetic fields surrounding every electric field allow calculating electric curl. Here the method implicitly applies The Faraday and Ampere laws. Significant disadvantage of this method is that magnetic and electric fields are not defined at one and the same point and therefore the Pointing Vector requires averaging of electric or magnetic field. In the time domain the Yee’s algorithm calculates the E and H components at temporal instants that differ of half time step t/2. On Figure 2.5.1 is shown simplified 1D visualization of the method in k space domain.
Figure 2.5.1: The 1D space-time Yee algorithm showing central differences for the space derivatives and leapfrog over the time derivatives, k represent electric field node numbers and n the time steps.

Figure 2.5.2: Position of electromagnetic field components in Yee cell.

The FDTD algorithm was implemented for an arbitrary system of coordinates. It has been shown that the discrete version of Maxwell’s equations is valid for any arbitrary grid. In the real
space domain an insight into the method one can get from Figure 2.5.2.53 In Cartesian coordinates in linear, isotropic, nondispersive three dimensional media the Maxwell equations become:

\[
\begin{align*}
\frac{\partial E_x}{\partial t} &= \frac{1}{\varepsilon} \left[ \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x \right] \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\varepsilon} \left[ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y \right] \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\varepsilon} \left[ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right] \\
\frac{\partial H_x}{\partial t} &= \mu \left[ \frac{\partial E_y}{\partial y} - \frac{\partial E_y}{\partial y} \right] \\
\frac{\partial H_y}{\partial t} &= \mu \left[ \frac{\partial E_z}{\partial z} - \frac{\partial E_z}{\partial z} \right] \\
\frac{\partial H_z}{\partial t} &= \mu \left[ \frac{\partial E_x}{\partial x} - \frac{\partial E_x}{\partial x} \right] 
\end{align*}
\] (2.16)

Here the spatial points are given by \((i, j, k) = (i\Delta x, j\Delta y, k\Delta z)\). The quantities \(\Delta x, \Delta y\) and \(\Delta z\) are the spatial step along the three directions \(x, y\) and \(z\) and the three integers \(i, j\) and \(k\). Using the space and time discretization, the time derivative of the \(x\) component of the electric field is:

\[
E_{x,i,j+1/2,k+1/2}^{n+1/2} = \left(1 - \frac{\sigma \Delta t}{2\varepsilon} \right) E_{x,i,j+1/2,k+1/2}^{n} + \frac{\Delta t}{\varepsilon} \left[ \frac{H_{y,i,j+1/2,k+1/2}^{n} - H_{y,i,j+1/2,k+1/2}^{n} - H_{y,i,j+1/2,k+1/2}^{n}}{\Delta y} \right] \left[ \frac{H_{z,i,j+1/2,k+1/2}^{n} - H_{z,i,j+1/2,k+1/2}^{n}}{\Delta z} \right] \] (2.17)

One can write down analogous expressions for all other components of the electric and magnetic fields. However, they are not needed for the current discussion.

Looking at the equation 2.17 the first advantage of this technique emerges. Any new value of any electromagnetic component at any special point depends only on its value a time step before and the values of adjacent points. There several other advantages related to the second order accuracy and continuity of tangential components of electric and magnetic field.
FDTD method allows simulations either of TE or TM polarized light. In the case of AARH PhC and AARH PCS which are the focus of this thesis there is no periodicity in z direction as the wave uniform then all electromagnetic derivatives are zero. The TM modes then are using equations:

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} \right)
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} \right)
\]

\[
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_z}{\partial y} - \sigma E_z \right)
\]

The TE modes are using equations:

\[
\frac{\partial E_x}{\partial t} = -\frac{1}{\varepsilon} \left( \frac{\partial H_z}{\partial y} - \sigma E_x \right)
\]

\[
\frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon} \left( \frac{\partial H_z}{\partial x} + \sigma E_y \right)
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_y}{\partial y} - E_y \right)
\]

The PCS then could be characterized by the propagation of polarized electromagnetic wave through its structure or its refractive and reflective properties. In order to achieve this one need to discretize the above equation:

\[
E_{x,j-1/2,i+1}^{n+1} = \left( 1 - \frac{\sigma \Delta \mu}{2 \varepsilon} \right) E_{x,j-1/2,i+1}^{n} + \left( \frac{\Delta \mu}{\varepsilon \Delta x} \right) \left( H_{y,j-1/2,i+2}^{n} - H_{y,j-1/2,i+1}^{n} \right) + \left( \frac{\Delta \mu}{\varepsilon \Delta \mu \Delta x} \right) \left[ H_{y,j-1/2,i+2}^{n} + H_{y,j-1/2,i+1}^{n} \right]
\]

\[
H_{x,j-1,i+1}^{n+1} = H_{x,j-1,i+1}^{n} + \left( \frac{\Delta \mu}{\varepsilon \Delta \mu} \right) \left[ E_{x,j-1/2,i+1}^{n+1} - E_{x,j-1/2,i+1}^{n} \right]
\]

\[
H_{y,j-1,i+2}^{n+1} = H_{y,j-1,i+2}^{n} + \left( \frac{\Delta \mu}{\varepsilon \Delta \mu} \right) \left[ E_{x,j-1/2,i+1}^{n+1} - E_{x,j-1/2,i+1}^{n} \right]
\]

\[
20
\]
\[
E_{x,i,j+1/2}^{n+1/2} = \left(1 - \frac{\sigma \Delta t}{2 e} \right) E_{x,i,j+1/2}^{n-1/2} + \left(\frac{\Delta t}{\sigma \Delta t} \right) \left[ H_{z,i,j+1/2}^{n} - H_{z,i,j}^{n} \right]
\]

\[
E_{z,i-1/2,j+1}^{n+1/2} = \left(1 - \frac{\sigma \Delta t}{2 e} \right) E_{y,j-1/2,j+1}^{n-1/2} + \left(\frac{\Delta t}{\sigma \Delta t} \right) \left[ H_{z,j-1,j+1}^{n} - H_{z,j,j+1}^{n} \right]
\]

\[
H_{z,i,j+1}^{n+1} = H_{z,i,j+1}^{n} + \left(\frac{\Delta t}{\mu \Delta y} \right) \left[ E_{y,j+1/2,j+3/2}^{n+1/2} - E_{y,j+1/2,j+1/2}^{n+1/2} \right] + \left(\frac{\Delta t}{\mu \Delta y} \right) \left[ E_{y,j-1/2,j+1/2}^{n+1/2} - E_{y,j+1/2,j+1/2}^{n+1/2} \right]
\]

CrystalWave can show the space propagation for each of \( H_x, H_y \) and \( E_z \) components of TM polarized light and the propagation of \( E_x, E_y, H_x \) and \( H_y \) components of TE polarized light. The best insight though is available with the intensity propagation in space domain. It is possible also to look at the distribution of Poynting vector inside the photonic device.

One can also write the condition of numerical stability of Tee algorithm. For 2 dimensional simple square lattices it is:

\[
\Delta t > \frac{\Delta x}{c_0 \sqrt{3}}
\]

Here \( c_0 \) is the speed of light in vacuum and \( \Delta x = \Delta y \).

FDTD method is computer resources intensive especially in its 3D variant. In order to lower its intensity and save computer storage one need to minimize the space and time regions of computation but still enclose the PCS. The truncation of the computational domain should absorb and attenuate all electromagnetic wave coming from the PCS and to be perpendicular to the surfaces of the PCS. This could be achieved by specifying boundary conditions at the edge of the computational region.
Several boundary conditions have been proposed starting with a simple Dirichlet boundary condition. It sets the solution to zero at the boundary of the grid. The disadvantage here is the lack of information of the reflective properties of given structure. Another popular set of condition is Absorbing Boundary Condition\(^5^4\) though it is suitable only in the case that leaking from the PCS is a single plane wave. It is extrapolating the field from the interior grid points to the edge grid points. Unfortunately this method is rather good for one dimensional structures but not for much more important two and three dimensional simulations.

The CrystalWave simulation tool is using the Perfectly Matched Layers method that is probably the most popular one. At the edges of the grid a new absorbing layer is added that is entirely independent from the boundary conditions. The medium should be constructed in such a way that the waves do not reflect at the interface between the structure and the new layer. This condition exhibits one important advantage that it works even in inhomogeneous media as photonic crystal waveguides.

Perfectly Matched Layers are situated at the upper and bottom layer of slab and absorb the light waves scattered in z direction from the elements of the photonic structure. They are shown schematically on Figure 2.5.3.
Figure 2.5.3: PCS active layer is in orange color, cladding is in gray and Perfectly Matched Layers in green some distance from the cladding layers.

Perfectly Matched Layers can be treated as uniaxial anisotropic absorbers\textsuperscript{55} whose permittivity and permeability tensors are specified according to the following relations.\textsuperscript{56}

\[
\hat{\varepsilon} = \varepsilon \hat{\Lambda} \\
\hat{\Lambda} = \begin{pmatrix}
\chi & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & \chi^{-1}
\end{pmatrix}
\]

(2.23)

Here $\chi$ is the relative permittivity of the adjacent medium, $\chi'$ is real and $\chi''$ positive. These conditions make possible complete absorption of all plane waves coming from the PCS from all angles and with all frequencies. However discretization of field and material properties result in a
not entirely transparent barrier on the interface between computational domain and Perfectly Matched Layers. It means that significant reflection can occur and some light starts propagating back into the crystal. The problem can be solved with replacing the constant $\chi''$ with a spatially varying function.

$$\chi'' = \frac{\sigma |z + z_0|^n}{L^n}$$ (2.24)

Here the plus and minus signs signify the upper and bottom boundary layer, $L$ is the constant thickness of the layer, $n$ is a constant parameter and $\bar{\sigma} = \sigma / \omega$ decaying rate inside the Perfectly Matched Layers. Optimization of those parameters is not a trivial task and lead to significant differences between results obtained from different computational software using different method of optimization.

There are two very important limitations for PML boundary conditions. One is that the absorption is angle dependent from the waves coming from the source. Therefore there are certain practical conditions for placing the source of simulated radiation. The second one is related to the stability of the numerical simulation when inhomogeneous dielectric pattern create unusual solution – negative refraction. Usually in such case other techniques are used mostly for two dimensional PhCs.

In this thesis the simulation methods used are 2D and 3D PWE that gives the dispersion relation in k-space. It can also expose the Bloch modes, isofrequency contours in k-space and 3D frequency surfaces. For every data point can be retrieved a treasure of information about the real and phase speed of the simulated light, the effective refractive index, etc. A resolution of 34 for investigations of the existence, frequency positions of PBGs and their relation to different properties of the PhC. This resolution was deemed proper for mass calculations. For several other
simulations like matching 3D PWE and 3D FDTD method a resolution of 64 was used. Still, there are some little discrepancies between higher and lower resolution dispersion diagrams.

Additionally, 2D and 3D FDTD methods were used. The frequency domain FDTF provides information on transmission properties of the PhC. Several sensors are simulated in front and behind the PhC. They measure the electric, magnetic field strengths of incident light, its refracted and reflected components. It is possible to measure the loss of the electromagnetic wave due lack of vertical light confinement in PCSs. The pulse is sinusoidal of 5 or 10 femtoseconds depending on the desired range. Resolution also varies with simulations that match PWE simulation reaching 100000 steps. Usual resolution is of 20000 steps where increasing them does not provide more accuracy but is consuming enormous amount of resources.

The 2D and 3D FDTD method can be used in real space domain. The light is propagating as a plane monochromic wave. The intensity of the light is presented in every point of space. Hence, it is possible to present the incident, refracted and reflected light. It is also possible to observe surface, edge and cladding modes. This is the method that can reveal the existence of negative refraction and superlensing in the photonic structure.

Maxwell equations are scalable, so everywhere the units are normalized frequency. Still there are some real space and wavelengths restrictions. The photonic elements of the PhC may be just half of the wavelength of propagating light bet the grid on which they are spaced should be at list 10 times smaller. Here the rule of stability is everywhere fulfilled and it is presented as:

\[
c\Delta t < \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}} \quad (2.25)
\]
Chapter 3 General Properties of Photonic Crystals

By definition a PhC is a material in which its refractive index is periodically modulated, hence: periodic material. The features of the PhC should be comparable to the wavelength of the light that propagates through it. “Feature” has many definitions but generally it is the smallest repeating element of the PhC. Overall, there are many analogies with the solid state crystals and the laws of electric charge and photonic propagation. When a beam of photons fall on the surface of a PhC and continue through the periodic interfaces of different dielectric index regions, it scatters coherently and is modulated in several ways. These scatterings lead to certain directions and energies that are forbidden for certain frequencies of the propagating photons. The frequency regions that are forbidden are called complete photonic bandgaps. The nature of these bandgaps could be very different for different PhC structures and depend on characteristics like dimensionality of the PhC, polarity of the light, initial and final surface of the crystals etc.

3.1 Dimensionality

While we are living in a 3D world the PhC may exhibit periodicity in 1, 2 or 3 of its dimensions. 1D PhC are stacks of 2 or more planes with different refractive index. They are useful in several applications as holography, brag mirrors and holography.

1D PhCs have continuous translational symmetry in x and z direction and discrete translational symmetry in y direction. Therefore the primitive lattice vector is a 1D constant $a = a\hat{y}$ and the reciprocal lattice vector is $b = \frac{2\pi}{a} \hat{y}$. Usually 1D structure has mirror symmetry so their Irreducible Brillouin Zone is in the range $0 \leq k \leq \pi / 2$. Classical choice of materials is a stack of
GaAs and air (dielectric constant $\varepsilon = 13$) and GaAlAs and air (dielectric constant of $\varepsilon = 12$). Unfortunately, there many important issues related to their optical qualities. They are also useless if the light is not exactly incident perpendicularly on the PhC surface.

In general every 1D PhC exhibits a PBG. If it is simple two layers structure though, its PBG is usually small. High quality photonic devices can be manufactured with multilayered stack of many different dielectric materials. One can observe interesting optical resonances with carefully chosen dielectric constants of the layers. As for the 2D PhC case, a practical problem is the light loss for the direction where the light is not confined. In the case of 1D PhC these are both x and z directions. It is increased if the optical quality of the dielectric materials in the stack is increased. A typical 1D PhC is shown on Figure 2.3.1 (a).

2D PhCs are very diverse in their structures. They have periodicity in x and y directions. If periodicity is not the same in x and y axis, PhCs are chiral. They can also be quasi crystals if certain level of disorder is introduced in their structure. Periodicity may be also long ranged with disordered elements in small scale and short ranged without disorder. The two classic PhCs structure are rods in air and holes in semiconductor as shown on Figure 3.1.1. The issues of topologies will be discussed in “Topologies” section bellow.

For computational purposes it is introduced ideal 2D PhC where the z component is disregarded. These crystals are widely used for qualitative description of photonic structure. The lack of confining in z axis for the real PCSs leads to impossibility of complete PBG. Still incomplete PBG along part of the k – space contour are possible and exhibit many useful features. These issues are going to be discussed further in their respected sections.
3D PhC are hard to manufacture until recently when 3D nano writing technology became available. Theoretically 3D PhC can exhibit enormous up to 80% PBGs. In reality the geometries with complete PBG are rather rare. The reason is the large 3D Brillouin Zone. The PBG should cover all nexuses, lines and volumes of the zone. Even very large dielectric constants do not open PBG even in most symmetric and promising geometries. The reason is that there is no 3D spherical Brillouin Zone and the PBGs for different k-space directions open up at different frequencies. There is need for significant dielectric contrast that should widen up the PBGs enough, so that they start to overlap. The closest to spherical structures is the Diamond and Face Centered Cubic geometries for the Brillouin Zone. They share the same lattices and generally are considered most promising for achieving complete PBG in 3D PhC. Nevertheless, many complete PBG were found for several other classes of lattices. It seems that the same engineering tricks that work for opening of PBGs in 2D PhC work also for their 3D version. On Figure 3.1.1 are shown the two most common topologies for 3D PhC: Woodpile and Spheres.

