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Terahertz Photonic Crystals

by

Zhongping Jian

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APPROVED, THESIS COMMITTEE:

[Signatures with names and titles]

Daniel M. Mittleman
Associate Professor, Chair
Electrical and Computer Engineering

Frank K. Tittel, J. S. Abercrombie Professor
Electrical and Computer Engineering

Vicki L. Colvin, Professor
Chemistry

HOUSTON, TEXAS

APRIL 2006
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ABSTRACT

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This thesis describes the study of two-dimensional photonic crystals slabs with terahertz time domain spectroscopy. In our study we first demonstrate the realization of planar photonic components to manipulate terahertz waves, and then characterize photonic crystals using terahertz pulses.

Photonic crystal slabs at the scale of micrometers are first designed and fabricated free of defects. Terahertz time domain spectrometer generates and detects the electric fields of single-cycle terahertz pulses. By putting photonic crystals into waveguide geometry, we successfully demonstrate planar photonic components such as transmission filters, reflection frequency-selective filters, defects modes as well as superprisms. In the characterization study of out-of-plane properties of photonic crystal slabs, we observe very strong dispersion at low frequencies, guided resonance modes at middle frequencies, and a group velocity anomaly at high frequencies. We employ Finite Element Method and Finite-Difference Time-Domain method to simulate the photonic crystals, and excellent agreement is achieved between simulation results and experimental results.
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Table of Contents

Abstract

Acknowledgements

List of Figures

1 Introduction

1.1 Motivation

1.2 Overview

2 Background Information of Photonic crystals

2.1 Brief History of Photonic Crystals

2.2 Photonic Band Gaps and Defect Modes

2.3 Superprism Effect of Photonic Crystals

2.4 Negative Refraction of Photonic Crystals

2.5 Quantum Information and Photonic Crystals

2.6 Computational Methods for Photonic Crystals

2.6.1 Basic equations

2.6.2 Finite Element Method (FEM)

2.6.3 Finite-Difference Time-Domain method (FDTD)

2.6.4 Plane-Wave Expansion Method

3 Terahertz Waves

3.1 Terahertz waves

3.2 Generation of Terahertz Pulses

3.3 Detection of Terahertz Pulses
3.4 Terahertz Time Domain Spectroscopy ................................................. 29
3.5 Applications of Terahertz Pulses ...................................................... 31
3.6 Waveguiding Terahertz Waves ......................................................... 33

4 In-Plane Properties of Two-Dimensional Photonic Crystals ................. 36
4.1 Introduction ...................................................................................... 36
4.2 Experimental Setup ......................................................................... 39
4.3 Photonic Crystal Samples ................................................................. 39
4.4 Transmission Results and Discussion .............................................. 41
   4.4.1 Band Structures ......................................................................... 41
   4.4.2 Time-Domain Waveforms .......................................................... 42
   4.4.3 Frequency Response .................................................................. 45
   4.4.4 Group Velocity ........................................................................... 47
4.5 Conclusion ......................................................................................... 51

5 Defect Modes and Reflection Spectra ................................................. 53
5.1 Introduction ...................................................................................... 53
5.2 Experimental Setup ......................................................................... 54
5.3 Defect Modes ................................................................................... 55
5.4 Reflection Spectra ............................................................................ 58
5.5 Conclusion ......................................................................................... 59

6 In-Plane and Out-of-Plane Dispersion and Homogenization .............. 61
6.1 Introduction ...................................................................................... 61
6.2 Experimental Setup ......................................................................... 62
6.3 In-plane Dispersion and Effective Refractive Index ............................ 64
6.4 Out-of-Plane Dispersion and Effective Refractive Index ........................................... 66
6.5 Finite Element Method Simulation ................................................................. 69
6.6 Conclusion .................................................................................................... 73

7 Broadband Group Velocity Anomaly in Photonic Crystal Slabs .................. 75
7.1 Introduction .................................................................................................. 75
7.2 Experimental Setup ...................................................................................... 78
7.3 Group Delay .................................................................................................. 79
7.4 Conclusion .................................................................................................... 82

8 Guided Resonance Modes in Photonic Crystal Slabs .................................. 84
8.1 Introduction .................................................................................................. 84
8.2 Temporal Behavior of Guided Resonances .................................................. 86
8.3 Transmission Spectra of Guided Resonances .............................................. 88
8.4 Dispersion Relation ....................................................................................... 90
8.5 Short-Time Fourier Transform .................................................................... 91
8.6 Conclusion .................................................................................................... 93

9 Angled Incidence and Displacement Sensitive Structures ........................ 94
9.1 Introduction .................................................................................................. 94
9.2 Angled Incidence ........................................................................................ 95
9.3 Two-Slab Structure ...................................................................................... 99
9.4 Conclusion .................................................................................................... 103

10 Summary of Results and Future Prospects .............................................. 105
10.1 Summary of Results ................................................................................... 105
10.2 Planar Photonic Crystal Devices .......................................................... 106
10.3 Superprism Effects .............................................................................. 108
10.4 Group Velocity Anomaly ..................................................................... 110

Bibliography ............................................................................................... 113
List of Figures

Figure 2.1. Typical one, two and three dimensional photonic crystals. In a 1-D photonic crystal, two materials with different refractive index are arranged periodically along one direction. In a 2-D photonic crystal, they are arranged periodically along two directions, and along three directions in a 3-D photonic crystal. .................................................................9

Figure 2.2. A Yeh cell shows the position of the electric and magnetic field vector components. .................................................................19

Figure 3.1. Figure 3.1 A typical Auston switch; black lines are electrodes made of gold, and the substrate is semi-insulating GaAs wafer. The two electrodes are DC biased. Ultrafast femtosecond pulses are focused onto the middle of the two gold lines to generate photocurrent, which radiates into free space and that is terahertz wave. .................................................................27

Figure 3.2. Top: schematic of the Terahertz Time-Domain Spectroscopy. Bottom: Photograph of the T-Ray 2000, by Picometrix Inc. T-Ray 2000 is a fiber coupled system which makes the free movement of the transmitter and receiver possible. .................................................................30

Figure 3.3. (a) A typical single-cycle terahertz pulse in time domain. (b) The amplitude spectrum of the pulse by Fourier transforming the detected time-domain waveforms. (c) The phase spectrum of the pulse, obtained by Fourier transform the time waveforms. .................................................................31
Figure 4.1. A schematic of the optics used to couple the THz radiation into and out of the parallel plate metal waveguide, into which the photonic crystal can be inserted. The polarization of the THz beam is perpendicular to the plane of the slabs, so only TM modes are excited. .................................................................39

Figure 4.2. Top: A schematic of the photonic crystal slab, consisting of an array of holes etched through a 305 micron- thick silicon wafer. Only half of the area of the wafer is etched, so that the un-etched portion can be used as a reference. Bottom: a top-down image of a portion of one sample fabricated using deep reactive ion etching. The diameter of the air holes is 360 microns and they form a hexagonal lattice, with a pitch of 400 microns. The thickness of the slab is 305 microns. ..................................................40

Figure 4.3. Left: Band structure for TM modes of the photonic crystal, with infinite thickness in the direction parallel to the axes of the air holes. This is computed using a plane wave expansion method [1, 2]. A complete band gap is denoted by the gray region. Dotted lines represent bands whose fields are anti-symmetric, and which therefore cannot be efficiently excited by the symmetric input field [3, 4]. The inset shows the two-dimensional Brillouin zone, with high symmetry points labeled. Right: Vertical components of the electric fields for bands between the \( \Gamma \) and \( K \) points. Those of bands 1, 3, and 5 are symmetric with respect to the \( \Gamma-K \) direction (denoted by the black line), while those of bands 2 and 4 are anti-symmetric. The key at lower right indicates which image corresponds to each band. .................................................................42

Figure 4.4. Typical measured time-domain waveforms, for the situations when the metal waveguide is filled with air, silicon, and the photonic crystal slab, from top to bottom, respectively. In each case, there are three samples with different lengths along the
propagation direction, and the lengths are 3.964 mm, 7.428 mm, and 14.356 mm, from top to bottom in each case, respectively. The air signals show no dispersion, and the silicon signals show a little dispersion resulting from multi-mode excitation of the waveguide. The photonic crystal signals are significantly dispersed, extending to hundreds of picoseconds. This dispersion results from the band structure of the photonic crystal, in particular near the edges of the band gap. ...........................................43

Figure 4.5. Calculated group velocity versus frequency for different modes, for the situations when the metal waveguide is filled with air, PC, and silicon, from top to bottom, respectively. Those modes in dashed lines are of odd parity and will not be excited by external waves. Up to 1THz, there is only one TEM mode for air, and two modes for photonic crystal, but there are four modes for etched silicon. This explains why the silicon signals in figure 4.4 are significantly dispersed. .............................44

Figure 4.6. (a) Measured power transmission spectrum of the photonic crystal inside the metal waveguide, for the Γ-K direction, along which the sample has 4 unit cells. This is computed using the Fourier transforms of the time-domain waveforms, with the air-filled guide as a reference. (b) Γ-K transmission spectrum computed using a transfer matrix method, for comparison with the experimental result. The comparison is quite good, except for a systematic red shift of about 0.025 THz, attributed to the finite thickness of the photonic crystal which is not considered in the numerical calculation. ...........................................................................................................46

Figure 4.7. (a) Measured power transmission spectrum of the photonic crystal inside the metal waveguide, for the Γ-M direction, along which the sample has 10 unit cells. This is computed using the Fourier transforms of the time-domain waveforms, with the air-filled
guide as a reference. (b) Γ-M transmission spectrum computed using a transfer matrix method, for comparison with the experimental result. A red-shift of the theory with respect to the experiment is observed, similar to the results of figure 4.6. ..........................................................47

Figure 4.8. Short-time Fourier transform false-color plots of the three waveforms along Γ-K direction. Here, red indicates high amplitude and blue indicates low amplitude. In the upper plot, the air-filled waveguide is dispersionless, so all of the spectral components of the THz pulse arrive at the same time. In the middle plot, the small dispersive effects arise from multimode excitation of the waveguide. In the lower plot, large dispersion is observed near the edges of the band gaps in the photonic crystal. ..........................................................50

Figure 4.9. Short-time Fourier transform false color plots of the THz pulses transmitted through three different samples along the Γ-M direction. In these samples, the thicknesses are 5, 10, and 20 unit cells, from top to bottom respectively. As a result of the increasing propagation distance inside the dispersive medium, both the transit times and the dispersion increase. The solid black lines are calculated as described in the text. These are plotted using only one adjustable parameter: the frequency shift due to the finite thickness of the crystal, mentioned in the context of figures 4.6 and 4.7. This parameter is the same for all three panels. ..........................................................51

Figure 5.1. (a) The experimental transmission spectrum for the photonic crystal, relative to a solid silicon slab of equal thickness. Solid squares are for the perfect lattice, and hollow circles are for the same lattice but with three holes filled, in the pattern shown in
the inset. A defect mode appears at \( \sim 0.28 \) THz. (b) the solid line shows the TMM calculation for a perfect photonic crystal, and the dashed line is for the lattice with a three-point defect. The material filling the holes is assumed to be a uniform dielectric with \( \varepsilon = 5.0 \). (c) The difference in the spectral phases of the two measured waveforms which gave the spectra in (a). The signature of the defect mode is evident at 0.28 THz. The shaded area denotes the region of the full photonic band gap, where the transmitted intensity is not large enough for an accurate determination of the phase.

Figure 5.2. Upper: Time-domain waveforms reflected from an un-patterned silicon reference slab (solid) and a photonic crystal (dotted). The inset shows a schematic of the reflection geometry. In these measurements, \( \Gamma-M \) direction is perpendicular to the incident surface of the photonic crystal. Lower: The power spectra of the two waveforms shown in the upper plot, on a log scale. The photonic crystal result (squares) exhibits enhanced reflection in certain spectral regions (indicated by arrows), due to the high reflectivity of band gap regions.

Figure 6.1. A schematic of the out-of-plane experimental arrangement. The photonic crystal slab is illuminated at normal incidence to the plane of the periodicity. The THz beam spot size is large enough to illuminate many holes.

Figure 6.2. (a) The transmission and (b) relative phase for in-plane propagation (TM polarization), along the \( \Gamma-M \) direction. The vertical dashed lines indicate the edges of the first (partial) photonic band gap. The slanted dashed line in (b) is a guide to the eye to indicate the linearity (and the zero intercept) of the in-plane phase at low frequencies. (c)
Effective refractive index versus frequency, for propagation in the plane of the slab. The predicted homogeneous value of $n_{\text{hom}} = 1.9585$ (horizontal solid line) is precisely consistent with the measurement at low frequencies, $n_{\text{meas}} = 1.958\pm0.011$. Deviations are observed only as the frequency approaches that of the band gap (vertical dashed lines).

Figure 6.3. (a) Power transmission coefficient and (b) relative phase $\Delta \phi$ for transmission perpendicular to the photonic crystal slab. The phase is measured relative to the case of no sample in the THz beam path. In (a), the solid line is the result of a finite element method (FEM) simulation, while in (b), the solid line is a finite-difference time-domain (FDTD) simulation. Both simulations account for the finite thickness of the sample along the propagation direction, and both reproduce the frequency-dependent features of the data.

Figure 6.4. Effective refractive index versus frequency, for propagation normal to the plane of the photonic crystal slab, for the frequency range below the first guided resonance. The horizontal dashed line indicates the predicted homogeneous limit of $n_{\text{hom}} = 1.6448$, which is smaller than the measured low-frequency value of $n_{\text{meas}} = 1.73\pm0.07$. The dotted curve shows the dispersion predicted by a band structure calculation for out-of-plane propagation in an infinite-thick photonic crystal, based on a plane wave method [2]. The solid curve is the FDTD simulation from figure 6.3(b), which is in excellent agreement with experimental results.

Figure 6.5. Top: a schematic of a unit cell in our photonic crystal. Bottom: power distribution at the region denoted by the bold-line area, calculated with FEMLAB. With
the increase of frequency, power moves to the silicon region, making the effective index
increases with frequency. .................................................................69

Figure 6.6. A schematic to show how to choose the minimal modeling area in FEMLAB.
As the holes are periodically arranged, a unit cell such as the hexagon in yellow
represents the whole pattern. However, according to symmetry properties, we do not
need to model such a big area; instead, it is enough to modeling the rectangle in
red. ........................................................................................................71

Figure 6.7. (a) the geometry of modeling area. The center part is the red area shown in
figure 6.6. The two sides are needed to simulate the propagation of waves perpendicular
to the slab. (b) meshed geometry. The center part has more meshing elements, as it has
finer structure. .................................................................72

Figure 6.8. A solved model, with power distribution shown at different planes along the
wave propagation direction. The distribution is more uniform at two sides than at the
center, as the center part has a more complex structure. ..................73

Figure 7.1. The measured relative phase, $\Delta \phi = \phi_s - \phi_r$, for (a) a solid silicon slab and (b)
a photonic crystal slab. In (a), the solid curve is a calculation of the Fabry-Perot phase,
using the known thickness and refractive index. This shows that the measured results are
reliable up to at least 1.5 THz. In (b) the solid curve is a finite-difference time-domain
(FDTD) simulation. Above 0.9 THz, the relative phase is nearly constant, indicating a
group velocity equal to the vacuum speed of light in this broad spectral
range. .................................................................79
Figure 7.2. Time-domain waveforms after propagating through air, a solid silicon slab, and the photonic crystal slab. These have been filtered to remove all spectral content below 0.9 THz, as described in the text. The solid curves show the pulse envelopes, while the dashed curves show the real electric field. The group delay (transit time) through the photonic crystal slab is identical to that of air, whereas the middle (solid silicon) waveform is delayed by $\Delta t = (n_{si} - 1)L/c$ relative to the other two. Curves vertically offset for clarity.

Figure 7.3. The amplitude transmission coefficient, $|E_s(\omega)/E_r(\omega)|$, for (a) a solid silicon slab and (b) a photonic crystal slab, corresponding to the two phase measurements shown in figure 7.1. As in figure 7.1, the solid curve in (a) is computed from the Fabry-Perot effect, demonstrating the reliability of the measurement up to at least 1.5 THz. The spectrum in (b) shows no obvious signatures corresponding to the abrupt change in the phase spectrum at 0.9 THz.

Figure 8.1. Typical time domain waveforms. From top to bottom, the top three signals are for air, un-etched silicon wafer, and photonic crystal slab, respectively. The bottom two curves illustrate the deconvolution of the air signal from the silicon wafer and photonic crystal slab signals, respectively. These deconvolved signals highlight the interaction of the radiation with the samples under study.

Figure 8.2. Power transmission spectrum, computed using the Fourier transforms of the time-domain waveforms, with the air signal as a reference. Upper: Results for the silicon wafer from measurement (square) and theoretical calculation considering only the Fabry-
Perot effect (solid). Lower: Circle line shows the experimental results for the photonic crystal slab. Finite Element Method is used for simulation and it (solid line) agrees very well with the experimental results. Limited by our computation power, we can only reach frequencies up to about 0.75THz at this moment. .........................................................88

Figure 8.3. Upper: phase spectra of the silicon wafer, subtracted by that of the air reference signal, from experiments (gray) and theoretical calculations (solid line). Lower: phase spectra of the photonic crystal slab, subtracted by that of the air reference signal. Results from the experiments are shown as square and those from FDTD are shown as the solid line. Excellent agreement is obtained between the two. The thin black arrows denote the positions of guided resonances. .........................................................89

Figure 8.4. The dispersion relation from photonic crystal slab. Triangle shows the experimental results and solid line shows the FDTD simulation. The blank area between the two dashed lines denotes the region where there are phase jumps resulting from guided resonances, so an accurate determination of the dispersion for this region is not available. .................................................................91

Figure 8.5. Short-time Fourier transform false color plots of the THz pulses transmitted through silicon (top) and photonic crystal slab (bottom). The Fabry-Perot effect in the silicon sample is manifested by the reflected pulse following the main input pulse. In the PC signal, at low frequencies, the arrival time increases with frequency, indicating the increase of effective index. At the middle frequencies, at many picoseconds later, there are still components. At high frequencies, almost all frequency components arrive at the same time, indicating the broadband group delay anomaly discussed in chapter 7. ........................................................................................................92
Figure 9.1. A schematic of the out-of-plane experimental arrangement. The photonic crystal slab is illuminated at normal incidence to the plane of the periodicity. The THz beam spot size is large enough to illuminate many holes. .............................................95

Figure 9.2. The deconvolution of the air signal from photonic crystal slab signals measured at different incident angles, ranging from 0 up to 30 degrees, respectively. Although measured at different angles, these signals have similar profile, while changes also exist, such as the amplitude of the initial pulse decreases with the increase of the angle. ...........................................................................................................96

Figure 9.3. Gray lines are experimental power transmission spectra for waves detected at different incident angles, computed using the Fourier transforms of the time-domain electric waveforms with the air signal as a reference. They are offset for clarity. The black dashed line shows new guided resonance modes emerge with the change of the incident angle. .............................................................................................................97

Figure 9.4. Phase spectra of the photonic crystal slab, subtracted by that of the air reference for four representative incident angle $\theta=5, 10, 20$ and 30 degrees, from top to bottom, respectively. These curves are offset for clarity. They are almost the same, indicating there are almost same dispersive effects, guided resonance modes and group delay anomalies no matter what is the incident angle. .................................................98

Figure 9.5. Phase spectra of the photonic crystal slab, subtracted by that of the air reference signal for different incident angles. An extra guided resonance modes is highlighted in the gray circle. This result echoes what we obtained in the transmission spectra. ..................................................................................................................99
Figure 9.6. Schematic of the two-slab structure experiment. The black arrows denote the direction of the incident waves. The transmission spectra depend significantly on the separation t and the lateral shift s between the two slabs.

Figure 9.7. Transmission spectra through a two-slab structure, with the spacing of 390 and 610 microns, respectively. Solid lines are experimental results, which agree well with the FEM simulation results shown in gray dashed lines.