The Spheres topology can be either dielectric spheres in air or air spheres in dielectric. The most important parameter here is the radius of the sphere exactly as in the radius of rods and holes for 2D PhCs. The first practically realized 3D PhC is the Yablonovite\textsuperscript{58} with centimeter sized features that correspond to microwave region of electromagnetic spectrum. It was discovered by Eli Yablonovitch in 1989 and achieved complete PBG of 19 %. Its topology is like to interpenetrating diamond like lattices of air and dielectric spheres.

The Woodpile topology was the first one that achieved 3D complete PBG in 1994 for micron range.\textsuperscript{59} It is a rectangular or rhomboid stack of dielectric rods oriented horizontally with altering orthogonal directions (several attempts were done with non-orthogonal orientations). Its
main advantage is that the fabrication procedure is similar to that in the electronics manufacturing. In 1999 a complete PBG was achieved for frequency of close to information frequency of 1.5µ.\textsuperscript{60}

However, even that the 3D stack of AARH PCSs proposed in this thesis is possible, the computer resources and software support were insufficient for deeper investigations, so it is left outside the scope of current thesis.

![Examples of 1D, 2D and 3D PhCs with simple topologies.\textsuperscript{61}](image)

**Figure 3.1.1:** Examples of 1D, 2D and 3D PhCs with simple topologies.\textsuperscript{61}

### 3.2 Symmetry and symmetry breaking in photonic crystals

For the purpose of engineering PhC with useful properties symmetries are somehow two edged sword. On one hand the very existence of symmetries creates the basis for defining certain dielectric medium periodic. On other hand symmetries lead to mode degeneration at high symmetrical vertices in k space and close any PBG that could exist. Therefore a careful balance is needed when constructing periodic structures.
For low dimensional PhCs one unescapable type of symmetry is the continuous translational symmetry. It can be found in the isotropic direction of 1D and 2D PhCs. Its most important property is that it conserves the wave vector $\mathbf{k}$ along the symmetry directions. Along those directions the medium is isotropic and therefore dielectric index is constant. The modes become:

$$\tilde{\mathbf{H}}_k (\vec{r}) = \tilde{\mathbf{H}}_0 e^{i\mathbf{k}\cdot\vec{r}}$$  \hspace{1cm} (3.1)

Solving the master equation one can obtain the dispersion relation that is $\omega = c \left| k \right| / \sqrt{\varepsilon}$. The frequencies depend only on the wave vector and its direction. Realistic PhC are not infinite in any direction which means that soon or later the propagating light will meet an interface boundary with different dielectric index that will change its frequency.

Total internal reflection is a phenomena derived from Snell Law. If the light propagating from a medium with higher dielectric index hit at small angle medium with low dielectric index the light is confined in the first region. In real life scattered light propagating from the PhC may fall at every possible angle on the boundary. The waves going back into the PhC consist of “guided modes” while the waves leaving the construct, exponentially decay in free space and are described as evanescent modes. The frequency boundary between these two kinds of modes is called light line. The frequency region above the light line is called light cone and its wave vectors are imaginary. The important result of this split of frequencies is that the guided modes now possess discrete frequencies while the evanescent modes are continuous.

Being periodic medium, PhC exhibit discrete translational symmetry as it has discrete regions of different dielectric index. If there is no such symmetry the medium is classified as photonic quasicrystal or disordered PhC. Periodicity of the medium is the factor defines the band
structure of the crystal. The solutions and dispersal relation due to this symmetry were described in the Bloch – Flouquet section in Chapter 2.

Rotational symmetry is another important property of PhC. PhCs without 90° rotational symmetry are called Chiral and will be described later. The overall result from rotational symmetry is that frequency bands have additional redundancy in the Brillouin Zone.\(^{62}\) Frequencies that undergo rotation by rotational operator \(\hat{R}\) remain the same as the original \(\omega(\hat{R}\vec{k}) \equiv \omega(\vec{k})\) and there is no need these \(\vec{k}\) to be considered in the Brillouin Zone. When all redundant \(\vec{k}\) points (due to rotation, reflection and inversion) are dismissed, the \(k\)-space region with unique frequencies bands is described as Irreducible Brillouin Zone.

The mirror symmetry is especially important for 2D PhC and 3D PCS. It leads to field polarization and allows solving the dispersion relations for two independent classes of modes. In the first case the field components of \(E_x, E_y\) and \(H_z\) form the TE modes while \(H_x, H_y\) and \(E_z\) field components form the TM modes. In the case of PCSs the two polarizations include the “even” modes with field components \(H_x, E_y\) and \(E_z\) and “odd” modes with the field components of \(E_x, H_y\) and \(H_z\). The behavior and properties of latter are so like the 2D variant that when discussing PCSs the odd modes are referred as TM modes and even modes are referred as TE modes.

The inversion symmetry is common for all 2D PhC and 3D PCS and need no discussion here.

On Figure 3.2.1 (a) is shown the full set of symmetries for square lattice 2D PhC, on Figure 3.2.1 (b) The First Brillouin Zone and its reduction due to symmetries into Irreducible Brillouin Zone (the shaded region).
Due to translational, two mirror and two rotational symmetries the Irreducible Brillouin Zone becomes just $1/8$th of the original Brillouin Zone. One can describe them as follows: Translational symmetry reduces periodicity of the structure as $\varepsilon(\vec{r}) = \varepsilon(\vec{r} + n\hat{a} + m\hat{a})$ where $n$ and $m$ are integers and $a$ is the lattice constant. It is worth noting that if the two lattice vectors were unequal $\vec{a}_1 \neq \vec{a}_2$ the PhC will become Chiral and high symmetry points $X$ and $X'$ would become unequal. In such case the light propagation from bellow and from aside with be described with different dispersion relations. Dispersion relations for light wave incident from an angle would have unique properties and often exhibiting unusual reflection and refraction.

There are two mirror symmetries for the given PhC: along $x$ axis and along $y$ axis. The invariance can be expressed as $\varepsilon(x, y) = \varepsilon(-x, y)$ and $\varepsilon(x, y) = \varepsilon(x, -y)$. 

Figure 3.2.1: (a) Example of various symmetries in a 2D PhC with square lattice (b) Larger First Brillouin Zone and much smaller shaded Irreducible Brillouin Zone.
Rotational symmetry is expressed by $C_n$ which means invariance under rotation of $2\pi / n$. In this case the PhC exhibit two symmetries $C_2$ and $C_4$ – rotation of 180° and 90°.

Periodic structures have some disadvantages due to their high symmetry. Most important among them are the degeneration of modes that close the PBGs and unescapable difficulties during fabrication process that results in less than ideal cases. Recently, a lot of studies had been aimed at PhC configurations with reduced symmetry. Anomalous characteristics arise mainly due to high rotational symmetries in PhCs. Translational symmetries could be broken in quasi – periodic structures without lessening the widths of PBGs and in some cases even improving them\textsuperscript{63}. Disordered or reduced symmetry structures were found to possess many superior characteristics in their transmission, reflection, refraction, diffraction and nonlinear optical properties.\textsuperscript{64}

There are several ways to reduce high symmetrical PhC.\textsuperscript{65} Most of the proposed in the literature PhC structures intentionally or not break certain symmetry of the classic triangular or square unit cell. The unit cell of classical PhC are highly symmetric in their structural pattern that leads to high symmetry of the reciprocal unit cell space. Complete PBG are rarely observed mainly because of degeneracy between their modes. The degeneracy is probably due to highly symmetric points in the reciprocal BZ that cause equivalent points along the k–space contour. It is believed that solving this degeneracy by breaking equivalent points will remove the mode degeneracy and open up TE PBG in rods in air and TM PBG in holes in semiconductor PhCs. Reducing the of BZ is called BZ folding.

The dielectric function depends directly on the structure and filling factor of the PhC. In the reciprocal space this dependence can be expressed as.\textsuperscript{66}

\begin{equation}
\epsilon(G) = f \epsilon_{\text{rods}} + (1 - f) \epsilon_{\text{background}} \quad \text{for } G = 0 \\
\epsilon(G) = (\epsilon_{\text{rods}} - \epsilon_{\text{background}}) S(G) \quad \text{for } G \neq 0
\end{equation}

\begin{equation}
33
\end{equation}
The quantity \( \varepsilon(G) \) is the dielectric matrix of square lattice of rods in air background. The quantity “\( f \)” is the filling factor which can be expressed either as percent or fraction like 
\[
f_i = \frac{b r}{2\pi}.
\]
The quantity \( S(G) \) is the structural factor that depends on the geometry of the dielectric unit and can be expressed by the integral:

\[
S(G) = 2f \frac{J_1(G r)}{G r}
\]

Here \( J_1 \) is a Bessel function of first order. For rectangular unit cell with two arrays there is going to be superposition of two structural factors: one for rods and one for holes. This will shift in a various way the bands and therefore lift the degeneracies at various points. Integration is taken by the unit cell in real space with area of \( A \). It is clear that the change of the structural factor directly influence the dielectric matrix and the TE and TM bands become completely different for even small change.

![Brillouin Zone folding](image)

Figure 3.2.2: Brillouin Zone folding when in a (a) triangle unit cell is added another array of elements (b) with different dielectric constant.

On Figure 3.2.2 is shown the significant transformation of BZ when to a classic triangle lattice PhC Figure 3.2.2 (a) is added second array of photonic elements with different dielectric
index, shown on Figure 3.2.2 (b). The original Brillouin Zone exhibit 12 folded rotational symmetry where all vertices X’, M, X, K… are identical. All 12 contours like ΓX’M, ΓMX… are the same and all components b_{ΓX’}, b_{ΓM}, b_{ΓX}… of the reciprocal vectors are equivalent equal to b. The addition of second array increases the surface of real space unit cell and therefore decreases the surface of the Brillouin Zone. The shape of AARH PhC is transformed into rectangle with two unequal components of reciprocal vectors: \( b_{ΓX'} = b / 2 \) and \( b_{ΓX} = b / \sqrt{3} \). The number of equivalent high symmetry points is reduced. Adjusting several characteristics of these arrays enables one to observe many cases of negative slopes in isofrequency contours. Without exception negative slopes indicated the existence of either partial PBGs or left handed characteristics of light propagation. All of them appear due to degeneracy lifting of certain points in K space. In 3D PCS the degeneracy lifting influenced only XM and X’M parts of the overall K space contour. In the 2D case degeneracy lifting caused opening of large complete PBGs along all of the k-space contours.

Important observation is that the first bands of low symmetry PhCs for both TE and TM modes behave very much like in isotropic medium. It means that symmetry breaking rarely open up complete PBGs between lower bands. However the higher the bands the stronger is the influence of the symmetries. Therefore large PBG can be expected between bands higher than 2\textsuperscript{nd} order. The breaking of C\(_4\) symmetry allows the light to take different paths through PhC. Isofrequency contours folds into themselves and the effective refraction index becomes negative which leads to negative refraction, superlensing, and other unusual effects. In fact dielectric index remain positive in other regions of the k-space which directly leads to divergence of photonic bands. This divergence opens up the distance between the bands and creates PBG or enlarges
existing ones. The AARH structure presented in this investigation exhibit numerous TE and TM PBGs for even relatively small dielectric contrast $\varepsilon \sim 6$ to 7.

### 3.3 Chirality

There are many materials in the nature that though isotropic, exhibit different chemical and physical properties along their spatial axes. Sometimes it is due to different structure of their molecules along x, y or z axes. These are denoted as stereoisomers and are useful for many important applications. In Chemistry, Biology and solid State Physics such structures are further subdivided according the symmetry break of their order. As was shown in previous section symmetry break may be meritorious for achieving large, complete PBGs and unusual refraction properties. Therefore, breaking certain symmetries of the unit cell leads to emergence of analogous chiral PhC or PCS. Hence, one can expect that chiral PhC will display different reflection and refraction properties along different axis.67 These differences of optical responses may have huge impact on engineering optical elements like optical gates and switches.

However it was proven that the break out of space inversion symmetry of chiral dielectric materials has effect very similar to the spin-orbiting coupling of electronic band states. The result is helical propagation of the electromagnetic wave through the PhC – gyrotropy. In such way one can make analogy between the photospin transport and electrospin transport and expect similar effects of these wave propagations.68

One of the main feature of the proposed AARH and AARH PCS is that there are very strong degeneration of the bands in one direction $\Gamma X'$ and lack of it in direction of $\Gamma X$. Further investigations are needed on the physical meaning of this effect. Slight changes of the PhC
properties lead to strong chiral resonances that completely transform the dispersion relations in both directions.

3.4 Topology

The rods in air and holes in semiconductor PhCs exhibit the same symmetry but due to their different topology their dispersion diagrams are quite different. PBGs are possible for both topologies but are more often observed with the triangular space unit cell. The reason is that the irreducible Brillouin Zone is smaller for triangular lattice and therefore it is easier to be covered with forbidden frequencies. On other hand triangular lattice is highly symmetrical which leads to degeneracy of its modes that often destroy any nascent PBG. In order to lift such degeneracies, other engineering tricks are often used. Degeneracies around highly symmetrical point X for quadratic lattice will play significant role in the following chapter.
Figure 3.4.1: Classic topologies of 2D PhC (a) Rectangular lattice and its irreducible Brillouin zone (b) Triangular lattice and its irreducible Brillouin zone.

On Figure 3.4.1 (a) the diagram on the left shows the square lattice in real space. The diagram on the right shows the reciprocal lattice of the Brillouin zone and the shaded region is its Irreducible Brillouin Zone. The crystal is invariant to a 90° rotation so its properties are the same irrespectively if the propagating light falls from x or y direction. This invariance is translated in k-space. There are 8 Irreducible Brillouin Zones in the first Brillouin Zone. The real space and reciprocal vectors are:
\[ \bar{a}_1 = a (1,0) \]
\[ \bar{a}_2 = a (0,1) \]
\[ \bar{b}_1 = \frac{2\pi}{a} (1,0) \]
\[ \bar{b}_2 = \frac{2\pi}{a} (0,1) \]  

(3.4)

On Figure 3.4.1 (b) the diagram on the left shows the triangular lattice topology in real space. The diagram on the right shows the Brillouin Zone in reciprocal space. The shaded Zone is the Irreducible Brillouin Zone. The rotational symmetry is even higher for this type of PhC. There are 12 Irreducible Brillouin Zones in its first Brillouin Zone. Its real space and reciprocal vectors are:

\[ \bar{a}_1 = a \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \]
\[ \bar{a}_2 = a \left( \frac{1}{2}, -\frac{\sqrt{3}}{2} \right) \]
\[ \bar{b}_1 = \frac{2\pi}{a} \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right) \]
\[ \bar{b}_2 = \frac{2\pi}{a} \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right) \]  

(3.5)

In both topology \( a \) is the lattice constant.