Figure 9.8. Phase spectra of photonic crystal slabs, subtracted by that of the air reference signal. The gray circles are from a single slab, and multiplied by two. The black squares are from a two-slab structure with the spacing t=0 microns. The triangles are for two-slab structure whose spacing t is 80 microns. These curves are offset for clarity. There are only minor differences between those curves, as indicated by the inset which is the difference between the top two curves.

Figure 9.9. Phase spectra of two-slab structures with spacing t=80 microns, subtracted by that of the air reference signal. From top to bottom, the black circles, the gray square, the black diamonds, and the gray triangles correspond to lateral shift of 0, 80, 160, and 305 microns, respectively. These curves are offset for clarity. These curves are more or less the same, and all have dispersive effects, guided resonance modes and group delay anomaly from low to high frequencies.

Figure 10.1. Schematics of two-dimensional photonic devices made from photonic crystals. (a): a waveguide bend. (b): a waveguide splitter. (c) a channel add-drop filter. (d) a waveguide branch. Here those circles can be considered as the air holes etched in a
solid slab, or as solid rods standing in air, even more generally, as one material standing in another material of different dielectric function. .................................................107

Figure 10.2. (a) Band structure of our photonic crystals with infinite thickness. The horizontal axes are in-plane wave vectors. A band gap can be clearly seen from the surface. (b) Equi-Frequency contour. The red dotted line is the projection of the mode that has its frequency of 0.67 c/a onto the bottom plane, and the solid line is the projection of the mode which has its frequency of 0.06 c/a. The solid line is a circle, which is symmetric, while the red dotted line is highly asymmetric. This asymmetry is where the superprism comes from. .................................................................109
Chapter 1

Introduction

1.1 Motivation

Terahertz waves are electromagnetic radiations at frequencies between 0.1 to 10 THz [5]. This is the spectrum region where electronics meets optics -- below the gap, electronics is the dominant paradigm for technology and scientific instrumentation; above the gap, the paradigm is optics. Various research opportunities exist at this frequency range. For example, in semiconductors, electronic excitations in quantum systems confined to one and two dimensions have excitations in the THz regime; in Physics, rotational excitations in molecules, Rydberg transitions in all Coulomb bound systems, and excitons in solids exist at the terahertz spectrum; in Chemistry and Biology, gas phase spectra and dynamics, membranes, and self-assembled monolayers are all amenable to THz studies. These have made the spectrum a scientific frontier and it holds great application potentials. Various applications of terahertz waves have been proposed, such as imaging, sensing and spectroscopy [5]. To fully appreciate the potential of the waves, optical components and techniques that can manipulate those waves are highly desired. There are many ways to make optical components, depending on specific function requirements. In this thesis I will present our work on terahertz photonic crystals. This, on one hand, provides functional photonic devices to manipulate terahertz waves; and, on the other hand, terahertz waves are used as a valuable tool to characterize photonic crystals.
Photonic crystals are materials with periodic dielectric functions [6, 7]. They are widely studied for various applications, such as waveguides [8], sensors [9], negative refraction [10-12] to make superlenses, and quantum information processing [13-16]. Despite many impressive theoretical and experimental results, however, some fundamental issues still exist. For example, there are usually more or less unintended defects or disorder in many of studied samples. The existence of these defects introduces complexity into samples and they induce complicated effects, which makes the explanation of experimental results difficult. Studies of photonic crystals that are free of defects are therefore necessary. Also, most experimental studies use narrow-banded sources and only integrated intensities of waves are detected, which does not provide any information of dynamics of how phase and electric field evolve with time.

Here we design photonic crystals at the scale of micrometers, which can be fabricated with virtually no defects. The photonic crystals are then studied with terahertz time domain spectroscopy, a technique which can be used to generate and detect electromagnetic waves of frequencies from 0.1 to 2 terahertz. The technique directly yields time resolved electric fields, which makes the dynamics information readily available. By Fourier transforming measured electric fields, one can get spectral information easily. Since Maxwell’s equations are scale invariant, our results can be related directly to any other frequencies.

1.2 Overview

In this thesis, I present our study of photonic crystals using terahertz waves. We studied the in-plane and out-of-plane properties of photonic crystals. In the in-plane
measurement, we observed band gaps and defects modes in both transmission curves and phase spectra, which are in excellent agreement with theory. For out of plane measurements, we observe very strong dispersion at low frequencies part, guided resonance modes at middle frequencies, and zero group velocity delay at high frequencies. We employed Finite Element Method and Finite Difference Time Domain methods to simulate the photonic crystals, and excellent agreement is achieved. The whole thesis is organized as follows.

Chapter 2 introduces background information of photonic crystals. A brief history of photonic crystals is given first, followed by introduction of interesting properties of photonic crystals, such as band gaps, defect modes, superprism effects, negative refraction, and quantum information processing using photonic crystals. To verify experimental results, one needs to solve Maxwell’s equations numerically. The computational methods we use include Finite Element Method, Finite-Difference Time-Domain method and Plane-Wave Expansion method. The last part of the chapter introduces all those methods.

Chapter 3 describes the experimental technique we use to generate and detect terahertz waves throughout our study, that is, Terahertz Time-Domain Spectroscopy (THz-TDS). There are several ways to generate and detect terahertz pulses, and the focus of this thesis is on the photoconductive switching method. Terahertz Time Domain Spectroscopy has many advantages, such as high temporal resolution and the ability of providing the electric field of the terahertz pulses, as well as polarization sensitive measurement. Applications of the technique will be described, together with the development of waveguides to manipulate terahertz waves.
In chapter 4, results on in-plane propagation in two-dimensional photonic crystals are presented. Power transmission reveals the existence of photonic band gaps, which agree well with theoretical calculation results. Results for photonic crystals with different lengths in the propagation direction are compared. From the measured electric fields, we directly extract the phase spectra and the group velocity, which are in good match with theoretical computations. These results confirm that our device is an excellent band pass filter.

The above photonic crystals are defect-free. We have also introduced defects into the otherwise perfect crystals by adding artificial defects. Chapter 5 describes such effort, and we observe defect modes in the photonic band gap, in both power transmission spectra and phase spectra. We have also measured the reflection spectra of photonic crystals, and it shows the photonic crystals are very good frequency selective filters.

In previous chapters we investigate the in-plane properties of our photonic crystals. Beginning from Chapter 6, we start to study their out-of-plane properties. Chapter 6 describes the study of in-plane and out-of-plane dispersion properties. Excellent agreement is achieved between experimental results and theoretical calculations. The effective in-plane refractive index is the volume-weighted average refractive index, while the out-of-plane dispersion is significant and exhibits a complicated spectral dependence, which is explained by Finite Element Method simulations.

At high frequency region of our spectrum, we observe a broadband group delay anomaly for out-of-plane propagation of terahertz waves. We obtain that by measuring the complex transmission coefficients. The group delay is equal to that of empty space
despite the fact that the volume-weighted average dielectric of the slab is not even close
to 1. Our results are consistent with finite-difference time-domain simulations. All these
are detailed in Chapter 7.

In Chapter 6 and 7 we discussed the out-of-plane dispersion at low and high
frequencies. The middle-frequencies part between the two is also interesting. In Chapter
8 we describe what we observed at the middle frequency range, that is, guided resonance
modes. In the time domain, we observed the two stages of guided resonance modes: an
initial transmission pulse and a long decaying tail. In the frequency domain, signatures of
guided resonances are observed to be superimposed on a large dispersive effect. Those
results are in good agreement with Finite Element Method simulation.

Summarizing the Chapter 6, 7 and 8, we observed significant dispersive effects at
low frequencies, guided resonance modes at middle frequencies, and group delay
anomalies at high frequencies. In all those cases, terahertz waves are illuminated onto the
photonic crystal slabs in the direction perpendicular to the slab and there is only one
single slab. In Chapter 9 we investigate the case where the terahertz waves are incident
onto the slab at an angle with respect to the slab. We find there are similar effects at
different frequency range. By putting two photonic crystal slabs next to each other, we
have made a displacement sensitive structure, and those three effects are also present in a
two-slab structure.
Chapter 2

Background Information of Photonic crystals

What are photonic crystals? What are their properties? Why are they interesting? In this chapter, I will answer those questions. I will first introduce the concept of photonic crystals, and then discuss some of their interesting properties and applications. To reveal properties of photonic crystals, one needs to solve Maxwell’s equations with proper boundary conditions. As photonic crystals are complex structures, analytical solutions generally do not exist and one has to rely on numerical solutions. In this chapter, I will introduce three most widely used simulation methods for photonic crystals. They are Finite Element Method, Finite-Difference Time-Domain method and plane-wave expansion method (MIT MPB package). All those methods are widely used in my study.

2.1 Brief History of Photonic Crystals

Semiconductor crystals provide a periodic potential for electrons in the materials. Those periodic potentials induce energy bands which electrons have to fall into when traveling in the materials. Between those energy bands are gaps, where the propagation of electrons are prohibited. By introducing impurities in the materials, one can gain control over the properties of those bands and band gaps, which thus enable the invention of transistors which revolutionizes our lives.

Inspired by what happened in the field of electronics, people begin to look for “photonic semiconductor crystals” (thereafter we call them photonic crystals), which
should have a periodic potential for photons in the materials and therefore induce photonic bands and more importantly, band gaps, in which electromagnetic waves cannot propagate in any direction. A good example of a photonic crystal is the naturally occurring gemstone opal, whose opalescence comes from Bragg diffraction of light on the crystal's lattice planes. Many biological objects also have photonic-crystal-like structures, from butterfly wings, to crabs, and to fossil animals of billions of years old [17]. However, to have the control over the properties of those bands and band gaps, one has to build artificial crystals. The search for artificial photonic crystals began in the middle of 1980's, when Yablonovitch [6] and John [7] first proposed the concept of photonic crystals. In 1989, through trial and error, Yablonovitch et al. identified the first structure which has a photonic band gap. This structure consists of a periodic array of spherical holes arranged in a face-centered-cubic lattice. This finding spurred further development of the field.

Motivated by the experimental findings, and also to avoid the blindness in searching by experimentalists, theorists began to step into the field. The calculation methods become more and more complex, and employ more and more computation power. Initial work employed "scalar wave approximation", in which the two polarizations of electromagnetic waves were assumed to be independent [18, 19]. This dramatically simplifies the problem into two scalar wave equations. However, although the computation results match with experimental ones sometimes, most of time they do not. This suggests one can not decouple the two polarizations of EM waves, and a more advanced method has to be developed. The vector wave solution of Maxwell's equations
are then developed, which employ plane wave expansion of electromagnetic waves [2, 20-22].

Once the existence of photonic band gaps is verified for one structure, the search for more structures began. One dimensional photonic crystal, which is most widely known as Bragg reflector or dielectric mirror, was already in wide use such as in distributed feedback lasers. Two dimensional crystals, either in the form of high-refractive-index rods standing in low-index materials, or in the form of low-index rods standing in high-index materials, are studied with a variety of different parameters. The rods were circular, square, or rectangle; the rods formed different lattice structure, such as square lattice, rectangle lattice or hexagonal lattice; and different filling ratios of rods were studied [8]. One of the most widely studied two-dimensional photonic crystals is called photonic crystal slab, which consists of periodic air holes in a solid slab of finite thickness [23-26]. This structure is of particular interests due to its compatibility with planar photonic devices, and also its ease of fabrication, as it can be fabricated with high precision using standard semiconductor fabrication facility. Light is confined in the slab plane by photonic crystal band gaps. The confinement of EM waves by two-dimensional photonic crystals is, however, not complete, as in the third direction the wave is confined only through total reflection [27, 28]. A three-dimensional structure offers the complete confinement ability. However, fabricating a three-dimensional structure has been challenging. A variety of ways have been tried, such as colloidal self-assembly method (an excellent review in this field can be found in [29]), and wood-piling small rods [30-33]. Those methods are still far from ideal, such as there are many defects in self-assembled structure, and constructing structures with wood-pile method is not efficient.
The search of better fabrication method for three-dimensional method is still under development.

Photonic crystals were first proposed to inhibit the spontaneous emission in a material. This phenomenon was directly observed a few years ago. But other than that, much more properties have been found and applications have been proposed, for example, waveguides, filters, superprisms, and negative index of refraction. Here I am going to introduce some of those interesting properties and applications.

2.2 Photonic Band Gaps and Defect Modes

One of the standard ways to describe photonic crystals is via its band structure: between bands are band gaps, in which waves of certain frequencies are forbidden to propagate along certain directions. If waves cannot propagate along all directions, the band gap is called a complete band gap. A complete band gap requires three dimensional photonic crystals, which consists of two materials with different refractive index distributed periodically along three directions, as shown in figure 2.1. Also shown in figure 2.1 are one dimensional and two dimensional photonic crystals.

Figure 2.1. Typical one, two and three dimensional photonic crystals. In a 1-D photonic crystal, two materials with different refractive index are arranged periodically along one direction. In a 2-D photonic crystal, they are arranged periodically along two directions, and along three directions in a 3-D photonic crystal.
When waves are incident into photonic crystals, there are transmitted waves and multiply reflected waves inside the crystals. Those waves can interfere coherently with each other. The result is that certain waves with right frequencies are not allowed to propagate through the crystals, instead they are all reflected. This is the origin of the band gap. This band gap itself is already interesting enough, as it is a filter through which waves with frequencies in the bands will pass and those in the gaps will be blocked.

As in the case of semiconductors, more interesting things happen when new modes are introduced into the band gaps. In both cases, the way to introduce new modes is to break the periodicity of the periodic potential. Similar to adding other materials into semiconductors as donors or acceptors, one introduces other materials to an otherwise perfect photonic crystal to break the periodicity. This perturbs the periodic potential locally around the defects and changes the properties of the structures, making unsupported modes in a perfect photonic crystal supported or partially supported. A point defect, for example, would behave as a microcavity, which can have very high Quality factor (Q is equal to the ratio of the center frequency to the bandwidth) [34].

If the defect is a line, then it is a perfect waveguide for waves whose frequencies are in the band gaps, as those waves have nowhere else to go but along the line [35, 36]. This kind of waveguide has very small loss and very small scale – only at the scale of wavelength. It can be used to solve the long-standing challenge facing the optical fiber, where the loss is too large as the light transmits through a sharp bend. By playing with the shape of defects, many more devices can be made for communication applications, such as a waveguide bend [37], a T waveguide branch [38], and channel add/drop filter [39] and so on [8].
2.3 Superprism Effect of Photonic Crystals

A structure with a complete band gap, however, turned out to be quite hard to fabricate. Many methods have been tried, such as wood-pile method, colloidal method, semiconductor method and so on. Still, there is a long way to go to achieve a method that can fabricate photonic crystals with high accurate positions and high efficiency. This severely limits the applications of photonic crystals.

But, many other properties have also been discovered in photonic crystals, which do not need a complete band gap and can still be used to manipulate the flow of light. For example, some bands of photonic crystal can be quite flat, which means the group velocity of light is small and that can be used to build optical delay lines [40, 41].

One of those interesting properties is superprism effect. This effect is first observed by Kosaka et al, where they found the output direction of light changed dramatically when the incident angle changed slightly [42]. Later the output direction is also found very sensitive to other parameters such as wavelength [43], and polarization [44].

To understand this effect, we can refer to dispersion surfaces of photonic crystals. Dispersion surfaces are obtained by calculating the band structure in various directions within Brillouin zone. In conventional crystalline optics, the surfaces correspond to index ellipsoids, where the length from the center (Γ point) to the surface corresponds to the refractive index. On the other hand, in a photonic crystal, the surface can present kinds of shapes, as decided by pitch, lattice type, filling factor, and index contrast. To make thing simpler, one may take cross-sections of the dispersion surfaces at constant frequencies to get equi-frequency contours (EFCs). The shape of the EFC is very
important, as it determines the propagation direction of group velocity $v_g = \nabla_k \omega(k)$, which is the same as that of energy velocity in a lossless photonic crystal. If the EFC is circular, which indicates an isotropic medium, waves would keep their directions unchanged when propagating through a photonic crystal. However, if the shape is not symmetric, or is anisotropic, waves would propagate in the photonic crystal along completely different directions as those of the incident waves. This is the origin of the superprism effect. As the shapes of EFCs are different for different frequencies, the effect is highly sensitive to frequencies. Since the shapes can be highly anisotropic, the incident angle can have a huge influence on the frequencies. Also, the shapes are different for different polarization, which explains why the effect is related to the polarization.

The effect opens up new possibilities to design optical devices, by engineering the dispersion properties of photonic crystals. There is no need for complete band gaps, thus, no need for 3-D photonic crystals, which makes the fabrication much easier. A variety of devices have been proposed based on the effect, such as prisms [42, 44-46], spot-size converters [43], waveguides and spatial beam routers [47-50]. Those devices hold the promise for better control of waves, and smaller sizes at the same time.

2.4 Negative Refraction of Photonic Crystals

Another interesting property of photonic crystal is negative refraction. Refraction is one of the most basic electromagnetic phenomena. When waves are incident onto an interface between two different materials, the direction of the output waves and that of input waves is connected by well-known Snell’s law, which is related to the indices of
refraction of the two materials. The refractive index $n$ is defined to be $n^2=\mu \varepsilon$, where $\varepsilon$ and $\mu$ are the permittivity and permeability, respectively. For most frequencies, naturally existing materials almost all have positive $\mu$ and $\varepsilon$, thus the refractive index is positive. However, at high frequencies such as optical ones, $\varepsilon$ of metal can be negative, and at low frequencies such as microwaves and THz waves, $\mu$ of ferromagnetic systems could be negative [51].

In 1968, Veselago first discussed the consequences when both $\varepsilon$ and $\mu$ are negative [52]. He concluded that no fundamental physical laws would be violated for such cases, as $\varepsilon$ and $\mu$ always appear as a product in Maxwell’s equations; therefore it would not matter whether they are both negative or are both positive. The difference for the two situations, however, is that the refractive index $n$ will be negative when both $\varepsilon$ and $\mu$ are negative.

As no natural materials exhibit both $\varepsilon$ and $\mu$ at the same time for a frequency band, artificial materials has to be found to get those properties. These materials are called left-handed materials or metamaterials. The first metamaterial with both negative $\varepsilon$ and $\mu$ was successfully fabricated in 2001 at microwaves frequencies, which consists of a two-dimensional array of repeated unit cells of metal strips and split ring resonators [53]. However, using the same methods would be problematic for higher frequencies, as metal is lossy for those frequencies. As a result, artificial structures composed of lossless dielectrics are preferred.

Photonic crystal, which is made of periodically arranged dielectrics, is an excellent candidate to realize negative refraction. As a photonic crystal is not a homogeneous medium, it is inappropriate to define its values of $\varepsilon$ and $\mu$. However,
photonic crystals can still present negative refraction, as Bragg diffraction inside photonic crystals can result in dispersion relationships similar to those in metamaterials. That is, the frequency disperses negatively with wave vector.

Negative refraction in photonic crystals is first observed by Kosaka et al. in 1998, together with the superprism effect [42]. Since then, many new structures have been investigated [10, 11, 54-56]. New applications have also been investigated, such as superlens [57], and imaging, which can have sub-wavelength resolution [58].

2.5 Quantum Information and Photonic Crystals

As discussed earlier, by introducing defects into photonic crystals, one breaks the periodicity of refractive index distribution and makes unsupported modes now supported. This makes many interesting devices possible, such as waveguides that can guide light and bend it at sharp angles. If one constructs a defect and then introduces photo emissive materials such as III-V semiconductors into such defect, a laser can be built [13]. This kind of laser can have very narrow linewidth, because although the materials emit light in a wide spectral range, only the wavelength that matches the wavelength of the defect mode is amplified as it can propagate freely through the material. Light at other wavelengths is trapped within the photonic crystal and cannot build up.

One of the most interesting devices is probably related to quantum information processing in a cavity quantum electrodynamics (QED) system. A cavity QED system consists of a few atoms interacting strongly with photons confined in a high-quality optical cavity. In this system, the intrinsic quantum mechanical coupling dominates losses due to dissipation, which therefore provides a setting in which one can
quantitatively study the dynamics of an open quantum system under continuous observation. Furthermore, the presence of a single atom or photon is sufficient to affect the properties of the system in this strong coupling regime. Thus quantum state mapping between atomic and optical states becomes possible, which could lead to the realization of quantum information processing [14].