For comparison on Figure 3.4.2 are shown the real space unit cell on the left and its reciprocal Brillouin Zone on the right for the proposed AARH PhC. AARH PhC lacks 90° rotational symmetry. The high symmetry points X and X' are now unequal and the light propagates differently if incident from on x or y direction. The shaded zones represent the Irreducible Brillouin Zones for the two cases. The darker circles represent high dielectric index material (\( \varepsilon = 6 \sim 12 \)), white circles air holes (\( \varepsilon = 1 \)) and the medium in between is low dielectric medium (\( \varepsilon = 2.5 \)). As
the cell includes many elements it is referred “supercell”. It is the same regardless whether its origin is in the high dielectric circles or in the air holes. Its real and reciprocal vectors are:

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

(3.6)

Figure 3.4.2: Topology of proposed AARH PhCs. (a) Rectangular real space unit cell and (b) rectangular reciprocal supercell. The two shaded regions are the Irreducible Brillouin Zone for two chiral directions.
3.5 Refractive index contrast

The classical rods in air and holes in semiconductor PhCs are produced by two elements and the difference between their refractive indexes is called refractive index contrast. In general, the higher the contrast between low and high contrast material the stronger the possibility of PhCs useful properties like PBG. Usually there is pretty high minimum contrast at which PBG is opened up. Computational simulations of high dielectric constant structure are useful for understanding mechanisms of creations of PBGs. Also, high dielectric constant semiconductors are often used in experimental manufacturing of photonic structures. However, it is worth simulating low refractive contrast architectures. Materials used in them often have the advantage of high optical quality. In order to open PBGs in them, one needs more complicated topologies. In PhCs such as AARH PhC the contrast is harder to define but is still useful in explanations of its dispersion properties.

While materials are more often referred to with their dielectric index, the PhC as a whole is described by its effective index \( n_{\text{eff}} \): 

\[
\frac{\varepsilon_1 + \varepsilon_2 + \ldots + \varepsilon_N}{N}
\] 

for PhC with \( N \) different photonic elements with dielectric index \( \varepsilon \). This index can be widely different in different space regions of the PhC. Even if one postulate strict periodicity of the dielectric index, the effective refractive index for different surfaces can be positive, negative or in some rare case close to zero. In each measured point of dispersion diagram, this quantity may differ resulting in flat or negative isofrequency contours of photonic modes. It is especially true for the proposed AARH PhC and AARH PCS where frequency surfaces are contorted and phase velocity of light may be at all possible direction with any magnitude including zero and infinity.

All PhC exhibit the very important feature of scalability. Due to scalability of Maxwell Equations the solution for propagating light of one frequency is exactly the same for all other
frequencies proportionally to the lattice constant. For a simple rod base or hole base 2D PhC doubling the lattice constant will half the frequency of the energy mode. For this reason the normalized frequency $\omega a/2\pi c$ is invariable.

### 3.6 Filling Factor

The relative size of the main photonic element is called filling factor. It can be measured as fraction like for example $f=r/a$ where $r$ is the radius of the rod or hole and $a$ is the lattice constant. There is certain ambiguity in defining the lattice constant when the PhC is made of more than two photonic elements. This causes some difficulties in annualizing the results from computational simulations as different software are using different conventions. Conversions from frequencies to wavelengths become non-trivial when the special and reciprocal vectors are different for different directions and $k$ space contours. For such structures sometimes it is advantageous to use surface ratio for various dielectric regions. For example the effect of near zero effective refractive index is impossible to be explained without taking into account the magnitude of the relative surfaces of the photonic elements. In this investigation the filling factor is simply the radius of photonic elements rods or holes. However, in many figures it is additionally normalized to better match the real frequencies of the photonic modes using PWE method. Filling factor is also modified for FDTD simulations when the chirality of the PhC is taken into account. There are other conventions like measure of percent area of the PhC. In the case AARH PhC there are defined two different filling factors for the two different arrays respectably. More theoretical investigations are needed to get understanding of surface filling factor play in some of the most extreme effects in reflective and refractive properties of propagating light.
Filling factor plays important role in the opening of PBGs and creation of overlapping TE and TM PBGs. In AARH PhC it controls to what degree the structure is more hole-like or more rod like. For practical reasons it is best that the filling factor is moderate. Very small one is making the structure more homogeneous and smears the differences of refractive index. Smaller photonic elements are also harder to manufacture. Similar effects exist with high filling factors where the overall size of elements should be decreased as compensation. High filling factor for holes and rods also leave tiny connected regions for the medium that are posing obstacles of their practical realization.
Chapter 4 Photonic crystals with alternate arrays of rods and holes: 2D Treatment

4.1 Optimization of 2D photonic structures

In this section there is an overview of some of the most successful attempts to reduce symmetries of various PhC constructs and achieve complete PBG. One cannot pretend to be exhaustive and there are may be many other publications outside ones attention. Mostly the overview is on investigations that were inspirational in this attempt to construct original and useful photonic structure. However this thesis argues that AARH PhC and AARH PCS structures allows for some quite unique features and enables practical manufacturing.

In the past 15 years a large number of PBG structures have been developed. Constructs that has been producing complete PBG through Finite Difference Time Domain (FDTD) and Plane Wave Expansion (PWE) simulations can be categorized according their lattice structure: simple periodic structures,\textsuperscript{69-73} quasicrystals,\textsuperscript{74,75} disordered structures,\textsuperscript{76,77} and PhC with two or more photonic patterns.\textsuperscript{78} The greatest difficulties come from the fact that all attempts have to be compromised by using unnaturally high dielectric contrast or impossible to fabricate complex photonic structures.

An example of rich PBG structures is PhCs with honeycomb lattices. Though the said lattice is promising its PBG structure is not much different from triangle lattice as the shape of its BZ. In both cases a significant modifications were needed to decrease the inherent symmetries of the unit cell in order to achieve overlapping PBG from both polarizations. One example is investigation\textsuperscript{79} of two-dimensional photonic structures consisting of rods covered with a thin dielectric film arrayed in a honeycomb lattice. Though the computer simulations exhibit complete PBGs the cladding of rods introduces new complicated feature that should be just several
nanometers thick. Similar problem occurs in another example\textsuperscript{80} where a honeycomb lattice is constructed from two sets of holes with different radiuses. Though the technology is improving with every year its small radius of holes are still too hard feature to be realized correctly. Other structures\textsuperscript{81} interpose two or more patterns in one 2D PhC and consistently achieve large complete PBG but still have problems with too extreme filling factors and therefore their practicality. In the most of classical structures rod only and hole only PhCs and PCS the dielectric constant of medium or of rods is rather large usually $\varepsilon \sim 12$. While there are many semiconductors that can play such role, the issues of low optical quality of solid semiconductors and the loss remain important. AARH PhC that is going to be presented in the next section exhibit convenient complete PBG with medium of dielectric constant of 2.5 and rods with dielectric constant of 7. The former corresponds to UV – curable SU8 resin and the latter correspond to variety of quantum dots like materials like CdSe with high optical quality.

Serious research was given on modulation of classical PhC by changing the shape of photonic atoms into triangles,\textsuperscript{82} ellipses\textsuperscript{83} and etc. The problems here stem mostly from the band shift toward higher frequencies which as a result close PBGs. Gaps were observed mainly at higher than 10\textsuperscript{th} order bands. Also, when converted into realistic PCSs, an issue with uniformity emerges. Sharp angles and high ellipticity make them difficult to manufacture. Attempts were focused on investigation of far more complicated lattices like Kagome, Pirochloric\textsuperscript{84} or disordered quasicrystals.\textsuperscript{85} Of them a lot promised was found in quasicrystals that carry some similarity with AARH PhC. They are type of structures\textsuperscript{86} which building blocks are arranged periodically but lack translational symmetry. It is proven that they exhibit diffraction patterns and unusual transmission of light. As it is mentioned later AARH PhC exhibit large unit cell with many elements in it but still is periodic in x and y translational directions. A problem with long-ranged ordered PhCs is
that the photonic atoms or elements should be far smaller than the wavelength of propagating wave. In this case it is the supercell that should be in the order of the wavelength for the crystal to exhibit the properties of PhC.

The proposed structure of AARH PhC achieve one very important result that is missing in many of the above investigations: it is the strong modulation of the PhC at even small changes of structure’s parameters. These parameters are also large in number which increases significantly the flexibility while constructing the PhC. These are: dielectric constant of rods $\varepsilon_{\text{rods}}$, dielectric constant of medium $\varepsilon_{\text{medium}}$, radius of rods $r_{\text{rods}}$, radius of holes $r_{\text{holes}}$ and the lattice constant (correspondingly the unit cell vectors). The TE and TM bands respond in different way to changes of these parameters and the existing PBG shift their frequencies with different rate.

The proposed AARH PhC structure is also very rich in both TM and TE PBGs. For 8 TE and TM bands 2D PWE method predicted at cases with 3 TE AND TM PBGs each. It allows with careful choice of parameters to achieve comparatively large complete PBG. In several sets of parameters our computations showed more than one complete PBG. The frequency position is very sensitive to variety of factors. Tuning them allow us to achieve PBG between lower frequency bands and set them in the optical region without unrealistically small features of the structure. In contrast the aforementioned complete photonic bands achieved by heavy modulation of the lattice show complete photonic bands well after 10th order.

Apart from complete PBGs the proposed structures exhibit properties that are typical for metamaterials. At wavelength close to but outside the complete PBG, the computer simulations of light propagation show negative refraction. The significance here is that metamaterials are prone to excessive loss, even at microwave ranges with losses making them completely impractical close to optical region. Purely dielectric PhC have intrinsically less losses as lower dispersion and
absorption. The metallic characteristics of metamaterials create certain difficulties for computer simulations and ambiguities at calculating refractive angles. Computer simulations with AARH PhC clearly show the surface waves that cause effects like superresolution. Related but different effect is the self-wave guiding where most of wavevectors in the PhC point in ΓX or ΓX’ direction. Negative refraction leads to possibility of creating flat lens – effect observed on variety of wavelengths. One direct consequence is that in a realistic Photonic crystal slab the evanescent waves are going to behave unusually and subwavelength resolution becomes reality. Their interaction with the left handed material’s surface leads to several other effects like Smith – Purcell, Cherenkov radiation and reverse Doppler Effect.

Another motivation is that the proposed ideal 2D structure can be manufactured as a Photonic Crystal Slab using the latest accessible technologies as photo-lithography and 3D writing. A two-step process with two different photo-masks was developed and is currently implemented in the Advance Science Research Center of City University of New York. As the two photomasks may have independent from each other features the radiusses of the back – filled rods\textsuperscript{87} and holes could differ significantly. This introduces another asymmetry in the unit cell and additional parameter that could be tuned to achieve complete PBG.

4.2 Relevance of 2D simulations of photonic crystals

Along the years many attempts were made to engineer 2D and 3D PhC with properties that include existence of overlapping TE and TM PBGs, negative refraction, superlensing and others. The greatest hurdle is that realistic PCSs mostly exhibit different characteristics than their 2D PhC analogies. In this thesis there are two versions of two arrays PhC: 2D AARH PhC and 3D AARH
PCS. In the more realistic 3D AARH PCS due to lack of confinement in vertical directions, complete PBG for all k-space is not possible. Still it is possible to open partial PBG in XM or X’M direction and even to overlap the TE and TM PBGs. There are significant differences in band diagrams for 2D PhC and 3D PCS with the same lattice structure and unit cell. Still after extensive comparison between the band diagrams of our AARH PhC and AARH PCS we believe that there is direct relation between the results. Some of these comparison are shown in Chapter 5. In order to get a quantitative picture of PCS optical properties one have to simulate it both by 3D PWE and 3D FDTD methods. Still the qualitative picture of the structure: the k-space points of degeneracy lifting or degeneracy of modes at certain direction, rate of frequency shifting with change of parameters could be provided by 2D PWE method. Mapping of various PBGs is much easier with 2D PWE which is far less recourses hungry than its 3D analogue. The complex nature of AARH PhC unit cell requires very high resolution in order to characterize correctly the structure. It also requires simulations for both ΓX and ΓX’ k-space contours with PWE method and light propagation by both physical directions with FDTD in both frequency and space domains. Besides, it is pointed out that the method allows computing the field distribution for each of eigenstates of the PhC which is extremely convenient when designing PhC-based active devices as well as investigating PhC fibers. In addition, it is attempted to clarify the mechanisms of opening overlapping TE and TM PBGs, something that is not so easy when looking at highly degenerated bands close to the light cone for 3D PWE diagram of PCS. Certainly there should be further investigations on the relations between these two types of diagrams.
### 4.3 Structure

The schematic structure of the proposed AARH PhC is shown in Figure 4.3.1(a). The hosting medium is a dielectric material with low dielectric constant such as UV-curable polymers with dielectric constant, $\varepsilon = 2.5$. The photonic atoms are two different kinds: semiconductor rods with the high dielectric constant $\varepsilon$ between 5.0 and 15 and air holes $\varepsilon = 1$. The k-space Brillouin Zone is shown on the Figure 4.3.1 (b). In the Irreducible Brillouin Zone there are two unequal contours $\Gamma X M \Gamma$ and $\Gamma X' M G$ that produce very different band diagrams.

Hope is that a method has been found of creating large number of complete PBG in 2D PhCs that could be additionally tuned in for specific frequencies and widths. The attempt is to modulate the structure of classical PhCs using their already well known physical properties. Symmetry breaking is a well-researched way to lift degeneracy of bands in certain points in k – space. Related to it is the Brillouin Zone folding of supercells that reduces the size of the irreducible BZ and often leads to new chiral optical responses as light propagates from different real space directions. Lastly an advantage was taken of the fact that rod-based PhC tend to open more TM PBGs, while hole-based PhC tend to open more TE PBGs.\textsuperscript{89} By interposing these two types of PhCs in a two arrays PhC with large and complex supercell it is achieved a manipulation of the resulting rich in PBGs structure into opening large overlapping TE and TM PBGs at suitable frequency region. Finally, dielectric properties of the materials used in the computer simulations are realistic like those of UV-curable SU8 polymer for the hosting medium and processable soluble semiconductors with high optical quality like CdSe quantum dots for the semiconducting rods.
4.4 Consequences of adding alternate arrays of rods and holes

There is no known rule for opening complete PBGs by symmetry breaking. The intricacies of symmetry breaking are clarified in Chapter 3. At low filling factor classical air - hole PhC exhibits a single TE PBG, while semiconducting rod PhC produces a large TM PBG and a smaller higher frequency TE PBG. Superimposing these two classical types of PhCs creates a complex superlattice with two alternating arrays of rods and holes. This imposes additional periodicity and significantly modifies the photonic band diagram. The TM PBGs are predominant due to the high
dielectric constant between the rods and medium. Symmetry breaking already creates some large TM PBG and at some cases small complete PBGs. The effect of interposing the hole-based structure is that the TM bands are slightly shifted upward in frequency that additionally increases the width of PBGs. The TE bands though are dramatically shifted upward with different rate for each photonic band. This lifts the degeneracy in several points of k-space and opens PBGs. It was observed that if the structure was only hole-based then all bands would have been at much higher frequency. The shift in frequency can be controlled by changing the parameters of the PhC like radiuses of photonic atoms or dielectric constant of rods. Choosing different UV-curable polymer with different dielectric constant also modifies the photonic band structure. The result is that TE bands could be positioned to overlap entirely with the second TM PBG and create large complete PBG. In many cases it is possible to open more than one complete PBGs. Additionally, the AARH PhC not only reduce various real space symmetries but introduces a new feature: the TE and TM polarizations are faced with modified effective dielectric potential $\varepsilon(G)$ and modified effective dielectric contrast $\Delta \varepsilon$. 
On Figure 4.4.1 are presented the consequences for TE and TM bands when two arrays one of rods Figure 4.4.1 (a) and one of holes Figure 4.4.1 (c) with the same unit cell are merged Figure 4.4.1 (b). Computations are along ΓXMIΓ contour. The radiuses of both photonic structures are \( r = 0.375 \) and dielectric constant of rods is \( \varepsilon = 9 \), the medium dielectric constant as everywhere is \( \varepsilon = 2.5 \). Two overlapping TE and TM PBG are opened as photonic bands are shifted upward and TE band degeneracies are lifted. The higher frequency complete PBG has a width of about 6%. The rod-only structure exhibit larger PBGs than hole-only structure as its dielectric contrast is significantly larger. The frequency of hole-only structure is also much higher than the rod-only one.
Figure 4.4.2 clarifies the mechanism of complete PBGs creations, showing the same structure but only for TE bands. The merge of the two arrays removes the degeneracy in region A. It also shifts frequencies upward opening a TE PBG that overlaps with the PBG for TM polarization. A similar phenomenon is observed for regions B1 and B2 that are also shifted in frequency and open larger complete PBG.
Figure 4.4.3 shows the change for TM bands. It is much smaller than for TE bands due to larger dielectric contrast between rods and medium compared to the dielectric contrast between holes and medium. In both (a) and (b) the structure is much more rod in air like. Still in (b) the last band is inverted at the wings as compared to part (a) which increases the width of the TM PBG. In (c) there is no PBG whatsoever which is expected for air hole only photonic structure.

4.5 Alternate arrays of rods and holes with large filling factor

As it is shown on the PBG maps the proposed AARH PhC exhibit rich band structure even with small filling factor and with low dielectric contrast. In order to exhaustively investigate its
characteristics, here is presented AARH PhC with exaggerated set of parameters that expose them clearly. The dielectric constant of rods is $\varepsilon = 12$, dielectric constant of medium is $\varepsilon = 2.5$ and the filling factor is $f = 0.45$. The last quantity is too large to be realistic in a manufacturing process as the medium connecting features between the rods and holes are too small. However, the large filling factor tend to enlarge the PBGs especially in $\Gamma X M \Gamma$ direction and make it easier to compare it with the band structure of $\Gamma X' M \Gamma$ contour.

![Figure 4.5.1: Omnidirectional three TM and two TE 2D PBGs along the whole k-space contour $\Gamma X M \Gamma X' M \Gamma$ of a high contrast, high filling factor 2D AARH PhC](image)

On the Figure 4.5.1 is shown the dispersion relation for 8 TE and TM bands along the whole Irreducible Brillouin Zone $\Gamma X M \Gamma X' M \Gamma$. The structure exhibit two large TM PBGs, one tiny TM PBG, and two relatively small TE PBGs. As the simulation is along both contours these PBGs are omnidirectional and exist independently of the direction of incident light. Along the
The contours of the bands are shaped not very differently from the classical rods in air or holes in semiconductor PhCs. The structure is more like rods in air and exhibit larger TM PBGs. The first TE and TM bands are undisturbed by the break out of symmetry and do not form PBGs. It is the third TM and TE band that is shifted upwards and opens up the first order PBG.

The dispersion relation along ΓX’MΓ is significantly different. The bands degenerate two by two in X’M segment which allows for opening up of large regions of forbidden frequencies.
Figure 4.5.2: There is significant difference in dispersion relations along (a) ΓXMΓ and (b) ΓX’MΓ
On Figure 4.5.2 are shown the dispersion relations for each k-space contour. The PBGs along $\Gamma X M \Gamma$ are nearly identical with those on Figure 4.5.1 (a). The picture is very different along $\Gamma X'M \Gamma$ shown on Figure 4.5.2 (b). The first order TE PBG is dramatically enlarged due to upward shift of the 3rd TM band. The second order TM PBG is also enlarged and both PBGs now overlap to present complete PBG for all polarizations. This effect is probably due to reduction of the length of $X'M$ contour relative to $XM$ contour. One can easily see that the shape of the bands in $\Gamma X$ and $\Gamma X'$ directions are very similar. Degenerations of bands play important role also in the dispersion relations of AARH PCS and allow for incomplete overlapping PBGs.

4.6 Resolution

Each software for computer simulations exhibit slightly different set of parameters that allow correct computation of dispersion relations for simulated PhCs. In the case of CrystalWave after setting sizes of PhC atoms dielectric constants and features still there is one more parameters that strongly influences the resulting diagrams. The resolution parameter sets the number of points where calculations are performed between any two vertices. For classic rods in air or holes in semiconductor PhC due to simplicity of the periodic structure 8 points are pretty enough. The AARH PhC supercell is anchored at four photonic atoms to create rectangular lattice. Inside it there are two different photonic atoms and two more are halved by two of its sides. There is a need of strong representation of this complicated structure and it can be achieved by increasing resolution – the points between the vertices. Unfortunately every doubling of resolution leads to squaring the time needed for calculations. With increased resolution the computer resources needed for calculations also increase exponentially. In this work several different resolutions were used depending on the volume of calculations needed.
Figure 4.6.1: Dispersion diagram along ΓXMΓ for three different resolutions

Fig 4.6.2: Dispersion diagram along ΓX’MΓ contour for three different resolutions
It is clear that at low frequencies the computer simulations are pretty accurate even with low resolution. The problems emerge at higher frequency where the low resolution simulation lowers the TE bands and exaggerates the TE PBGs. This leads to “ghost” PBGs at higher frequencies. It is unclear why the TM PBG is nearly unchanged with increasing resolution. The hypothesis presented in this investigation is that the higher dielectric constant between rods and medium increases the accuracy of simulations for TM PBGs. The much lower dielectric contrast between holes and medium shifts the frequencies of the bands higher, but simulation software smears rods and medium at lower resolution and creates air hole PhC like structure in high dielectric background. The same problem exists in simulations of AARH PCS which makes their simulations extremely recourse hungry for resolutions correctly representing dispersion relations.

4.7 Isofrequency contours and frequency surfaces

When the light propagates through an AARH PhC it scatters and reflects due to the many surfaces inside the structure. Each photonic element becomes scattering center interacting with its neighbors inside the unit cell. This leads to difficulties in description of its effective refractive index. At low frequency there are several mathematical techniques to homogenize the structure of PhCs. However, anomalous refraction, slow light, reversed Doppler Effect and many other interesting phenomena occur only in high frequency regime. Here the high frequency regime is defined as wavelength of propagating light comparable to the period of the structure.

One way to get around this problem is to consider PhC as array of interfaces where the propagating light scatter on their surfaces. Using PWE method one can calculate the isofrequency contours for each energy mode of certain PhC or PCS.
The chirality of the proposed structure is revealed from the fact that $k_x$ and $k_z$ are unequal. The 1\textsuperscript{st} mode on Figure 4.7.1 (a) is not that different from modes in homogenized space or in free space. In free space the isofrequency contours should have been concentric circles. Here they are elliptic and ellipticity is proportional to the difference of effective refractive index along the $k_x$ and $k_z$. For all frequencies the slopes of the contours are positive and curved. It means that at those modes one can expect usual transmission properties of homogeneous material with higher than one refractive index.
However, the breaking of Brillouin Zone’s symmetry influences strongly higher modes. On Figure 4.7.1 (b) one can see how the curvature of the contours are flattened along $k_z$ which usually leads to superlensing effect and negatively sloped along $k_x$ which is an evidence of negative refraction. Figure 4.7.1 (c) and (d) shows even more distorted slopes that enable for such effects like reverse Doppler Effect and infinite speed of phase of light.

Figure 4.7.2: The isofrequency contour of the first 4 modes for TM polarization: (a) 1$^{\text{st}}$ mode, (b) 2$^{\text{nd}}$ mode, (c) 3$^{\text{rd}}$ mode, (d) 4$^{\text{th}}$ mode.
The TM isofrequency contours are similar to TE for lower frequencies but rather different at higher modes. An interesting observation is that 2D simulated TM modes are close in shape and magnitude to the 3D simulated modes.

The frequency surfaces define the permitted wave vectors and are expressed as:

$$\omega(\vec{k}) = \omega_0 = \text{const.}$$ \hspace{1cm} (4.1)

Another important quantity is the group velocity that is a gradient of the frequency surface in certain point \((k_x, k_y)\):

$$\vec{v}_g = \vec{\nabla}_{\vec{k}} \omega(\vec{k})$$ \hspace{1cm} (4.2)

As a result of this correlation the group velocity points inward when the slope of the band is negative and outward when the slope of the band is positive. In free space the frequency surfaces are conical and the slopes are all positive. When the space is modulated by insertion of periodic structure this could change. The scattering around photonic atom deforms the frequency surfaces and could lead to zero valued or negative slopes. The flat slopes are related to superlensing effects while negative slopes to negative refraction. However the two effects are strongly coupled and the structure exhibiting one of these properties usually exhibit the other on same or similar frequency.

On Figure 4.7.3 and Figure 4.7.4 are shown typical TE and TM isofrequency contours and mode frequency surfaces of AARH PhC. While the firs mode is mostly regular except for the corners, the higher modes exhibit many regions of negative slopes that are evidence of complex refractive phenomena. Part of them is due to chiral nature of AARH PhC that modulates these surfaces in highly asymmetric ways.
Figure 4.7.3: Frequency mode surfaces of the first 4 TE modes: (a) 1^{st} mode, (b) 2^{nd} mode, (c) 3^{rd} mode, (d) 4^{th} mode.
Figure 4.7.4: Frequency mode surfaces of the first 4 TM modes: (a) 1\textsuperscript{st} mode, (b) 2\textsuperscript{nd} mode, (c) 3\textsuperscript{rd} mode, (d) 4\textsuperscript{th} mode.

Note, that mode frequency surface is plotted over the whole rectangular area of the Brillouin Zone not only the one of Irreducible Brillouin Zones. The isofrequency contours are projected on the bottom of the diagrams.

Though similar in many ways to the Fermi surfaces of the solid state crystals, the frequency surfaces of PhC exhibit far more complicated structure due to several differences. The anisotropy of PhC leads to modification of Snell’s law in a sense that the refractive index is now angular dependent. Hence it is not possible to expressed it as simple index ellipsoid as is the case of solid state crystals and some naturel transparent optical crystals. The modified Snell’s law now is dependent on incident angle:
\[
\sin \theta_1 / \sin \theta_2 = n(\theta_1)
\]  

This expression exemplifies the difficulties to engineer all angle PBG or photonic mirror. In a sense the PBG is an extreme case of negative refraction. As is shown on Figure 4.7.3 and Figure 4.7.4 the contours are so different from circular or elliptic shapes that some of the waves are canceling each other creating forbidden for propagation frequency zones. Hence the observation that negative refraction, superlensing and other effects are happening all at the edge or very close the PBG. It is worth mentioning that highly symmetrical points tend to attract the energy modes that lead to degeneration and closing of PBG. Also they tend to curve the frequency surfaces in positive direction making negative slopes rare. The symmetry breaking used to open wider PBG is a suitable method of engineering PhC with highly irregular refractive properties.

4.8 Plane wave expansion photonic band gap maps

Computer simulations show complete PBG at large number of parameter combinations. These parameters could be the radiuses of rods and holes photonic atoms, dielectric constants of medium and semiconducting material. One or two complete PBG are observed at many frequencies for any PhC with dielectric constant of rods \( \varepsilon > 6 \) and radiuses \( r/a > 0.125 \).
Figure 4.8.1 Map of PBGs depending on the filling factor of holes with constant filling factor of rods, (a) AARH PhC with $\varepsilon = 12$ (b) AARH PhC with $\varepsilon = 9$
Figure 4.8.2 Map of PBGs depending on the filling factor of rods with constant filling factor of holes, (a) AARH PhC with $\varepsilon = 12$ (b) AARH PhC with $\varepsilon = 9$
Figure 4.8.3 Map of PBGs depending on the filling factor of both rods and holes, (a) AARH PhC with $\varepsilon = 12$ (b) AARH PhC with $\varepsilon = 9$
The filling factor for constant radiuses is set to $r/a = 0.375$ as PBGs exhibit larger width. Such PhC slabs are easier to manufacture due to their larger features. The general characteristic of the AARH PhC is the large number of both TM and TE PBG that can be engineered to overlap. In many cases it is possible to simulate two complete PBGs at the same frequency. At the extreme case where filling factor is closing to 0.5 the PhC behaves as common hole - array in semiconductor and at filling factor of zero PhC behaves as rod - array in air. For rods what remain are the two large TM and high frequency TR PBG, for holes only the second TE PBG at high frequency.
Figure 4.8.4 Map of TE, TM and Complete PBG depending of dielectric constant of rods at constant radiuses of holes and rods (a) AARH with $r_{\text{rods}} = r_{\text{holes}} = 0.425a$ (b) AARH with $r_{\text{rods}} = r_{\text{holes}} = 0.375a$. 

[Graphs showing frequency and dielectric constant for both cases.]
Figure 4.8.4 shows the relation between dielectric constant of semiconducting rods and existence of PBG. One unexpected result is that the TE and TM PBG increase in width as shown in others authors computer simulations, the widest Complete PBG is achieved at $\varepsilon_{\text{rods}} = 6 – 8$. The results were confirmed by similar computer simulations using 3D FDTD and 3D PWE computation methods for PhC slabs with similar parameters. These results show the usefulness of 2D computer simulations that could predict the existence and relative frequency of PBG in PhC slabs even if the gaps there are incomplete due to lack of vertical confinement of light. Another feature of the AARH PhC is the large number of TM and TE PBGs as we observed as many as 6 of them for 8 TM and 8 TE bands. The great flexibility in choosing the dielectric constant of rods allows in experimental settings the implementation of high optical quality index-of-refraction materials such as a solution processable polycrystalline semiconductor compounds.

Figure 4.8.5 PBG for a 2D PhC with $\varepsilon_{\text{rods}}=7$, $\varepsilon_{\text{holes}}=\varepsilon_{\text{rods}}=0.375$ (a) computed by PWE method (b) computed by FTDT method.
On Figure 4.8.1 is shown comparison of results from computer simulation using PWE and FDTD methods for 2D PhC with the same parameters. The PWE exhibit idealized Complete PBG and several TE and TM PBGs. The 2D FDTD method generally confirms the existence of these gaps with some noise. The net flux is the initial flux of plane wave light from a source passing through a sensor in front of the PhC minus the negative flux reflected by the PhC passing through the same sensor. When the net flux is close to zero it means that the PhC is acting as a mirror and the light cannot enter it. The net flux usually is not zero as some of it is absorbed by the medium and/or the first row of rods. Some light is also deflected by surface modes that are more relevant for PhC slabs computations. The data for the frequency region below 0.9 µm and above 2.5 µm is considered unreliable for this FDTD simulation.

4.9 Negative Refraction and Zero refraction index

Theoretically, negative refraction had been proposed for long time. Recently, two types of materials realized such effect: Metallic structures called metamaterials and PhCs. Metamaterials are isotropic structures where the group velocity vector is antiparallel to the wave vector which leads to left handedness of their refractive properties. One of the advantages of Metamaterials is that negative refraction can be realized in the first energy band. A disadvantage is that loss due to its metallic character is very high. In the case of PhCs there are two mechanisms of achieving negative refraction. One is engineering a dielectric structure for which the second but usually higher energy band has a negative phase refractive index. The second mechanism is to design a PhC that is highly anisotropic and though its phase refractive index is positive, its group refractive index is negative. The latter are deemed more promising as they allow greater flexibility and diversity of design.
PhCs allow for much less loss than metamaterials. In many cases there exist wide frequency regions where transmission may reach 90%. On other hand PhC exhibit PBGs in frequency not far from those for maximum transmission. Hence the ability to design complex photonic structures suitable for many applications. Another advantage is that negative refraction can be significantly enhanced by modifying the front and back of the PhC. Though there are still difficulties in obtaining negative refraction effect for the lowest energy band, there were investigations showing that this is not impossible. Achieving this effect for the lowest band gives the advantages of high transmission and single beam propagation.

The proposed AARH PhC is highly anisotropic and exhibit many unusual reflective and refractive properties. Its chirality allows to achieve atypical propagation properties of the light depending on which side is the incident beam. Also, small changes of frequency of the incident light lead to completely different sets of reflected and refracted beams. The loss can be controlled by changing the width of the PhC, its front and back surface and the angle of the incident light.