Almost all of the cavity QED experiments to date have used Fabry-Perot cavities, which require special efforts to stabilize. However, one can construct photonic crystal microcavities that localize photons into extremely small volumes, even smaller than a cubic optical wavelength [13]. The ability to localize light into very small volumes and with high quality factors in photonic crystal microcavities makes it possible to study cavity quantum electrodynamics (QED) phenomena in the solid state [15, 16], as well as to build novel quantum optical devices, such as efficient single- or entangled-photon sources [59, 60]. Photonic crystal cavities have several potential advantages over Fabry-Perot cavities for cavity QED study. The properties of a photonic crystal optical cavity are determined by its geometry, which can be controlled through the fabrication process. Photonic crystal microcavity can also be integrated with single atom trapping schemes using lithographically patterned magnetic microtraps [61].

2.6 Computational Methods for Photonic Crystals

2.6.1 Basic equations

The problem of waves propagating in photonic crystals is essentially an electromagnetic wave propagation problem. To get a complete solution, one needs to
solve Maxwell's equations with appropriate boundary conditions. Maxwell's equations can be written as:

\[
\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}
\]

\[
\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}
\]

\[
\nabla \cdot \vec{D} = \rho
\]

\[
\nabla \cdot \vec{B} = 0
\]

and the constitutive relations are:

\[
\vec{D} = \varepsilon_0 \vec{E} + \vec{P}
\]

\[
\vec{B} = \mu_0 (\vec{H} + \vec{M})
\]

\[
\vec{J} = \sigma \vec{E}
\]

These equations are a group of partial differential equations. Other than in a few simple cases, there is no analytical solution to those equations. Instead, one has to solve them numerically, and there are several ways to do that.

### 2.6.2 Finite Element Method (FEM)

Finite element method is a general numerical technique widely used to obtain numerical solutions to engineering and mathematical physics problems. It can be used to solve any partial differential equations. The method was first developed in 1940's by Richard Courant for use in structural analysis [62], and soon after that, it was used in a wide variety of engineering disciplines, including such as electromagnetics.

In the method, an entire continuous domain is replaced by a number of subdomains, that is, finite elements, in which the unknown function is represented by simple interpolation functions with unknown coefficients [63]. This makes the original problems with infinite number of degrees of freedom converted into a problem with a
finite number of degrees of freedom. The accuracy of the FEM method is closely related to the way of discretization. By refining the mesh, the accuracy can be improved. After the discretization, then those equations, together with applicable physical considerations, are applied to each element, and a system of simultaneous equations is constructed which minimizes the error based on variational method or weighted residual method. Finally the system of equations is solved for unknown values using the techniques of linear algebra or nonlinear numerical schemes, as appropriate.

In our modeling, we used the FEMLAB 3.1 from COMSOL, Inc [64]. It is installed in a Sun Workstation with dual AMD Opteron CPUs and 16 GB memory. The whole modeling consists of the following steps:

1. Geometry modeling
2. Physics settings to setup boundary conditions and subdomain settings
3. Mesh generation
4. Computing the solution
5. Postprocessing and visualization

2.6.3 Finite-Difference Time-Domain method (FDTD)

The FDTD technique is widely used as a propagation solution technique in photonic circuits and integrated optics. It is specially designed for electromagnetic modeling [65]. It solves Maxwell's equations by first discretizing the equations via central differences in time and space and then numerically solving these equations in software. As it solves the Maxwell's equations directly, there are no any approximations or theoretical restrictions. It is also a time-domain technique, so it can cover a wide
frequency range in a single run, instead of a monochromatic wavelength in most other cases.

In a region of space which contains no flowing currents or isolated charges, Maxwell's curl equations can be written in Cartesian coordinates as six simple scalar equations. Maxwell's equations describe a situation in which the temporal change in the H field is dependent upon the spatial variation of the E field, and vice versa. The FDTD method solves Maxwell's equations by first discretizing the equations via central differences in time and space and then numerically solving these equations in software.

The basic idea of FDTD is developed by Kane Yee back to 1966 [66], when he introduced the famous Yee cell, as shown in figure 2.2. In the cell, the vector components of the electric and magnetic fields are robustly represented and satisfy both the differential and integral forms of Maxwell's equations. The equations are then solved in a leap-frog manner; that is, all of the electric fields in the modeled space are solved at a given instant in time using magnetic fields at previous instant, then all the magnetic fields are solved using the newly obtained electric fields, and the process is repeated over and over again.

To use FDTD, we need to first establish a computational domain, then specify the materials in the domain, the source and the boundary conditions, and finally discretize the domain into many small cells. In our modeling, all those were done in a software package FullWAVE v3.0.1 from RSoft Design Group [67]. It is a commercially available package and we installed it in a Sun Workstation with dual AMD Opteron CPUs and 16 GB memory. I will discuss the procedures as follows.
Figure 2.2. A Yee cell shows the position of the electric and magnetic field vector components.

The choice of the computational domain must include the portion of the structure to be simulated. As FDTD method is computationally demanding, the larger the computation domain is, the more computation resources the simulation requires. It is then necessary to choose a right domain, so that it has the minimum size but in the mean time fully describes the structure.

To perform a simulation, one needs to specify the refractive index distribution n(r) as a function of space. FullWAVE utilizes the following formula to specify the material properties [68]:

\[
D = \varepsilon_0 \varepsilon_r E + \varepsilon_r (\omega) \cdot \varepsilon_0 E + 2\varepsilon_0 n n_2 \frac{I}{I_{sat}} \frac{E}{1 + \frac{I}{I_{sat}}}
\]

where the first term takes into account the linear index, the second term is related to the material dispersion, and the third term is the nonlinear term which is a function of the intensity in the structure. In our photonic crystals, we only need to consider the first term,
as the index in interested frequencies is frequency-independent and the field in the crystals is not strong enough to excite nonlinear effects.

To get the electric field as a function of space and time from a FullWAVE simulation, one also needs to configure the electromagnetic field excitation. That is, an initial launch condition $\Phi_L$ at time $t=0$ is needed, as well as a driving function in time. The excitation consists of both a spatial and temporal component, such as

$$\Phi(r, t) = f(r)g(t)$$

where $f(r)$ is the spatial excitation at the launch plane and $g(t)$ is the temporal excitation.

The boundary conditions at the spatial edges of the computational domain must be carefully considered. Many simulations employ an absorbing boundary condition that eliminates any outward propagating energy that impinges on the domain boundaries. One of the most effective is the perfectly matched layer (PML), in which both electric and magnetic conductivities are introduced in such a way that the wave impedance remains constant, absorbing the energy without inducing reflections. However, as we are dealing with periodic structures, we can set up periodic boundary conditions (PBC). In this case, the boundary condition is chosen such that the simulation is equivalent to an infinite structure composed of the basic computational domain repeated endlessly in all dimensions.

To discretize the computation domain into many small cells, care must be taken to specify the spatial grid sizes $\Delta x$, $\Delta y$, and $\Delta z$. On one side, the spatial grid must be small enough to resolve the smallest feature of the field to be simulated. Usually this is dictated by the wavelength in the material(s) to be simulated, but, in some cases, can be dictated by the geometry of the photonic device. Typically, the grid spacing must be able
to resolve the wavelength in time, and therefore usually be less than $\lambda/10$, where $\lambda$ is not the free space wavelength, but the wavelength in the material(s). On the other side, the spatial grid should be as large as possible, as the computation demands a lot of time and resources. Therefore, the grid sizes should be chosen in order to produce an accurate and efficient simulation.

Care must also be taken to configure temporal grid, as the FDTD algorithm is based in the time domain. The work is simplified as the temporal grid is related to spatial grid by the Courant condition [68]:

$$c\Delta t < \frac{1}{\sqrt{\left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)}}$$

where $c$ is the velocity of light. One can therefore choose the maximum $\Delta t$ allowed by the condition.

2.6.4 Plane-Wave Expansion Method

If there are no free charges or currents, that is, there are no sources of light, then $\rho=J=0$, and Maxwell’s equations would be

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \cdot \vec{D} = 0$$

$$\nabla \cdot \vec{B} = 0$$

Starting from these equations, we can make some assumptions. First, the field is weak, so that we are in the linear regime. Second, the refractive index of materials is
frequency independent. Third, the materials do not absorb much energy, that is, $\epsilon(\vec{r})$ is real. With those assumptions, after a series of deductions, the following equations govern the electromagnetic waves of a single frequency $\omega$ [8]:

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

$$
\nabla \cdot \vec{H}(\vec{r}) = 0
$$

The first equation is the master equation. Our goal is to solve this equation. Once we solve the master equation, we can have the magnetic field. We can then recover the electric field from the magnetic field.

To solve the equation, we can use plane-wave expansion method. In the method, $H(\vec{r})$ and $\epsilon(\vec{r})$ are expanded into a set of plane waves. As $\epsilon(\vec{r})$ is periodic, $H(\vec{r})$ should share the periodicity of $\epsilon(\vec{r})$. This amounts to that only plane waves whose wave vectors are reciprocal lattice vectors should be considered. Through this operation, the master equation is converted into a group of linear equations that can be readily solved in a computer.

In the plane-wave method, only linear equations are solved, therefore the computation time is minimized. There are two major places where errors could be introduced into the computation: the first happens when expanding $H(\vec{r})$ and $\epsilon(\vec{r})$. To get accurate solutions, significant numbers (which typically larger than 300) of plane waves must be included during the expansion process. The second place is regarding to meshing of the dielectric function $\epsilon(\vec{r})$. As $\epsilon(\vec{r})$ is not continuous but piecewise, it introduces significant convergence difficulties. One has to use appropriate interpolation schemes and more meshing elements to minimize this error.
The codes we use for this plane-wave expansion method are called MPB (MIT Photonic-Bands). MPB is developed by Steven G. Johnson and John D. Joannopoulos at Massachusetts Institute of Technology [2]. Detailed information can be found at website: http://ab-initio.mit.edu/mpb/
Chapter 3

Terahertz Waves

This chapter describes terahertz waves and the equipment used to generate and detect them -- Terahertz Time-Domain Spectrometer (THz-TDS). THz-TDS yields broadband single-cycle pulses whose frequencies are in the terahertz region, and it detects the time-resolved electric field $E(t)$ directly instead of the intensity $I(t)$, therefore fully characterize the terahertz waves. Some applications of terahertz waves will also be introduced in this chapter. Finally, the development of waveguides to manipulate terahertz waves will be discussed.

3.1 Terahertz waves

What are terahertz waves and why it is interesting?

Terahertz waves are electromagnetic waves whose frequencies locate between microwaves and infrared light. This frequency range has traditionally been hard to access due to the difficulty in generating and detecting it efficiently. For this reason, it remains largely unexplored and is called the final frontier of the electromagnetic spectrum. It is also referred to as THz gap.

This is a frequency range with rich science. Electrons in highly-excited atomic Rydberg states orbit at THz frequencies. Small molecules rotate at THz frequencies. Collisions between gas phase molecules at room temperature last about 1 picosecond. Biologically-important collective modes of proteins vibrate at THz frequencies. Frustrated rotations and collective modes cause polar liquids (such as water) to absorb at
THz frequencies. Electrons in semiconductors and their nanostructures resonate at THz frequencies. Superconducting energy gaps are found at THz frequencies. An electron in Intel’s THz Transistor races under the gate in ~1 picosecond. Gaseous and solid-state plasmas oscillate at THz frequencies. Matter at temperatures above 10 K emits black-body radiation at THz frequencies. The opportunities in the frequency are tremendous. Numerous applications have been proposed for terahertz waves, such as imaging, sensing, spectroscopy, package inspection, and so on.

Optics and electronics meet in the THz gap. This has led to unprecedented creativity in source development. Below the gap are electronic technologies. Motivated by the requirement for ever faster speed, electronic equipment is generating higher and higher frequencies. Above the gap are photonics industries, and they are trying to push down the frequencies one can generate with optical methods. Many ways have been developed to generate THz radiations, such as harmonic generation with microwaves, free electron lasers, photomixing, quantum cascade lasers, hybrid optoelectronic system with nonlinear crystals and photoconductive switching antennas.

In this chapter I will briefly introduce the method that we use throughout our experiments: the photoconductive switching method, which provides a broadband source and a coherent detection scheme and have high signal to noise ratio.

3.2 Generation of Terahertz Pulses

Photoconductive switching method is a powerful method to generate terahertz pulses. The key component in this method is the optoelectronic switch, which is usually referred to as Auston switch, as it was first demonstrated by Auston in 1984 [69].
A typical Austeron switch consists of two 5μm wide, 5μm thick gold electrodes separated by about 10μm. Those electrodes lie on a semiconductor substrate, as shown in Figure 3.1. In an emitter, the substrate is typically semi-insulating GaAs wafer. A DC bias of tens of voltages is applied across the two gold lines, which creates a strong electric field, and this field is further enhanced by the local field from deep traps present in semi-insulating wafers [70].

To generate THz waves, femtosecond laser pulses are focused into a small spot (diameter <10μm) close to the anode. Those pulses are about 100fs long, with their center frequency around 800nm and a repetition of 80 MHz. The pulses then excite photocarriers in the substrate, and under the acceleration of the strong DC field, a transient photocurrent is resulted. The current rises rapidly, and then decays with a time constant given by the lifetime of the semiconductor substrate. According to Maxwell's equations, this transient current radiates into free space, with the radiated electric field E(t)

\[ E(t) \propto \frac{\partial J(t)}{\partial t} \]

The resulted electromagnetic wave is terahertz wave. From the derivative expression, one can also see that the radiated field is dominated by the rising edge of the transient photocurrent, while the long decaying tails are mostly irrelevant to the radiated terahertz field.

The performance of the generators made this way is not optimized, however; specifically, most radiation is not directed into the forward direction and therefore is wasted. Fattinger and Grischkowsky [71] used a spherical sapphire lens on the back of the substrate to collect as much of the radiation as possible. The design and the position of the lens also affect the spatial profile of the radiation -- whether it is frequency
dependent or independent -- which has different applications such as in imaging \[72, 73\] or coupling into waveguide \[74, 75\].

![Figure 3.1](image)

\textbf{Figure 3.1} A typical Auston switch; black lines are electrodes made of gold, and the substrate is semi-insulating GaAs wafer. The two electrodes are DC biased. Ultrafast femtosecond pulses are focused onto the middle of the two gold lines to generate photocurrent, which radiates into free space and that is terahertz wave.

3.3 Detection of Terahertz Pulses

Now that we know how to generate THz pulses, the next is to detect them. There are several ways to do that. One is to use Fourier transform spectroscopy, which measures the linear autocorrelation of the beam and then calculates its Fourier transform. Greene et al. \[76\] first measured terahertz pulses with this method. The advantage of this technique is its broad frequency detection range, which responses for frequencies up to mid-infrared frequencies. However, its disadvantage is also obvious: here only the power spectrum is detected. One cannot recover spectral phase and cannot judge if there is any chirp present in the terahertz pulses. As a result, other detecting methods that can yield the electric fields directly are more widely used: one is electro-optic sampling and another is photoconductive switching method. The electro-optic sampling method uses the Pockels effect, which, in brief, is a second-order nonlinear effect. It was first utilized
to detect terahertz beams by several groups (such as [77, 78]). In our experiment, we use the photoconductive switching method.

The main advantage of the photoconductive switching method, as compared to incoherent detection methods such as by using bolometers, is that it measures directly the electric field, and therefore fully characterizes the terahertz pulse. In this method, an Auston switch is used again. But instead of being DC biased as used as the emitter, here when used as a detector, the two gold electrodes are attached to an ammeter. Although the substrate is still semiconductor, it is not semi-insulating semiconductor which has a relatively long carrier lifetime, but a low-temperature-grown GaAs or radiation-damaged Silicon, which has a short carrier lifetime and this is essential in the detection of the terahertz pulses.

When femtosecond pulses are focused onto the Auston switch, photocarriers are once again generated in the substrate of the detector. If at the same time an incident terahertz pulse reaches the detector, its electric field will drive those photocarriers and the corresponding electric field will be detected by the ammeter. To faithfully reproduce the electric field of terahertz waves, one would require the lifetime of the photocarriers much shorter than the terahertz pulse, so that the photoconductive switch acts as a sampling gate which samples the terahertz field at a shorter duration of time. This is exactly the reason why a low-temperature grown GaAs or radiation-damaged silicon is used here, as their carrier lifetimes are much shorter than the duration of terahertz pulses.

After detecting the electric field of terahertz pulses for certain time, one can vary the time delay of the femtosecond laser pulse with an optical delay line, so that the photoconductive gate will detect the electric field at another time. With this technique,
the whole terahertz pulse can be mapped out in the time domain, and this is the reason why it is called time domain spectroscopy.

3.4 Terahertz Time Domain Spectroscopy

Combining the generating and detecting techniques introduced above, one gets a complete terahertz time-domain spectroscopy system. The system in our lab is the T-Ray 2000, from Picometrix, Inc. The bottom part in Figure 3.2 is a photo of the Picometrix system we used in our experiment. It shows the fiber-coupled emitter and receiver modules, with two collimating silicon lenses standing between them. The brown box is the control center, with an optical delay line, splitter, and some electronic devices inside. The black box is the pumping Ti:Sapphire laser, which is a Vitesse Diode-Pumped Laser, from COHERENT Inc. The mode-locked power of the laser is 300 mw, and the center wavelength is 800 nm, with a bandwidth of 12.5 nm. The repetition rate of femtosecond pulses is 80 MHz, and the minimum diameter of the laser beam is 1.28 mm. The top part of the Figure 3.2 is the schematic of the complete terahertz system. Femtosecond pulse beams from the source are coupled into an optical fiber. Before the coupling, the beam passes through a pair of parallel gratings to compensate the group velocity dispersion that the beam will experience in the fiber. Then the beam will be split into two parts: one goes to the receiver, and the other goes to the optical delay line and then to the transmitter. A THz pulse is generated when a femtosecond pulse hits the transmitter. The THz pulse is collimated by parabolic mirrors, and the parallel THz beam produced is focused onto the sample of interest. Then the transmitted THz pulse is directed toward the detector.
Figure 3.2 Top: schematic of the Terahertz Time-Domain Spectroscopy. Bottom: Photograph of the T-Ray 2000, by Picometrix Inc. T-Ray 2000 is a fiber coupled system which makes the free movement of the transmitter and receiver possible.

When the THz pulse and the femtosecond pulse arrive at the detector simultaneously, a current proportional to the THz electric field will be generated and measured by the current meter, and then the information will be sent to a computer to be saved for further processing. The computer-controlled optical delay line is continuously sweeping to move the femtosecond laser pulse from the beginning to the end of the terahertz pulse to measure the temporal distribution of the terahertz electric field. The lenses used in the setup are either made of Silicon or Teflon, both of which have low absorption for THz radiations. To get a higher signal to noise ratio, a Princeton Applied
Research lock-in amplifier (Model 124) is used in the measurement. The chopper for the lock-in method is model SR 540 from Stanford Research Systems, INC.

Figure 3.2 shows the setup for a transmission experiment. We can also do reflection experiments by changing the setup so that the terahertz pulses reflected from the sample are collected and detected by the receiver.

3.5 Applications of Terahertz Pulses

Figure 3.3 shows a typical terahertz pulse. It is a single cycle pulse which lasts about 1 picosecond. The detected electric field gives not only the intensity information, but also the phase information. The inset shows its frequency components, which are from 0.1 up to 2 terahertz, a very broad bandwidth.

![Graphs of E(t), |E(\omega)|, and (\omega/\hbar)](image)

**Figure 3.3** (a) A typical single-cycle terahertz pulse in time domain. (b) The amplitude spectrum of the pulse by Fourier transforming the detected time-domain waveforms. (c) The phase spectrum of the pulse, obtained by Fourier transform the time waveforms.