On Figure 4.10.1 is shown a TE incident beam that after coming in contact with the AARH PhC splits into a reflective beam (i), positively (ii) and negatively (iii) refracted beams. The overall propagation of light inside the PhC is too complex to be trivially described but the three beams are very well spatially defined. There is even another low intensity beam that is probably back reflection from the original negative refraction inside the AARH PhC.
Figure 4.9.1: Plane monochromic wave is incident under an angle on AARH PhC: i) reflected component, ii) positively refracted component, iii) negatively refracted component of initial light, Dielectric constant of rods is $\varepsilon = 8.624 \quad f=0.2308$.

Figure 4.9.2: (a) Non-Snell’s Law propagation of (i) reflected, (ii) refracted light at $\varepsilon=11$ (b) Non-Snell’s Law angle of reflected light at $\varepsilon=9.36$ (c) Non-Snell’s Law propagation of (i) refracted , (ii) positively refracted, (iii) negatively refracted light at $\varepsilon=8$ (d) reflected light 180°shifted from Snell’s Law angle $\varepsilon=7.67$. The plane monochromatic wave is incident under an angle on AARH PhCs with different dielectric constant.
The four pictures on Figure 4.9.2 and differ only with the dielectric constant of rods. The frequency is the same as on Figure 4.9.1. The method is 2D FDTD. On Figure 4.10.2 (a) the light is divided into reflected electromagnetic wave and wave that activates surface modes. The surface modes are featured strongly in AARH PCS and will be explained in Chapter 5. The dielectric constant of rods is $\varepsilon = 11$, the filling factor is $f = 0.25a$. On Figure 4.9.2 (b) the light is mainly reflected from the crystal but the angle is not according Snell Law. Part of it is refracted through the AARH PhC. The structure therefore is more like PCS but features like thickness and cladding are exaggerated to create structure similar to 2D PhC. The dielectric constant is lowered to $\varepsilon = 9.36$. Lowering the dielectric constant further to $\varepsilon = 8$ destroys the PBG and the light propagates through the crystal shown on Figure 4.9.2 (d) and divides into (i) reflected, (ii) positively refracted and (iii) negatively refracted beam. On Figure 4.9.2 (c) at $\varepsilon = 7.67$ there is another PBG that reflects the light nearly 95% but reflection is 180° from what is expected according the Snell Law. All monochromatic plain waves are with TE polarization but waves with TM polarization exhibit similar properties but at different frequencies. The demonstrated effects are mostly close to the edge of PBG for given polarization. All attempts to find some general rule of predicting at what set of parameters and at what frequency they occur were unsuccessful.

On Figure 4.9.3 is a special case of unusual refraction obtained with 3D FDTD simulation method in space domain. The AARH PCS is the one with high filling factor and high dielectric constant. At the frequency region of the simulation there are no PBGs, though at lower frequency there is a region with high transmission and at higher frequencies region with high reflectivity. The angle of incident light is zero in both Figure 4.9.3 (a) and Figure 4.9.3 (b) simulations. According the Snell’s law the light should propagate straight through the AARH PCS as different surfaces reflect light symmetrically and do not redirect it. However in these simulations light is
redirected in case Figure 4.9.3 (a) to the right at normalized frequency of 0.172 and in the case Figure 4.9.3 (b) to the left at normalized frequency of 0.173. We hypothesize that the observed effect is one of zero refractive index. Generally it means that the phase velocity of light would be infinity. The reasoning is that the refractive index is a continuous function of frequency of propagating light. Hence there are should be a frequency where the effective refractive index should be zero. Our numerous simulations show that there are several beams refracted positively and negatively at the same time for one frequency. The angle of propagation depends on frequency but not on the angle of incident light that remains zero. We found specific non-linear function that controls the angles of propagation in a whole frequency region where the refractive index is vanishing.

Similar results but not as prominent were observed in other frequency regions in the vicinity of frequency where at X’ there is triple or even quadratic degeneracy of modes. They may be similar to Dirac–like dispersion cones that may produce similar results in metamaterials.
Figure 4.9.3: Example of very unusual refraction. (a) Monochromic plane wave at normalized frequency 0.233 (i) refracted wave, (ii) transmitted wave (b) Monochromic plane wave at normalized frequency 0.231 (i) refracted wave, (ii) transmitted wave

Zero refractive index may have numerous applications especially with low loss PhCs. They could include optical switches, design of various wave fronts, lenses etc. We intend to continue
work on this effect and widen it to include PCSs. Unfortunately the frequency region where this particular effect occur is very small. Prediction of this effect from dispersion diagrams is also difficult. PCSs demand far larger computational resources and time for simulations. Results for zero refractive index in AARH PCS are presented in the section related to thickness of photonic slabs as that parameter proved to be critical for many 3D properties of the photonic structure.

4.10 Superlensing

Conventional lenses based on positive index materials are constrained in their efficiency by Abbe’s diffraction limit. These materials with curved surfaces cannot resolve details that are smaller than half wavelength of the light. The observed diffraction limit is a consequence the fact that the waves carrying information about the sub wavelength details of given object decay exponentially in free space. It had been proposed that overcoming this problem should include periodic mediums with negative refractive index. In such medium the evanescent waves can grow exponentially and compensate for the decay. The result should be that all Fourier components of the given object could be recovered in the image that would have a resolution bellow the diffraction limit.

Supercolimation effect arises from the dispersion properties of PhC. The important quantity of the propagating electromagnetic energy is the group velocity. For a two dimensional plane wave with wave vector $\mathbf{k}$ the group velocity is defined by:

$$
\hat{v}_g = \frac{\partial w}{\partial k_x} \hat{x} + \frac{\partial w}{\partial k_y} \hat{y}
$$

(4.4)
Being a gradient, the group velocity is pointing at the direction of fastest increase. It is also perpendicular to the dispersion relation contour in k–space. In free space the isofrequency contours are infinite numbers of concentric rings around central point usually marked as Γ. The group velocity is represented by the simple expression \( \vec{v} = c \vec{k} \).

When the light propagates through a PhC the shapes of the contours are significantly modified.\(^91\,92\) Supercolimation is a product of deformation of the first band dispersion contour which arc is flattened. The meaning of this is that all plane waves will have the same group velocity in the flat section of the dispersion contour. Consequently the direction of energy propagation will not be the same as the phase. PhCs can be specifically engineered to exhibit supercolimating characteristics. The majority of the propagating energy is concentrated in the areas with higher dielectric index for both kinds of classical PhCs: rod-based and hole-based. Still there some specific differences between the two types of PhCs.

Supercolimation effect is observed usually at high frequencies where the band structure is strongly deformed. It is situated close to the PBG in frequency domain and is joined to other non-linear effects like negative refraction and birefringence.\(^93\) It is especially sensitive to properties like the angle of the incident light and frequency. The best simulation results can be achieved by using a spherical source of light.

There are several ways to achieve superlensing. The use of metamaterials takes advantage of their left hand behavior. The left handiness a PhC means that one can assume negative refractive index. This is the case when the three vectors \( \vec{k}, \vec{E} \) and \( \vec{H} \) form left hand set of vectors \((\vec{S}.\vec{k} < 0)\) where \( \vec{S} \) is the pointing vector. If a photonic structure has an index of refraction \( n=-1 \) then after propagating through it the light restores not only its phases but also the amplitudes of evanescence.
waves. The latter are responsible for the tiniest subwavelength details of the source. Therefore it opens the possibility of enabling subwavelength imaging. These possibilities were realized by the use of silver metamaterial slab.\textsuperscript{94,95} The greatest impediment is the high energy loss in the PhC\textsuperscript{96,97} due to the use of metallic metamaterials. Another drawback was the metamaterial superlens can operate at only single frequency due to transverse magnetic wave requirement. After electric and magnetic waves are decoupled the limitation for superlensing is that $\mu=-\mu_{\text{medium}}$ where $\mu_{\text{medium}}$ is the magnetic permeability of the medium interacting with lens.

Sometimes in complex photonic structures the isotropic dielectric index cannot be defined. Still several investigations\textsuperscript{98} were able to achieve negative refraction and superlensing without metamaterials. Thorough research of superlensing in PhC showed that at each dielectric layer the refraction follows simple ray optic physical lows. Therefore it is possible to engineer PhC with more than two interfaces and using the Snell’s law of refraction to achieve effective refractive index $n_{\text{eff}} = -1$ from common right handed dielectric materials.\textsuperscript{99} Another very important advantage of using dielectric is that the negative refraction is achieved in the lowest frequency band which means better focusing and transmitting.

Some investigations\textsuperscript{100} have shown that air-hole PCS possess good left handed behavior for TM modes, and a rod type PCS prefers TE modes. The two arrays in AARH ensure that superlensing effect may be exhibited for light of both polarizations. Similarly, as with the engineering of complete PBG the relation between superlensing and the height of the AARH is not trivial. The dielectric constants of $\varepsilon_{\text{rod}} = 6$ and $\varepsilon_{\text{rod}} = 12$ seems to also maximize these left handed properties.
The two arrays of rods and holes in AARH PhC exhibit many surfaces inside the PhC that have different effective dielectric constant and refract the incident light in complicated way. The superlensing is observed for both chiral directions but is much more visible along ΓX’MGΓ direction. The filling factor used is $r=0.25a$ for both rods and holes. The computing method is 3D FDTD. The slab has a height of 2a is confined by two cladding layers also with height of 2a. Dielectric constant of rods is $\varepsilon_{\text{rods}}=8$, and of polymer medium $\varepsilon_{\text{medium}}=2.5 \ f=0.231$. The perfectly matched layer boundary condition was used. The simulation source is spherical and is at different distance to the PhC. The effect is of flat lens and superlensing.

Figure 4.10.1: All angle Superlensing with flat PhC lens for different distances to the PhC. (a) 20a, (b) 5a, (c) 2.5a. The source is from the left, the image to the right. The propagating quantity is the light intensity.

The width of the AARH PCS is very important for the quality of the image. The partial reflective waves can easily destroy the image. The image is dipole like and on Figure 4.10.1 (a) is inside the AARH PCS, in (b) is partially outside, and in (c) entirely outside the slab. The inside of the slab presents a complicated superposition of standing waves, partially reflected, partially refracted and evanescent waves. Still the refracted waves out of the AARH PCS are near perfectly cylindrical waves matching the waves produced by the source from the left side of the slab. The loss is significant and in this case is about 35%.
On Figure 4.10.2 is presented the effect of spherical lenses. They produce a sharp image inside the AARH PhC and then are reflected backwards with very small amount of loss. The termination of the AASP is the most important characteristic. In the inner side of the lenses some of the rods and holes on the surface are with reduced radiuses. Several combinations of rods and holes with different radiuses were attempted leading to large difference in the sharpness, coherence and size of the image.

Figure 4.10.2: AARH is acting as spherical mirror. The image is magnified close to the focal point of the mirror. The frequency is in the range of the PBG and the loss of the light entering the AARH PCS is less than 10%.

The present PhC lens with negative refraction has several advantages when compared to the one with positive refraction. Lenses with reduced geometric aberrations produce sharper image with enhanced resolution and find numerous applications. Larger radius of curvature gives the
advantage of reduced aberration in the image formed. A PhC lens having the same focal length as that of a conventional lens weighs far less, and is attractive to space applications. The tailor made refractive index achievable in PhCs\textsuperscript{101} allows further control on the focal length and thereby helps to reduce the size of the optical systems.

The PhC flat lens slab also supports surface waves\textsuperscript{102} (if surface terminations are properly designed), which can enhance evanescent fields, thus leading to reconstruction of subwavelength details of an object at the image plane. From an effective medium approximation of the PhC,\textsuperscript{103} different surface terminations can be shown to lead to different excitations of surface modes.

![Figure 4.10.3: The mechanism of dipole focusing. Inside the AARH PhC the light refract both positively and negatively. Not on scale.](image)

There are three hypotheses related to the formation of double focus:

Hypothesis 1: Light is exhibiting both positive and negative refraction. The medium that divides the positively and negatively refracted waves is not the bulk of crystal but its surface. The most important fact here is how the surface is terminated. The boundary is splitting the wave and
then refocuses it at the other side. AARH PhC can be terminated by variety of ways and then it
can be finished differently at its other side. Computer simulations though did not show
significantly different optical response to termination. While the optical paths on Figure 4.10.3 are
clearly existing in the AARH PhC they very well could be explained in different ways.

Figure 4.10.4: Simulation of double focus for circular source of light.

Hypothesis 2: This is a reverted dipole image of the circular source. Circular sources in
software CrystalWave are in fact dipoles interposed toward observer in a way that it see only the
intensity without polarization. In several simulations it was observed change of the polarization of
the incident wave if it was falling from circular source. It is possible that double focusing is an
unknown effect or simply artifact of a known one related to dipole nature of simulated source.
Hypothesis 3: As it can be seen on Figure 4.7.3 and Figure 4.7.4 the AARH PhC exhibit many negatively sloped regions. It can be said that for the second order mode band more regions are focusing the propagated light that dispersing it as it is expected for positive slopes. More importantly, the modes are degenerating two by two. This creates a curious situation when part of the beam is showing negative refraction and part of it positive as it was shown in the section for Negative refraction. One can ask what will happen if both degenerating modes exhibit negative refraction? The possible answer is that on certain frequency there will be negative refraction in two different regimes. Such is the possible explanation to double focusing by AARH PhC: the two focuses are related to different modes showing negative refraction on one and the same frequency.

4.11 Optical Switches

Semiconductors exhibit high dielectric constant and can be used as materials for PhCs. Materials like GaAs have static dielectric constant around $\varepsilon = 12$ and can be considered in computational simulations. One of their important feature is the strong absorption nonlinearity. While in the linear absorption the light is absorbed within one optical frequency, nonlinear absorption is spread along several frequency ranges and allows for certain level of control. The effect of nonlinearity originates from the two photon absorption of free p or n carriers in semiconductors. Therefore, the optical properties of a PhC with semiconducting elements can be significantly altered with injection of such carriers by a controlling pulse beam perpendicular to the PhC. As a result a propagating wave beam with frequency right at the edge of a PhC PBG can be transitioned through the crystal or met with PBG by small change of dielectric constant of semiconducting elements in the PhC.
The Kerr effect in high dielectric constant materials is rather small with only 0.1% change of dielectric constant. In order to be able to control the optical properties of the PhC, it should exhibit inherently steep PBG edge with abrupt jumps of reflective and refractive properties. There are several propositions for devices that can perform optical switches based on these properties.\textsuperscript{105,106} Simulations of such devices revealed two main problems: not enough third order nonlinear optical susceptibility for popular semiconductors and not fast enough nonlinear response time for PhCs.\textsuperscript{107} The first problem is related to material science and is outside the scope of this investigation. The second problem may be ameliorated by the proposed AARH PhC as it is showing rich PBG structure with huge difference in its optical properties even for close frequencies.

If light is shined perpendicularly on AARH PhC from above there are possible two kind of optical responses. It is possible that the dielectric rods change their dielectric constant or/and low dielectric index medium change its dielectric constant. In the simulations the medium dielectric constant is chosen to be $\varepsilon = 2.5$ to match the properties of the popular organic UV curable polymer SU-8. One can judge that changes in the dielectric constant of medium are not sufficiently fast to be used in optical switching devices. There are several ways to improve these properties. For example some polystyrene like polymers exhibit ultrafast nonlinear response time. Certain Ag-doped polymers with dielectric constant close to SU-8 compound also possess strong third order nonlinearity. Unfortunately these materials are still hard to simulate with CrystalWave computational software. Therefore investigations were focused on the optical response of dielectric rod in AARH PhC. Here there are two possibilities to explore. The high dielectric elements as $\varepsilon = 12$ are possibly semiconductors. They provide high dielectric contrast inside the AARH PhC and ensure existence of several PBG including complete PBGs. A serious
disadvantage is their poor optical quality that impedes many practical applications. Fortunately, the AARH PhC also exhibit PBGs and diverse transmission properties for relatively low dielectric materials $\varepsilon = 6 \sim 10$. For practical applications such materials could be high optical qualities quantum dots some of which also exhibit strong third order nonlinearity.

\[ \frac{\Phi_{\text{transmitted}}}{\Phi_{\text{incident}}} \times 100 \]

Figure 4.11.1: Percent of refracted light relative to change of dielectric contrast of rods.