Since a terahertz pulse is quite short, it has all the applications of short pulses, such as exploring very fast phenomena. Its unique characteristics such as its phase information, broad bandwidth of ~1 THz, and high temporal resolution of sub-picosecond make it possible to be widely used in imaging, spectroscopy, tomography, package
inspection control and online process monitoring [5, 72, 79] and parameterizing materials [80]. Among them, imaging is currently a topic under intensive research and is called “T-Ray imaging”, by analogy to the name X-Ray imaging. Because the frequency components of the terahertz pulses are located in the far-infrared, where rotational energy levels of many polar molecules are also located, the terahertz pulses can also be used to detect and identify gases by their unique absorption fingerprint [81]. This can serve as a complementary tool to the well established mid-IR techniques, and can expand the number of gas species that can be detected.

The ability to determine phase information is one of the unique properties of THz-TDS. As we know, most detectors, such as CCD cameras and photon counters, can only provide intensity information. This phase information can allow us to have more freedom when considering its applications. For example, when constructing an image, we can use the intensity information, or we can use phase information. In certain situations, the phase image will give information that the intensity image cannot provide, or cannot provide very well. For instance, if objects to be imaged are transparent, it will provide no contrast with their environment, hence the intensity of the incident wave will not change much, but the phase of the incident wave will be altered because the optical thickness of such objects varies from points to points as either the actual thickness or refractive index or both vary. In those situations it will be desirable to see “phase” objects.

Excellent reviews about terahertz imaging can be found in [5, 73], in which the authors discuss not only transmission imaging and reflection imaging, but also near-field imaging and tomography. Not only is the intensity used to construct images, but also the
phase information. Using T-Ray for medical imaging, which might play an important role in future medical diagnosis, is also introduced in [73]. There are several advantages for terahertz pulses to be used in biological imaging. First, their energy is low, therefore they cause less damage to tissues, comparing with X-rays, for example. Second, their wavelength is long, which means they will be scattered less than visible or infrared radiation and can penetrate into the skin deeper. This is an advantage comparing with other higher-frequency light source. Third, the spectroscopic ability of terahertz imaging allows chemical-specific imaging/fingerprinting, which is a superior property comparing with ultrasound and X-Ray imaging. Of course, THz pulse has its own disadvantages for biological imaging. One of the main limiting factors is the absorption of THz waves by liquid water.

There are also some disadvantages for terahertz pulses imaging, for example, at this moment its acquisition time is long; the system is expensive and bulky, which limits its use in industry. Nevertheless, with the development of technologies, those issues could be solved. For example, the bulky issue could be solved, by replacing Ti:Sapphire laser with ultrafast fiber lasers, which have much smaller sizes.

3.6 Waveguiding Terahertz Waves

To develop potential applications of terahertz waves, one prerequisite is the ability to manipulate the waves. If they can only propagate efficiently in free space, their applications will be significantly limited. As terahertz pulses are transform-limited broadband pulses, finding a way to manipulate them is not easy, since dispersion is a serious issue for broadband pulses. Various waveguides have been developed, such as
metal wires, which provide a low-loss and low-dispersion guide of the waves [82, 83]. Another low-dispersion waveguide consists of two metal plates which are separated by a few tens or hundreds of micrometers [75]. TM waves can propagate with very small loss between the two plates. By changing the spacing or the material between the two plates, one can control what modes to excite and operate in a single-mode region.

These two waveguides allow the development of new modalities for spectroscopy and applications. For example, one can put materials to be characterized on the surface of metal wires, and then detect the transmitted terahertz waves. One of the issues associated with the metal wire waveguide is that the efficiency of coupling free-space terahertz waves to the surface of metal wire is low, as the free-space waves is linearly polarized, while that on the metal wire is radially polarized [82]. New sources of transmitter are being developed, which would promise better coupling efficiency [84, 85].

Recently, direct guided wave generation of terahertz pulses in parallel plate waveguide has been demonstrated [86, 87]. This development significantly minimizes the loss in coupling free space terahertz pulses into the waveguide, and therefore accelerates further development of the field. One can put samples to be characterized into the waveguide to do the spectroscopy. This provides an excellent way to characterize those samples that are not suitable for traditional free-space THz-TDS. For example, spectroscopy of water layers of nanometer size have been demonstrated [88]. It could potentially be extended to any thin samples, such as thin films, proteins, and DNA and so on. However, to develop this subject further, and also to develop integrated terahertz optoelectronics, optical components are needed to manipulate terahertz waves
inside the waveguide. At present mirrors are realized inside the waveguide [89]. But more components such as filters are needed.

There are many ways to construct optical components. Given their versatility and small sizes, photonic crystals are good candidates to start with to build a variety of components. Part of this thesis reflects our efforts in realizing this, and we have realized successfully band pass filters, and selective-reflection filters. I will introduce these work in the following chapters.
Chapter 4

In-Plane Properties of Two-Dimensional Photonic Crystals

Previous chapters introduce the photonic crystals and terahertz waves. Here we investigate in-plane properties of two-dimensional photonic crystals with terahertz waves. We observe that the temporal response of the photonic crystal slabs is significantly dispersed, indicative of strong dispersion near the edges of the photonic band gap. In the frequency domain, we observe several gaps whose sizes compare well with those from transfer matrix calculations. The group velocity dispersion is characterized using a short-time Fourier transform analysis, and the results are consistent with the predictions from the photonic band structure calculation.

Part of this chapter is published in [90].

4.1 Introduction

Much interest in terahertz (THz) radiation has been inspired recently by demonstrations of a variety of possible applications [5]. In particular, THz techniques offer the possibility for extremely broadband and secure communications channels. For these and other uses, new methods for manipulation of terahertz signals are required. One promising candidate is photonic crystals. Photonic crystals are materials that exhibit periodicity in the dielectric function in one or more dimensions [6, 7]. Because of the spatial periodicity, the dispersion relation for electromagnetic radiation, \( \omega = ck/\sqrt{\varepsilon} \), is modified. Certain frequencies of light may be forbidden to propagate in certain
directions, leading to a gap in the photon density of states. By selectively disrupting the
dielectric periodicity, one can introduce propagating modes into these gaps. This effect
can be exploited for switching, adding or dropping wavelength channels, or multiplexing
operations. Such localized modes can also be the basis for wavelength-scale cavities and
novel compact waveguide structures [8].

Although the majority of work on photonic crystals has been directed towards
their eventual use at telecommunications wavelengths, there have been several examples
of terahertz photonic crystals. Initially, these studies were motivated by the desire to
understand the optics of periodic media. Larger structures, designed for longer
wavelengths, can act as useful models of the behavior to be expected when the equivalent
design is fabricated for shorter wavelengths. Both two-dimensional [3, 4] and three-
dimensional [32, 33, 91-95] photonic crystals have been described. Recently, the value
of optical components specifically for THz applications has become a more compelling
factor, leading to an increasing interest in the THz properties of periodic systems [96-
105].

In this work, we focus our interests on two-dimensional photonic crystals, of the
type most commonly envisioned for optical telecommunications applications. The
specific design consists of a hexagonal lattice of air holes in a dielectric slab. In this
photonic crystal, propagating waves are confined in two dimensions by the periodic
modulation of the dielectric, and in the third by conventional waveguiding. The use of
this geometry is motivated by several factors. First, it is among the most thoroughly
studied photonic crystal systems [27]. We can take inspiration from these earlier works
for the design of specific waveguide or resonator structures. Second, this planar design
permits us to exploit recent advances in terahertz quasi-optic waveguide development. In a series of recent experiments, Grischkowsky and co-workers have demonstrated low-loss, low-dispersion guiding of single-cycle terahertz pulses in parallel plate metal waveguides [75, 89, 106]. By sandwiching a patterned dielectric slab between two parallel metal plates, we can achieve guiding in a system for which the only significant attenuation and dispersion arise from the photonic band structure. This unique configuration permits the direct study of the transmissive and dispersive properties of photonic crystal structures, without the need to correct for the loss or dispersion associated with the planar waveguide.

Here, we describe the characterization of a two-dimensional photonic crystal using terahertz time-domain spectroscopy (THz-TDS) [107, 108]. Comparing with other techniques, THz-TDS has its own advantages, especially in the characterization of dispersion properties. To date most of those investigations use interferometric techniques [109-112], which compare the pulse transmitted through a photonic crystal and a reference pulse. These methods could be challenging if the transmitted pulse is substantially reshaped, due to the nature of the correlation method. However, in a terahertz time domain spectroscopy system, one measures E(t) with a temporal resolution which is less than one cycle of the optical field. As a result, pulse reshaping and chirp can be characterized with very high accuracy. Using THz-TDS, we have directly measure both the amplitude and phase of the transmitted radiation, along two different high symmetry axes of the crystal. These results are compared to simulations based on a transfer matrix method [113, 114]. By displaying the results on a time-frequency plot,
we can directly visualize the dispersive characteristics near the edges of photonic band gaps.

4.2 Experimental Setup

A schematic of the experimental setup is shown in figure 4.1. Broadband single-cycle terahertz pulses are generated and detected using ultrafast photoconductive antennas. The terahertz radiation is first collimated and then focused into the waveguide by a plano-cylindrical lens. An identical setup is used at the output facet to collect the transmitted radiation. The waveguide consists of two parallel copper plates, which provide a nearly perfect metallic boundary for the guided wave. When the electric field of the input pulse is linearly polarized in the direction perpendicular to the plane of the plates, only the TM modes are excited inside the waveguide. The spacing between the waveguide plates is kept fixed at 305 μm.

![Figure 4.1 A schematic of the optics used to couple the THz radiation into and out of the parallel plate metal waveguide, into which the photonic crystal can be inserted. The polarization of the THz beam is perpendicular to the plane of the slabs, so only TM modes are excited.](image)

4.3 Photonic Crystal Samples

A schematic of the photonic crystal is shown in the top of figure 4.2, and only half of the area of the wafer is etched, so that the un-etched portion can be used as a reference. Shown in the bottom is a top-down photograph of our photonic crystal slab. It consist of
a hexagonal array of circular holes etched all the way through a 305 μm thick high-resistivity silicon wafer, using deep reactive-ion-etching (RIE) [103].

![Photonic crystal slab](image)

**Figure 4.2** Top: A schematic of the photonic crystal slab, consisting of an array of holes etched through a 305 micron-thick silicon wafer. Only half of the area of the wafer is etched, so that the un-etched portion can be used as a reference. Bottom: a top-down image of a portion of one sample fabricated using deep reactive ion etching. The diameter of the air holes is 360 microns and they form a hexagonal lattice, with a pitch of 400 microns. The thickness of the slab is 305 microns.