The proposed AARH PhC shows abrupt change of its reflective and refractive properties with small change of the refractive index of the rod atoms. The results on Figure 4.11.1 showed a
4% change of refraction at normalized frequency of 0.162 for 0.1% change of dielectric constant of rods atoms for certain combination of parameters. The larger scale simulations showed in the inset suggest rich structure with many abrupt maximums and minimums for refraction, reflection and absorption of light. If the change of dielectric constant is due only to changes of absorption, it is possible to find some optima; set of parameters for greatest effect. One easily enhanced parameter is the filling factor as larger filling factor enhances the absorption in parallel with increasing the surface area of rods elements.

Figure 4.11.2: (a) Transmission properties of two AARH PCS with $\varepsilon = 9.95$ and $\varepsilon = 10$. The change is $\Delta \varepsilon = 0.05$. The difference of transmission coefficients come from the fact that the modulation is maximized on the slope of the falling transmission quality. (b) Modulation of light in the vicinity of PBG.

On Figure 4.11.2 (a) is shown the overall change of transmission properties of light in the vicinity of PBG. The structure is the same as in Figure 4.11.1. The effect of increasing the dielectric index of rods is moving the maxima and minima of reflection to lower frequency. On Figure 4.11.2 (b) is shown the strong modulation of light for even smaller change of dielectric contrast. Unfortunately the modulation is strongest on the slopes of the transmission curves and about half
of the flux is lost. Still the effect is in the range of the expected Kerr Effect as the refractive and reflective modulations with $\Delta \varepsilon/\varepsilon=0.001$. Modulation is nearly 100%.

Figure 4.11.3: Shows that the proposed AARH [$\varepsilon_\text{r} = 8$, $r_\text{h} = r_\text{r} = 0.25 \, a$] can be used for the applications related to optical communication and computation. (a) No transmitted TE light at the normalized frequency of 0.2315 is detected from the light source (golden thin line above the PhC). (b) The majority (90%) light flux is transmitted to the other side of the PhC in which the relative dielectric index of the rods is changed by $\Delta \varepsilon/\varepsilon = 10^{-3}$.

Figure 4.11.3 shows FDTD simulations in space domain of AARH. At (a) the light is repulsed by the PBG at the given frequency. After small modulation of the dielectric constant the light is propagating freely through the PhC. Modulation is on the scale of the best results that could be found in literature.
Chapter 5 Photonic Crystals with Alternate Arrays of Rods and Holes: 3DTreatment

5.1 Photonic crystal slabs

The most interesting and complex PhCs are periodic structures in 3 dimensions. With them one can control the flow of light in all possible directions. Unfortunately 3D PhCs require high dielectric contrast as well as very accurate stacking of photonic elements. Even small defects in the structure destroy the PBGs. Even now the 3D PhCs are hard to manufacture especially in the infrared and optical regime.

An alternative to 3D PhCs is the PCS where the light is controlled in 2 dimensions by a periodic structure and in vertical direction by variety of claddings and low or high dielectric material sandwich-like structures. Confinement of light in 3rd direction is far from perfect and usually lead to enormous losses. This fact creates serious restriction on applicability of PCSs.

Discovery of complete PBG and left hand behavior in two dimensional crystals raised high hopes for manufacturing photonic structures and optical computing. However it was found that the properties of real PhC are rather different than their 2D approximations. On one hand 3D PhC exhibit far more complicated behavior and on other hand they were extremely hard to manufacture just couple of years ago.

The alternative is to design structures that are periodical only in two dimensions and finite in the third. Such structures could be reasonably easy produced using techniques such as NanoLithography, PhotoLithography and 2-photon absorption laser writing. They retain within limits many of the unique features of 2D crystals and could be realized even on nano-scale.

Photonic crystal slab (PCS) structures with various designs of unit cells are strong candidates for the building blocks of optical integrated circuits on a nano-scale. These PhC
structures can be fabricated using many effective techniques such as UV –photo lithography or nano-imprinting. One of main obstacles for the PCS related applications such as optical computing is that it usually exhibits a PBG only in a given polarization. Based on two-dimensional simulations, there are several PCS structures that exhibit overlapping PBGs for transverse magnetic and transverse electric plane-waves. However, the calculated results based the 2D model may not be adequate for realistic three-dimensional PCS. The inclusion of cladding layers on the top and bottom of PCS with finite thickness creates continuum “radiative” states, and therefore partially destroys PBGs for a 3D structure.

Like in 2D PhC there are two types of modes that are independent of each other and represent different polarizations. Their characteristics are so close to the characteristics of TE and TM modes in the 2D case that here this nomenclature is preserved. The bands that are odd in respect to reflections through slab surface are defined as TM and those that are even are classified as TE.

There are two basic topologies for PCS structures: cylindrical rods with high dielectric constant in the air and air holes in high dielectric medium. They were shown on Figure 3.1.1 in Chapter 2. Like 2D PhC a network of rods in air tends to produce TM-like PBGs, while a system of holes in high dielectric medium tends to generate TE-like PBGs. Hence, several works attempted to design nonconventional slab structures for obtaining the overlapped TM- and TE-like PBGs. One of difficulties is the degenerate tendency of the photonic bands for the case of TM-like modes in the hole-based PCS. Similarly, to achieve non trivial light propagation, one need to introduce some disorder and reduced symmetry in the structure. On Figure 4.3.1 is shown the AARH PCS which is finite in z direction.
5.2 Mode Structure

As in the two dimensional crystals the rod structures create TM PBG while air – holes tend to create TE PBG. The dispersion diagram exhibit conical structure in 3D and its 2D dimension is trapezoid. The region outside the boundary modes on the left and right of the band diagram is called Light Cone and represent the continuum of states. These states are also known as radiation modes and are extended outside of the PCS up to infinity. They still play important role in constraining and interacting with the guided modes which correspond to states localized to the plane of the slab. Result of this interaction could be surface modes and further confinement of light. The guided modes are extended infinitely in the periodic plane of the PCS. Once they reach the light cone they leave the plane and exponentially decay. The light is propagating mostly along higher dielectric index of the periodic PCS and is confined not unlike the total internal reflection on the boundary surface with the air outside PCS.

It is important to mention that an incomplete PBG in the case of PCS are frequency regions where the guided modes are forbidden. Along the borders of light cone there are radiative modes that are source of large losses as the light propagates through the PCS. Another consequence is that standing wave modes are impossible and resonance cavities will decay after some time. In the bandgap the light cannot pass through the PCS and radiates away in several ways. Firstly the light can reflect from the surface of the PCS acting like a mirror. This is the classical way to observe PBG as the simulated sensor will measure the incident intensity and then subtract from it the reflected one. Below are presented the expressions for net flux and the flux lost due to lack of confinement. Some more loss incur because the inherent absorption of dielectric material inside the PCS.
\[ \Phi_{\text{net}} = \Phi_{\text{incident}} - \Phi_{\text{reflected}} \]  
\[ \Phi_{\text{loss}} = \Phi_{\text{incident}} - \Phi_{\text{reflected}} - \Phi_{\text{refracted}} = \Phi_{\text{net}} - \Phi_{\text{refracted}} \]  

Secondly the light can propagate along the surface of the PCS and radiate away with the physical termination of the structure. Modes that propagate along the surface are called surface modes and can be detected only when a single monochromatic plane wave is simulated for given frequency. The third way of light propagation is along the vertical direction with some light reflected from cladding layer and passing back into PCS. The incomplete PBG therefore means that at least 10% or more of the light still enters the PCS. Simulations showed that although surface termination modulate some of the propagating light, its relation is more of the nature of incurring more losses if termination is jagged.

### 5.3 Photonic band gap optimization

The photonic bang gaps in PCS are very different from their 2D PhC counterpart. By definition they are regions in k – space where no guided modes exist. Radiation modes always exist and lead to incomplete confinement of light. On the 3D FDTD simulations this effect corresponds to less than 100% reflection of light in the PBG and high losses of light that propagates in the PCS outside of PBG. There are several ways to ameliorate these losses as they are very sensitive to the type of periodicity and the refractive index of the materials in the PCS. Putting additional dielectric layers over and under the PCS could also help controlling the losses and scattering of light. Still, the PCS could be used in most of photonic applications like waveguides, optical switches, flat lens, resonators and mirrors. Also, with careful modification of the photonic lattice it is still possible to create incomplete none – omnidirectional (in a sense of k – space) but
somehow omnidirectional in normal space PBG for both polarizations TE and TM. PBG was successfully used to create efficient LED as the light was allowed to radiate only outside of the PCS.\textsuperscript{111}

The width of the PBG is strongly dependent on the thickness of the PCS. If it is too thin very small amount of light propagates through the periodic plane of the slab and the PBG are too small. If it is too thick then the higher order modes are too close to the lowest one and prevent any gap of opening. However, even if PBGs along ΓX, MΓ and ΓX’ are always destroyed, it is possible to find not only PBG in direction of XM or X’M but also overlapping TE and TM PBGs. In his thesis Johnson has shown that there is a rule that can predict the optimal thickness of PCSs. Here there will be a brief explanation of this method and then will compare it with the results for AARH PCS.

The first postulate is that the optimal thickness for PBG should be the on the order of half the two dimensional gap bottom wavelength of its 2D representation. PhCs are themselves defined as dielectric structures on the scale of the wavelength of the propagating through them light. The justification is that if thickness is higher than the wavelength or smaller than half of it then the structure would not be classified correctly as PCS. Then, an effective dielectric constant is defined for PCS. The frequency of bottom gap mode can be evaluated using the calculation from Chapter 2 for 2D PhC. The resulting frequency is:

\[ \omega^2 = \omega_0^2 + \frac{c^2 \left\langle k^2 \right\rangle}{\varepsilon_{\text{eff}}} \]  

(5.3)

Here \( \omega_0 \) is the two dimensional frequency. The quantity \( \varepsilon_{\text{eff}} \) differ in case of TM and TE polarization. This means that the thickness should be different in case of rods in air and holes in semiconductor PCS. In the case of TE, the dielectric constant is weighted by the electric field. As
it is concentrated in higher dielectric for its lower bands the effective dielectric constant will tend to be close to the higher one. Conversely, in case of TM the effective dielectric constant will be closer to the lower one where the majority of magnetic field energy is. All this is assuming classic PCS with only two material with high and low dielectric constants. The final result is given by the expression:

\[ h_{slab} \sim \frac{1}{2\omega_{bottom-of-the-gap}\sqrt{\varepsilon_{eff}}} \]  \hspace{1cm} (5.4)

Assuming PCS width high dielectric constant of 12 and low one of 1 the result predicts 1.6\(a\) for rods in air PCS as opposed to PWE simulation result of 2.6\(a\) and 0.6\(a\) as opposed to 0.7\(a\) for holes in semiconductor PCS.

These results are posing significant difficulty for predicting the optimal width of AARH PCS as the optimal widths for the two arrays are very different.

**5.4 Dispersion diagram and its resolution**

The proposed photonic slab is the 3D version of the 2D AARH PhC. Its structure is a two interposing arrays of holes and high dielectric rods in a low dielectric medium. The most important question is if there is some kind of similarity in dispersion diagrams of AARH PhC and AARH PCS. In a first sight they are very different, but at closer look the picture becomes much more interesting.

In this investigation are presented two types AARH PCS. The first one is realistic structure with relatively low dielectric constant of rods and moderate filling factor. It is shown how one can tweak the properties of the AARH PCS to achieve overlapping TE and TM PBG. The simulations
are mostly using 3D FDTD method that is very resource hungry. It will be shown that overlapping TE and TM gaps exist and are rather large.

The second type of AARH PCS like its 2D analogue is with large filling factor and high dielectric constant of rods. This exaggerated structure is very suitable to investigate the finer points of AARH PCS properties. It will be shown the unambiguous analogy between the 2 and 3 dimensional versions of this structure. Also it will describe how the dielectric constant, width of the slab, cladding and other properties change the characteristics of light propagation through the slab and how one can take advantages of it.

![Dispersion diagram for high dielectric AARH PCS along all k-space contour ΓXMX’MΓ. The light cone prevents any complete PBG.](image)

Figure 5.4.1: Dispersion diagram for high dielectric AARH PCS along all k-space contour ΓXMX’MΓ. The light cone prevents any complete PBG.
On Figure 5.4.1 is presented the dispersion diagram of high filling factor AARH PCS. One can see the great difference between behavior of photonic bands in \( \Gamma X M \Gamma \) and \( \Gamma X' M \Gamma \) contour. In the first case the modes are distinct from each other and crisscross the XM segment, destroying any partial PBG. Along the second contour the bands are two by two degenerated which allows for large regions along \( X'M \) segment without bands. These regions form the incomplete TE like and TM like PBGs that overlap at certain sets of AARH PCS’s properties.

Fundamentally, the lowest two modes - first TE and first TM are entirely confined in the AARH PCS. At lower frequency and in \( \Gamma X/X' M \Gamma \) they are so mixed up that one can talk about polarizations only as reference. The two modes are separated just in the \( X/X'M \) direction only due to different dielectric contrast between the rods and medium on one hand and holes and medium on another. No state is allowed in the light cone for this modes due to total internal reflection into the cladding. Therefore if it was not for the internal scattering from the dielectric material these two modes would have been lossless. These modes are referred as guided modes.

These characteristics could change dramatically if the internal asymmetry of the AARH PCS is somehow increased. If one introduce AARH PCS with different radius of rods and holes it is possible to observe no guided modes at all. The relation here is very complicated and non-trivial. It is also different along the two contours \( X/X' \). Above the lowest modes are the leaking modes that can exist outside the slab but are exponentially decaying. Their existence is depending on the cladding material, effective dielectric contrast of the AARH PCS and thickness of the slab. In \( X' \) direction these modes degenerate two by two and open large frequency domains in \( X'M \) directions. The AARH PCS with high dielectric rods and large filling factor exhibit many higher modes that create many PBGs at higher frequency. Unfortunately this structure is very leaky and the more realistic lower dielectric constant AARH PCS is introduced carrying its own problems.
The simulations are done by 3D PWE method and resolution issue is even more important than in 2D variant. Here one needs to characterize correctly not only the physical layer of PCS but also the cladding and eventually a substrate on which the PCS lay and also an air layer from above the device. There are several techniques used in these simulations that should give as realistic as possible characteristics of the proposed structure. Calculations can be performed along the k-space contours of Irreducible Brillouin Zone or along every point of Brillouin Zone. In the first case like in 2D investigation the results are frequency bands and in the second the results are isofrequency contours and mode surfaces.

Figure 5.4.2: Simulations of AARH PCS with low (a), middle (b) and high (c) resolution.
The analyzes of Figure 5.4.2 follow to some degree the discussion at 2D AARH PhC. Lower resolution exaggerates the frequencies and PBGs. High resolution shows that the TE and TM modes are not significantly different in frequency. This is in agreement with fact that those modes are in reality mixture of Electric and Magnetic fields and closely situated in the same structure. Even at low resolutions the lowest two TE and TM modes are relatively well characterized. There will be more discussions on the nature of these lowest modes later in this chapter. It is worth mentioning that calculations of even higher resolution repeat the trend but differences are insignificant and mainly related to some discrepancies when comparing results of 3D PWE and 3D FDTD model. The high dielectric constant of rods and the large filling factor additionally increase the resource requirements beyond reasonable for simulations with higher resolution.

The main difference from 2D behavior is that at higher resolution both TE and TM modes are lowered in frequency. In 2D variation high resolution shifted TE modes upward leaving TM constant.

5.5 Isofrequency Contours and Frequency Surfaces

As it was before the modes of PCSs are mixed up but generally could be described as TE and TM modes. However it is not possible to do this if one simulate the frequency surfaces in k-space. Calculation is along the whole surface of the Brillouin Zone and surfaces are numbered without specifying if they are odd or even with TE or TM likeness. The reason is in the continuity of the measurement where at each point can be assigned all of electromagnetic vectors even if some of them are with zero strength. The analyses of these surfaces shown on Figure 5.5.1 and Figure 5.5.2
reveals that there are many frequency regions with flat contours describing possible superlensing characteristics and negatively sloped contours showing potential for negative refraction. One can easily see the degeneration of the first modes and then the double minima of higher modes that actually are opening a frequency gap of potential PBG.

Figure 5.5.1: The four lowest isofrequency curves and 3D frequency surfaces of the mixed TE and TM modes of AARH PCS.
One can see that asymmetry of the Brillouin Zone leads to dramatically asymmetric isofrequency contours and mode frequency surfaces. On $k_z$ component of reciprocal vector the corresponding to $\Gamma X'$ section the frequency for the higher modes have a steep minima exactly where the lower mode has a steep maxima which leads to degeneration of the modes seen on the dispersion diagram. On the $k_x$ component of reciprocal vector minima and maxima are not as steep and do not match numerically. This direction corresponds to $\Gamma X$ segment and shows no degeneration of modes. They cross each other and destroy any possible uncomplete PBG.
5.6 Cladding and thickness in alternate arrays photonic crystal slabs

The fabrication of PCS with more complicated lattice is rather hard if the background of the slab is air. Instead mediums like As$_2$S$_3$ chalcogenide glasses or organic polymers like SU-8 or IP – L 780 can be used both as dielectric medium inside of the PCS and as background medium that could sandwich the structure. These upper and bottom layer may have thickness of several wavelengths and then considered infinite. The result is a membrane like structure hanging in infinite solid medium.

In theory, PCS can be in a form of membrane: a core of periodic photonic structure surrounded in air. Simulations of such PCSs show wider incomplete PBGs better transmission properties and low losses. However integrating of such photonic element will mean putting it on a substrate which will mean high asymmetry of the top and bottom slab terminations. This asymmetry will lead consequently to asymmetry of the modes and therefore escalation losses. Simulations of classical rods in air and holes in semiconductor PCSs show that there is a need of “cladding” material to hold the top and bottom of the slab. Usually some kind of SiO is considered as it has dielectric constant close to that of air.

In the AARH PhC two layers are added on the top and on the bottom of the periodic layer. They are made of the same dielectric medium as the medium of the slab with $\varepsilon=2.5$. The reason of this is in the dramatic change of shape of the modes with different dielectric constant from the dielectric constant of medium. On one hand lower dielectric constant of cladding will diminish confining of light due to internal reflection, on other hand higher dielectric constant act as a magnet for certain modes and they migrate their energy toward it.
Cladding can heavily modify the TE and TM modes in such way that some of them could be called “Cladding” modes. They are situated mostly in the cladding physical region and on the light line in the dispersion diagram. Physically, they are bouncing between the termination of the slab and the surrounding material. In principle these modes are detrimental as light propagation un them destroys every eventual PBG. On other hand it is possible to minimize its effect and utilize the cladding as another method of gaining control over propagating light wave.

![Graph](image.png)

Figure 5.6.1: AARH PCS with different diameters of rods and holes and low dielectric constant of rods. The orange and green modes are the cladding modes along the two contours.

The dimensions of the cladding are also from certain importance. There are two regimes that can be observed on Figure 5.6.1 As the claddings increase in size the two overlapping PBG of 104
cladding size slightly lowers the sizes of PBGs and lowers all the modes frequencies. The lower PBG is closing at cladding of $4a$. Most of the calculations in this investigation are done with cladding of $5a$. The reason is that for lower dielectric constant of rods this relation is harder to observe and the cladding was left at sufficiently large width to be practically feasible. Therefore choosing advantageous width of cladding can maximize the incomplete PBGs and also shifts them in suitable direction. This additional control can also help choose AARH PCS that is exactly analogous to the 2D AARH PhC.

![Graph showing the overlapping TE and TM PBGs' dependence of the thickness of cladding.](image)

Figure 5.6.2: Overlapping TE and TM PBGs’ dependence of the thickness of cladding.

The cladding of AARH PCS is not optimal but many simulations of 2D AARH PhC were performed with 3D FDTD method that featured slab like structure with very large thick cladding. In order to keep the structures as similar as possible the thickness of cladding and thickness of periodic slab were exaggerated, not optimized for largest possible PBGs.
Simulations of PCSs face several new factors that must be taken care of. The slab thickness is of great importance but it seems that after Johnson’s work no more research was undertaken at this topic. The proposed AARH PCS structure is very complex and is without analogy in Johnson’s work. On Figure 5.6.3 is shown the PBG map for different thicknesses of AARH PCS. The method is 3D PWE simulated for both K-space contours.

The most important effect of slab thickness is in fact the symmetry or asymmetry of point M and X, X’. When the thickness of the slab starts to decrease the PBGs are actually increasing in width. At the same the asymmetry is also increasing and at some cutoff is destroying the PBGs as it is shown in Figure 5.6.3 with $t = 0.5a$. The modes around points X and X’ are so much higher in frequency that it is impossible to construe a forbidden frequency zone between the bands. Hence, on one hand if one needs PBG in visual region it needs smaller thickness of the slab as the smaller thickness move the PBG up, as is shown above on Figure 5.6.2. Therefore, one needs to choose thickness before the frequency cutoff where the PBG is destroyed. It seems that the best strategy of engineering AARH PCS is to choose thickness for maximizing the PBG and then cladding such as to achieve best match between two dimensional and three dimensional models.
On Figure 5.6.3 are shown the dependence of overlapping TE and TM PBGs for the three frequency regions between the degenerated four couples of degenerated bands. The simulations with different thickness show sharp cutoff around $0.75a$. At this thickness the degeneration of the bands is partially lifted and the bands cross along X’M direction. Also the modes are sharply rising towards higher frequency and TE and TM bands are separated into different frequency regions. Only the lowest modes of TE and TM polarization stay in mutual range. There is a strong feeling that the highest PBG is exaggerated and may not exist as it is missing in the 3D FDTD measurements. Close to the cutoff the PBGs are maximized but again the picture is different if one look at figure of merit. In a sense of frequency the gaps are becoming stable but the accuracy is decreasing and one can say that after $3.5a$ the data is unreliable and probably the PBGs does not
exist. This conclusion is supported by a single simulation with very high thickness – 5a that shows all degenerated bands crossing each other in the X’M region.

As it will be shown later the most reliable region with thickness between \( t = 1.5a \sim 2.5a \) is most intriguing as it resembles very much the band frequency structure of the 2D AARH PhC. This discussion is developed in the following section.

These simulations show no such clear cut relation between the thickness of the PCS and width of the PBG as it was proposed by Johnson et. al. It is possible that the other parameters of our complicated system are overwhelming the influence of thickness. Most of the simulations in this investigation are not performed with ideal thickness that maximize the width of PBGs. There are many other factors to consider and one very important is the question is it possible to match our 2D AARH PhC simulation results with our 3D AARH PCS simulation results.

### 5.7 Zero Refractive Index

In Section 4.9 had been demonstrated a possible zero effective refractive index of 2D AARH PhC. In the next section it will be shown that adjusting the thickness of the slab can make its properties identical to those of its 2D version. In this section are presented results of simulations which goal had been to repeat replicate the 2D results in the Section 4.5.0.
Figure 5.7.1: Plane wave light is propagating through AARH PCSs with different thicknesses (a) $t = 0.5a$ (b) $t = 1.25a$ (c) $t = 0.75a$ (d) $t = 1.375a$. The rest of the parameters are presented in the text.

On Figure 5.7.1 (a) one can see TE polarized light propagating upward through a AARH PCS with filling factor $f = 0.45a$, $\varepsilon_{rods} = 12$, $\varepsilon_{medium} = 2.5$ and thickness of the slab $t = 0.5a$. Cladding is with the same thickness as the active layer of AARH PCS. The normalized frequency is the same as on Figure 4.9.3 - $f = 0.233$. Most of the plane electromagnetic wave is transmitted by the crystal with small percent of it reflected and loss due to the lack of vertical confinement. On Figure 5.7.1 (b) is represented the simulation of the same AARH PCS on the same frequency but the thickness now is $t = 1.25a$. The light is entirely reflected by the AARH PCS except for the usual confinement related loss, indicating the existence of PBG. The gap is strictly TE and is not
presented on Figure 5.7.1. Its existence was proved by subsequent 3D PWE simulation which shows surprising jump of first order PBG toward higher normalized frequency.

Light direction of propagation can be further controlled by the thickness of the slab. On Figure 5.7.1 (c) is shown the same AARH PCS with propagating light on the same frequency but the thickness of the slab is $t = 0.75a$. The result is very similar to the result on Figure 4.9.3 with its 2D counterpart. The incident beam is perpendicular to the PhC but bends to the left as it is refracted through its bulk. Some of the light beam is disturbed by the edges of the slab. The result is an evidence that there are exist analogy between the properties of 2D AARH PhC and 3D AARH PCS and the properties of the 3D slab could be predicted by the properties of its idealized 2D variant if the thickness is carefully chosen.

A series of simulations for various thicknesses of AARH PCS were performed with the goal to find if there is a relation of the angle of refracted light and the thickness of the slab. The result was negative, and it appears that effects of zero effective refractive index could be found in vanishingly small frequency region as well as very small range of appropriate thicknesses. However a surprising result is shown on Figure 5.7.1 (d) where the refractive light is bended on the right. The AARH PCS is again identical but the thickness has a value of $t = 1.375a$. Overall the series of computational simulations show that on theory one can control the direction of refracted or/and reflected light through AARH PCS by change of thickness. The direction can be adjusted on any angle on 360° circle. To achieve desired direction one has to modulate variety of factors that increase the flexibility in engineering specific photonic structures. Possible applications were already enumerated in the previous sections.
5.8 Analogy between the two dimensional and three dimensional alternate arrays of rods and holes.

![Dispersion Diagram Comparison](image)

Figure 5.8.1: Comparison between (a) 2D dispersion diagram of AARH PhC along ΓX’MΓ contour and 3D dispersion diagram of AARH PCS along X’M section of the same contour.

While on first look there is little alike between dispersion diagrams of 2D AARH PhC and 3D AARH PCS when performed with the respectful 2D and 3D PWE methods one should keep in mind that AARH PCS allows for additional degrees of control of its properties. In the previous two sections it became clear that choosing carefully the thickness of the active layer of the slab and thickness of its cladding one can modes toward higher and lower frequencies. The trends shown before are non-trivial but it seems that lower photonic bands are not only similar in shape
to their 2D variation but are also somehow close as frequency. Without trying to maximize the PBGs an AARH PCS structure was chosen where its lower modes are on the 2D frequencies. On Figure 5.8.1 is shown that at thickness around $t = 2.5a$ there is clear analogy between the 2 and 3 dimensional structures. It is unclear if this number is by coincidence close to the result of Johnson given in the Section 5.1.5. One can argue that 2D results are somehow like low resolution 3D as they extend the modes into higher frequencies especially the TE like bands. Also, the TM modes are predominant due to higher dielectric contrast and less sensitive to changes of AARH PCS parameters. In fact this number is not exactly constant. It is in the region of $1.3a$ and $1.7a$ for reasonable set of parameters. Large differences between the radiuses of rods and holes completely destroy any possible relation. Very low filling factors also tend to increase difference between the frequency domains of these structures. In the example of low dielectric constant and low filling factor AARH PCS the relation is nearly the same.

Another way to tweak frequency regions of 2D and 3D AARH PCS is using the size of the cladding. In this case the cladding was chosen as $5a$ which is not the optimal one but simulate large nearly infinite size of the cladding.

All of these investigations were along $\Gamma X' M \Gamma$ contour. No such relation was observed along $\Gamma X M \Gamma$ contour for higher frequencies where the TE bands cross into each other and close any PBG in the region of XM. Only the TM PBG that is between second and third order band exist and is related as $t = 2.8a$. In general it is much harder to match 2D and 3D predictions along this contour.
5.9 Photonic band gaps detected by three dimensional finite difference time domain method

In this section is presented AARH PCS with somehow different parameters from the one with high dielectric constant of rods and large filling factor. It is presented on Figure 5.9.1. Here the dielectric constant of rods is chosen to be $\varepsilon = 7.1$ as dielectric constants of many kinds of quantum dots is between $\varepsilon = 6$ and $\varepsilon = 8$. For practical reasons the quantum dots are far superior as material for rods than semiconductors because of their higher optical quality. High dielectric semiconductors though are simpler to simulate, what was done in previous sections.

The fitting parameter is lowered too and is $f = 0.25a$ which makes the structure much more realistic. With high fitting factor of the previous AARH PCS the connected regions of the medium form very thin shapes that would be very hard to manufacture. With this configuration all features in the slab are with comparable size. The resulting dispersion modes in this case is shifted to higher frequencies which allows for PBGs in infra-red and optical regimes for comparatively large features.

The thickness of the cladding and slab were not optimized but still in the suitable region. The thickness of the active layer is $t_{\text{slab}} = 1.25a$ and cladding is $t_{\text{cladding}} = 2.5a$. Simulations with different combination of thickness of slab and clad gave much higher width of the PBGs. The disadvantage of these sets of photonic parameters is in the smaller difference of the rate of frequency shift between TE and TM PBGs, which is the point of this investigation.

By changing the values of dielectric constants of rods and hosting medium and radius of rods/holes, the TM- and TE-like PBGs in AARH PCS are found to shift in frequency at different rates. This feature allows us to engineer the PBGs for both orthogonal polarizations in a same
frequency range. The method of computations is 3D FDTD method in frequency domain. The results are transmission – frequency spectrum for each set of parameters. The PBGs are observed when the reflective index is maximized. The central TE and TM curves on Figure 5.9.1 represent the minimum peak of incident flux as calculated in expression 5.1. These center frequencies of TM and TE PBGs change as the values of dielectric constant and radius of rod/hole increase.

In order to demonstrate that the proposed AARH PCS possesses the overlapped TE and TM PBGs, we scanned the structure parameter space using the PWE method and found that the parameters of dielectric constant for rods and radius of rod/hole can be effectively used to tune the centers of the TM and TE PBGs. Furthermore, the center of PBG decreases at different rates for TE and TM PBGs as function of $\varepsilon_{\text{rod}}$ or filling factor $f$, enabling us to engineer the PBGs for both orthogonal polarizations in a same frequency range.

In the case of dielectric constant the central frequency for TE and TM incomplete PBGs are shifting downwards with the increase of dielectric constant of rods. It is worth mentioning that these are the first order PBGs. As was analyzed in the sections above first order overlapping PBGs disappear at higher dielectric constants and what was left was the second order. On Figure 5.9.1 (a) the two PBGs are shifting downwards and generate overlapping PBG range when the value of $\varepsilon_{\text{rod}}$ is in the range of 6 to 8. How the center frequencies of TE- and TM-like PBGs change with the filling factor is demonstrated in Figure 5.9.1 (b). The changing rate for the two polarizations is initially different, resulting in the overlapping PBGs when filling factor becomes $f = 0.225$ then the decreasing rate of PBGs for both polarization remains same until the filling factor becomes $f = 0.275$ when the two central lines of TE and TM PBGs start to diverge. The shaded regions in the diagram represent the average half-width of the PBGs. Generally, for this set of parameters it is 6% for TM and 5% for TE polarization, respectively.
Figure 5.9.1: the middle values of TM- and TE-like PBGs are plotted as function of dielectric constant of rods (a), and as function filling factor (b). The following initial structure parameters are used: \( \varepsilon_{rods} = 7.1 \), \( \varepsilon_{medium} = 2.5 \), \( f = 0.25a \), \( t_{slab} = 1.25a \), \( t_{cladding} = 2.5a \). The shaded areas are the average relative band gap width: 6% for TM- and 5% for TE-like polarizations.

The results here are only along ΓX’MΓ k-space contour which corresponds to direction of \( \vec{a}_2 \) real space vector on Figure 4.3.1. It is true that 3D FDTD simulations show overlapping TE and TM PBGs in \( \vec{a}_1 \) direction too but the data is much noisier and depends too much on how the AARH PCS is terminated. Example of an overlapping TE and TM PBG in this direction is presented in following section.

It is possible to show similar shift with the change of the low dielectric constant medium is \( \varepsilon_{m} \). It shows similar shifts bur in smaller scales. It also could be used for fine-tuning the frequency positions of the PBGs. Equalizing the dielectric contrast on one hand between the rods and medium and on another hand between the holes and medium lead to some interesting optical and transmission effects. However it is not clear how realistic is such arrangement, so the results
are not presented in this investigation. Further research on unusual set of parameters may achieve some interesting results.

5.10 Comparison between the three dimensional plane wave expansion and finite difference time domain methods

Photonic dispersion band diagrams for a given set of structure parameters ($\varepsilon_{rod} = 7.1$, $\varepsilon_m = 2.5$, $f = 0.25a$, thickness $t = 1.25a$ and cladding $t=2.5a$) are displayed in Figure 5.10.1: (a) along the $\Gamma X'M\Gamma$ contour and (c) along the $\Gamma XM\Gamma$ contour. The simulations were performed with very high resolution using 3D PWE method. The transmission – frequency spectrum is shown on Figure 5.10.1 (b) in $a_2$ direction and Figure 5.10.1 (d) in $a_1$ direction. The simulation was performed using 3D FDTD method with 100 steps per grid distance, Furrier Padding and no-reflections PML. In the first pair of simulations there are two overlapping TE and TM PBGs. On the dispersion diagram Figure 5.10.1 (a) they are incomplete and stretch only in $X'M$ segment of k-space. On the Figure 5.10.1 (b) diagram the overlapping minima of net flux are proof of overlapping TE and TM PBGs. The minima are not zero as unconfined light is radiated away as loss. Similar picture is seen on Figure 5.10.1 (c) where the dispersion diagram shows only one second order overlapping TE and TM PBG, and Figure 5.10.1 (d) it is matched with single overlapping TE and TM net flux minima. As was mentioned earlier the truncation of front and back side of AARH PCS along $a_1$ space direction strongly influences the 3D FDTD results. The large net flux is coming from significant scattering on the surface of the slab.

A peculiar feature can be observed on Figure 5.10.1 (a) and (b). On the dispersion diagram is observed only one large first order overlapping PBG while on the transmission frequency
diagram are observed two narrow net flux minima. The possible reason for this phenomenon is related in the next section.

Figure 5.10.1: Photonic band diagrams for the two independent contours of $\Gamma X'M\Gamma$ (a), and $\Gamma XM\Gamma$ (c) calculated by the 3D PWE method. The net flux is calculated by the FDTD method when a light beam is incident on the PCS along $\vec{a}_t$ direction (b), and when the beam is parallel to $\vec{a}_t$ direction (d).
This investigation confirms that the results of simulations using 3D PWE and 3D FDTD are very similar. The PBGs are good match and the transmission properties are related to the frequencies of the modes in the dispersion diagram. There is a hope that if not perfect these simulations are good prediction of the optical properties of the proposed AARH PCS.

5.11 Surface modes and edge modes

Surface waves on PCSs are localized at the interface of PCS and the outside medium. As an analogy one consider electronic scattering at the interphase of two different crystalline solids. Initially such waves were theoretically predicted in PCS but barely observed. It happened that the front and back surfaces of a PCS should be significantly modified to make those waves observable. Research of this phenomena was for long obstructed by the fact that these waves were deemed very undesirable due to large additional loss. Now surface waves are promising in engineering coupled waveguides and various flat lens optical devises.

In attempt to prove the accurateness of Figure 5.10.1 and understand the discrepancies between 3D PWE results in (a) and 3D FDTD results in (b) several simulation were performed with 3D FDTD method in space domain. With this method it is possible to simulate plane wave falling on the AARH PCS the same way as in the simulation of negative refraction in Chapter 4. Though calculation could show the spatial distribution of all components of electromagnetic wave, once again the intensity measurements were most informative. The simulation showed with good precision high reflective properties of the AARH PCS inside the region with incomplete PBG. The losses were also in the range of Figure 5.10.1. Below the first PBG and above the second one the light entered inside the slab and was transmitted with something between 20%~50 total loss. This
shows that this particular set of parameters do not produce PCS with good transmission properties. However high transmission can be achieved with small lowering of the radiuses of rods and holes. At such regimes transmission can reach 90% which with somehow lowered quality of reflection in the high reflective regions.

An unexpected result was obtained when plane wave was simulated in the frequency region between the two PBGs. The light did not propagate inside the AARH PCS but was redirected along its surface. At the edge of the structure it was reemitted not unlike circular source.

Given the information in the beginning of this section one can speculate that there was an observation of surface modes that otherwise cannot be detected with flux measurements wit 3D FDTD method in frequency domain. The reemission of incident light at the edge of AARH PCS could be recognized as edge modes. The references attempt the observation of the said modes in 2D while observing them in 3D simulations is very rare.

In the Figure 5.1.1 are shown several spatial distribution of intensity of light after leaving its source and propagating toward the AARH PCS. The simulation is both along ΓX’MΓ contour as the second ΓXMG contour did not exhibit such effects. The simulation results are showing the light intensity in space at the end of the simulation time period. The measurements were with medium resolution and time period of 5000 steps enough to encompass all of the device. The light intensity scale ranges from the highest in white-yellow color to the lowest in dark red-black. Inspecting this figure, it can be seen that the light is concentrated near the first two rows of rods and holes, instead of directly being reflected. The light beam is also being scattered from the edges of PCS. This simulation result explains why the net flux calculated by the 3D FDTD appears to be not consistent with the PBGs obtained by PWE method. To further clarify the frequency dependent transmission property through the PCS, a similar light beam resembling a TE polarized plane wave
but with a different frequency, located outside of the PBGs was simulated to pass the PCS. The light intensity distribution at the end of simulation period is shown in Figure 5.11.1. It is consistent with the PBG scenario that the light beam freely propagates through the PCS with negligible scatterings at edges. The simulation results using TM polarized light further support the notion that non-ideal reflection in the PBG region may be due to redirection of reflected beam toward the surface.

Figure 5.11.1: 3D FDTD measurement in space domain. The light intensity distribution is shown at the end of FDTD simulation period when a plane-wave-like light beam with TE polarization (a) and (c) and TM (b) and (d) is sent to the PSC in $\vec{a}_2$ direction. The normalized frequency of the monochromatic plane wave is $0.25$ for (a) and (b) and is $0.29$ for (c) and (d).
On Figure 5.11.1 (a) and (c) is shown the intensity of TE and TM respectively polarized light propagating toward the PCS at frequency inside the overlapping PBG but between the two reflectance peaks. Most of the field is concentrated at the first two rows of PCS and then propagates along the surface of the crystal. In the case of TE polarization nearly no light is reflected or refracted. In the case of TM polarization larger percent of light is reflected and the field extends to larger degree inside the crystal. PBG and reflectance for TM is significantly wider and stronger than for TE as dielectric contrast between rods and medium is larger than medium and holes. In principle TE modes prefer to propagate along connected structures (medium around holes) which is a factor enhancing the creation of surface modes. TM polarized modes prefer to propagate along disconnected structures (rods) and therefore its field penetrates deeper into PCS. On Figure 5.11.1 (b) and (d) are shown the intensities of TE and TM light of frequency outside the PBG region. The light is refracted through the crystal without much reflection. In this case the loss for both polarizations is similar. The existence of surface modes depends on the way the PCS is terminated. The incident light faces two very different surfaces in \( \vec{a}_1 \) and \( \vec{a}_2 \) directions: the reason why one of them generate surface modes the other not. 3D FDTD simulation with different modified surfaces showed large variety of effects from broadening of the photonic gap to its overall closing.

As there are several ways to terminate the TACS in \( \vec{a}_1 \) which correspond to light propagation along k-space \( \Gamma \mathrm{XM} \Gamma \) contour, several options were considered like “Pure hole wall”, ”Pure rod wall” and the two possible mixtures. Based our 3D FDTD data, it appears that the light beam incident to the surface parallel in \( \vec{a}_1 \) direction does not excite the any surface modes while it does when it is incident to the surface parallel to \( \vec{a}_2 \) direction. Once again this fact shows that k-space \( \Gamma \mathrm{X}' \mathrm{M} \Gamma \) contour exhibit is much richer photonic characteristics.
Chapter 6 Experimental design and future work

We propose to fabricate the AARH PCS characterized by computational simulations in previous chapters above, using the photolithography method. The fabrication processes can be implemented in the Advance Science Research Center CUNY using a two-step process that requires high resolution and excellent repeatability or the alignment of photomask and wafer. The new EVG Mask Aligner in ASRC is modern equipment that fully meets these requirements. The other equipment available in ASRC will be also used and they are: Brewer Science Spin coater for generating polymer thin layers, Blue M Oven for soft and hard baking, Bruker 3D optical Profiler, and Bruker Stylus Profiler.

Another possibility of fabricating our PCS structures is to use the newly purchased Nanoscribe 3D Lithography apparatus that uses 3D laser writing (two-photon absorption mechanism). It may allow us to drill both photonic arrays in a single rigid polymer making the highly-accurate alignment procedure unneeded, achieving much smaller features in comparison with the structures fabricated by the conventional photolithographic method. If this method is successful for our PCS structures, it enables us to characterize the proposed PCS structures using lasers in near infrared region rather than in mid-infrared region.

In the past months, an enlarged version of the AARH PCS was fabricated using initially nanoimprinting device available in Brooklyn College Photonic laboratory. In the process the many issues with physical and chemical properties of SU-8 and its applications were mastered and the Nano-imprinter was significantly upgraded for the need of our applications. Several procedures for two-mask photolithography were constructed as no such procedure exists in the literature. We are very thankful for the help and advices many researchers gave us on “MEMS Talk” website.
Later, the manufacturing process was moved to the Advanced Science Research center, where the fabrication process was advanced and concluded.

A detailed schematic diagram of the proposed fabrication process is given below on Figure 6.1.

Figure 6.1: Schematic diagram for the fabrication process of the proposed AARHC structures.
1) The glass (or silicon) wafer is cleaned and chemically processed for later detachment of the patterned structure. The SU-8 polymer is spin-coated and soft baked. Then it is cured by UV light. The photomask pattern is a group of white rings on black background.

2) The wafer and polymer are soft-baked again and then developed by a combination of SU-8 developer, Acetone and Isopropyl Alcohol. The result is a group of hollow cylinders of rigid polymer over the glass wafer and air in between.

3) The hollow cylinders are filled repeatedly with a solution processable to a polycrystalline semiconductor compound. After the solvent evaporation, the holes are replaced by rods of high-refractive-index semiconductor. The solution between the cylinders is removed by gently spinning the wafer.

4) SU-8 is once again deposited over the wafer with the existing semiconductor cylindrical rods. It is spun until polymer layer is barely thicker than the height of the cylinders. Then it is soft baked. For this procedure a different photomask is used. The second pattern is a group of black disks in between the arrays of white rings in the first photomask. This procedure requires a precise alignment of the second photomask relative to the processed wafer by the first mask.

5) The processed wafer is soft-baked and the SU-8 is developed. The second photomask creates series of holes in between the series of semiconductor rods.

6) The fully finished structure is detached from the glass wafer and the cladding layers are added on the top and bottom of the PCS (see Figure 4.3.1) for the light confinement in vertical direction.
From the very beginning the computational simulations were aimed at achieving complete PBGs and negative refraction effects in the optical regime. From practical point of view this is not easy as the features of any PhC modulating visible light should be on the scale of 100 – 200 nm. Of now such scale is achieved only in the most advanced national laboratories. Another difficulty is to find commercially available photomasks with high definition for tiny features. Hence the scale of the features are needed to be enlarged to about a micron. On such scale the PBGs for AARH PhC and AARH PCS in our simulations are situated in the infrared region around 4 – 5 microns. Such regime can be achieved with quantum cascade laser that is planned to be purchased in near future.

Figure 6.2: The final structure of fabricated AARH PhC.
Chapter 7 Conclusions

• The focus of the current research was on design and fabrication of complex photonic structures with large potential for future applications. A summary of key achievements are highlighted as following:

• A thorough study was conducted on properties of 2D and 3D PhCs. In the process several methods of creating overlapping TE and TM PBGs were recognized. Large number of different photonic structures were simulated and their dispersion relations explored.

• A new 2D photonic structure was introduces and designed with two alternate arrays of rods and holes. The PWE simulations showed large frequency regions where light is forbidden to enter. Adjusting the properties of the PhC like dielectric constant of rods or filling factors of rods and holes, it was possible to achieve overlapping of PBGs for both polarizations TM and TE. The design was refined using rigorous 2D and 3D FDTD simulations. The simulation results confirmed the existence of complete PBGs regardless of which numerical method had been used. On deeper inspection it was found that there are two prevailing mechanisms that are responsible for the creation of complete PBGs. On one hand the symmetry breaking in the k – space Irreducible Brillouin Zone lifts the degenerations at points of high symmetry. As a result some gaps are opening between the modes. Also, the TE modes are shifted to lower frequencies and their PBGs are now in the same frequency region as TM bands and PBGs in between. On the other hand on certain k – space contours, the Brillouin Zone folding leads to complete degenerations of
bands in XM direction. Thus, a PBGs are opened between each couple of photonic bands for both polarizations.

- Further exploration of the presented structure were executed using a third numerical method: 2D and 3D FDTD space domain. On the edge of PBGs were observed several effects of unusual light propagation like negative refraction and superlensing. Of great interest is the observation of “zero – refractive index propagation”. It was found that at certain frequency ranges the angle of refractive light propagation depends only on the frequency and not on the initial angle. The matter deserve additional research.

- Several attempts on simulation of optical switches using the Ker effect showed that the structure is flexible enough to accommodate the needed requirements.

- There is serious disconnect between 2D and 3D photonic structures as the former is deemed too idealized and the latter does not exhibit PBGs in the same sense as the 2D structure. It was found that for the novel AARH slab a combination of thicknesses of active and cladding layers make their dispersion diagrams in XM direction very similar to the 2D PhCs. This enables a fast and cheap design of 2D AARH of specific properties and then its direct implementation as a 3D slab.

- The AARH slabs exhibit complicated set of unusual properties of propagating light. Apart from negative refraction it was found that the direction of refracted light can be controlled by the thickness of the slab. At zero incident angle the light can go in nearly all possible directions including entirely transmitted through the crystal and entirely reflected as in a PBG. This result could be very useful in designing optical switches and optical transistors.
• A method was designed for overlapping the incomplete TE and TM PBGs for the 3D AARH photonic slabs. The method was greatly improved by exciting surface and edge modes. This had led to large increase of the width of the overlapping TE and TM PBG reaching in some cases up to 20%.

• In the end, a two photomask method of manufacturing for AARH was developed and partially implemented in a physics lab.
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