The holes have vertical side walls with diameters of 360 μm, and the lattice has a pitch of 400 μm. High-resistivity (greater than $10^4$ Ω-cm) silicon is chosen because the absorption is low enough to be negligible, and its refractive index is essentially dispersionless ($n = 3.418$) over the entire bandwidth of the THz pulses [115]. This index contrast (silicon vs. air) is large enough to open a sizeable complete band gap for both TE and TM polarizations. In the long wavelength limit, the photonic crystal behaves like a
homogeneous dielectric with a refractive index of 1.96, the volume-weighted average. We have prepared one sample with 4 unit cells for propagation along Γ-K direction, and along Γ-M direction, we have three samples, which have 5, 10 and 20 unit cells, respectively. Each sample has been etched over only half of the area of the wafer. We may use either the un-etched portions or simply an air-filled waveguide as a reference for our transmission measurements.

4.4 Transmission Results and Discussion

4.4.1 Band Structures

Using an available software package based on the plane-wave expansion method, we calculate the band structures for TM modes of our photonic crystal, assuming the thickness of the photonic crystal slab to be infinite [2, 27]. We note that the finite thickness of the slab leads to systematic shifts between the calculation and the experiment, as detailed further below. The calculated band structures are shown in the left side of figure 4.3. A complete gap is predicted between 0.30 and 0.33 THz. At the right side we show the calculated vertical (parallel to the center axis of air holes) component of the electric field, for the lowest five bands between the Γ and K points. Since the input fields are TM polarized, the vertical component is the only non-zero part of the electric field. As can be seen, the fields of bands 1, 3 and 5 are symmetric with respect to the Γ–K direction (denoted by the black lines), while those of bands 2 and 4 are anti-symmetric. Since the input waves are symmetric, these anti-symmetric bands cannot be efficiently excited by the input field. Thus, although the complete band gap covers only a small region of frequency, we expect much larger regions of low transmission due to uncoupled
modes [3, 4]. In the band structure diagram, the uncoupled modes are shown as dashed lines, indicating the larger regions of low transmission. For example, the apparent gap along the Γ–K direction extends from 0.22 to 0.33 THz, although only the high frequency portion of this region corresponds to the complete gap. A similar analysis for the Γ-M direction indicates that band 3 is an anti-symmetric (uncoupled) band in that direction.

![Band structure diagram](image)

**Figure 4.3** Left: Band structure for TM modes of the photonic crystal, with infinite thickness in the direction parallel to the axes of the air holes. This is computed using a plane wave expansion method [1, 2]. A complete band gap is denoted by the gray region. Dotted lines represent bands whose fields are anti-symmetric, and which therefore cannot be efficiently excited by the symmetric input field [3, 4]. The inset shows the two-dimensional Brillouin zone, with high symmetry points labeled. Right: Vertical components of the electric fields for bands between the Γ and K points. Those of bands 1, 3, and 5 are symmetric with respect to the Γ-K direction (denoted by the black line), while those of bands 2 and 4 are anti-symmetric. The key at lower right indicates which image corresponds to each band.

### 4.4.2 Time-Domain Waveforms

Figure 4.4 shows several typical detected waveforms, measured in transmission through the waveguide. When there is no silicon wafer inside the waveguide, we detected a single-cycle terahertz pulse, consistent with the previously reported results on parallel plate metal waveguides [75, 116]. The small irregular oscillations following the
main pulse are characteristic of the system, arising from electrical and optical reflections. For different propagation lengths, the amplitude is almost the same, indicating a small propagation loss.

![Figure 4.4 Typical measured time-domain waveforms, for the situations when the metal waveguide is filled with air, silicon, and the photonic crystal slab, from top to bottom, respectively. In each case, there are three samples with different lengths along the propagation direction, and the lengths are 3.964 mm, 7.428 mm, and 14.356 mm, from top to bottom in each case, respectively. The air signals show no dispersion, and the silicon signals show a little dispersion resulting from multi-mode excitation of the waveguide. The photonic crystal signals are significantly dispersed, extending to hundreds of picoseconds. This dispersion results from the band structure of the photonic crystal, in particular near the edges of the band gap.](image)

When the unetched silicon slab is inserted into the waveguide, the pulse is no longer a single cycle. This dispersion results mainly from multimode propagation inside the waveguide. When the high index material materials is placed inside the waveguide, the cutoff wavelength for each waveguide mode shrinks by a factor of the refractive index, $n=3.42$ [117]. Figure 4.5 shows the group velocity with respect to frequency, and those modes denoted by dashed lines are of odd parity and cannot be excited to input beams. While there is only one TEM mode for air for frequency up to 1THz, there are
four modes for unetched silicon. As a result, a larger fraction of the input pulse energy (which extends beyond 1 THz) overlaps with dispersive modes and the result is a net dispersion of the terahertz pulse. With different propagation lengths, the shapes of the pulses are almost the same, except those with longer lengths are delayed in time.

![Diagram showing group velocity versus frequency for different modes, with labels for different materials: Air, PC, and Silicon.](image)

**Figure 4.5** Calculated group velocity versus frequency for different modes, for the situations when the metal waveguide is filled with air, PC, and silicon, from top to bottom, respectively. Those modes in dashed lines are of odd parity and will not be excited by external waves. Up to 1THz, there is only one TEM mode for air, and two modes for photonic crystal, but there are four modes for unetched silicon. This explains why the silicon signals in figure 4.4 are significantly dispersed.

When the etched portions of the wafers (the photonic crystals) are inserted into the metal waveguide, the waveforms are substantially dispersed, extending to hundreds of picoseconds. In contrast to the case of the solid silicon wafer, this is primarily not due to waveguide dispersion. The lower average index of the photonic crystal pushes the cutoff frequency of higher order TM modes to larger frequencies. As can be seen in figure 4.5,
other than TEM mode, there is only one TM$_2$ mode in our frequency range. The dispersion is primarily the result of the dispersive effects of the photonic band structure, resulting from sharp spectral features in the photonic band structure such as the edges of the stop band [110, 118-120].

Incidentally, the effect of the lower average index can also be seen in the transit time of the earliest arriving portion of the THz signal through the waveguide, intermediate between the cases of air and solid silicon. The maximum of this earliest arriving signal can be used to estimate the effective refractive index of the photonic crystal structure. For example, we observe that the earliest peak of the signal arriving roughly 19 ps earlier than the corresponding peak in the case of the solid silicon waveguide for the Γ-K sample. Given the propagation distance (4 unit cells), we compute a mean dielectric of 3.9 for the photonic crystal, which is close to the volume-weighted average value of 3.86.

4.4.3 Frequency Response

In order to characterize the effects of band gaps and uncoupled modes, we plot in figures 4.6 and 4.7 the normalized transmission spectra in the frequency domain. Figure 4.6(a) shows the transmission coefficient of the sample in the Γ-K direction, relative to those of an air-filled waveguide. Two low-transmission regions can be observed. For comparison, we also compute the transmission spectrum using a transfer matrix method [113], which again assumes an infinite thickness for the photonic crystal slab. The result, as shown in figure 4.6(b), shows almost the same gap widths as those from the experimental result, except there is a systematic red shift of about 0.025 THz. This shift
has previously been attributed to the finite thickness of the photonic crystal slab [27, 103, 121].

![Figure 4.6](image.png)

Figure 4.6 (a) Measured power transmission spectrum of the photonic crystal inside the metal waveguide, for the \( \Gamma-K \) direction, along which the sample has 4 unit cells. This is computed using the Fourier transforms of the time-domain waveforms, with the air-filled guide as a reference. (b) \( \Gamma-K \) transmission spectrum computed using a transfer matrix method, for comparison with the experimental result. The comparison is quite good, except for a systematic red shift of about 0.025 THz, attributed to the finite thickness of the photonic crystal which is not considered in the numerical calculation.

Interestingly, the experimental transmission in the first gap is somewhat larger at the low frequency side of the gap (near 0.27 THz) than it is at the high frequency side (near 0.32 THz). This difference may be due to the fact that only the higher frequency portion of this region corresponds to the complete photonic band gap, while the lower portion corresponds to the region of uncoupled modes. A small residual amount of radiation may be coupled into these modes due to imperfections in the wavefront of the focused THz pulse, leading to a slightly higher transmission coefficient. This phenomenon is also seen in the second gap (near 0.42 THz), which also results from the anti-symmetric modes, and has transmission coefficients of the same order as those for the low frequency portion of the first gap. We note that the transmission coefficients in
the region of the complete gap are not as small as the theoretically computed transmission. This residual transmission reflects the noise floor of the measurement.

Figure 4.7 shows the measured and calculated transmission coefficients for the \( \Gamma - M \) direction. Once again, we observe a similar degree of correspondence between the two results, along with a similar red shift due to the finite thickness of the photonic crystal.

![Image of transmission spectrum](image)

**Figure 4.7** (a) Measured power transmission spectrum of the photonic crystal inside the metal waveguide, for the \( \Gamma - M \) direction, along which the sample has 10 unit cells. This is computed using the Fourier transforms of the time-domain waveforms, with the air-filled guide as a reference. (b) \( \Gamma - M \) transmission spectrum computed using a transfer matrix method, for comparison with the experimental result. A red-shift of the theory with respect to the experiment is observed, similar to the results of figure 4.6.

### 4.4.4 Group Velocity

As noted above, propagation through the photonic crystal leads to substantial dispersion of the time-domain waveforms, due to the strong group velocity dispersion associated with the band structure. This dispersion can be used for ultrafast pulse manipulation, including for example pulse compression [122, 123] and optical delay lines [40, 41]. There have been a few reports on using ultrafast pulses to probe the dispersion
at or near the band gaps of photonic crystals by measuring the difference of arrival times between one pulse transmitted through a photonic crystal and the other through a reference sample [118, 120, 124, 125]. Others have used interferometric techniques, comparing the pulse transmitted through a photonic crystal and a reference pulse [109-112]. Direct measurements of pulse group velocity have also been realized using nonlinear effects [119, 126].

Here we take advantage of the coherent nature of the THz-TDS measurement to investigate the dispersion associated with the photonic band structure. Because this technique permits sub-cycle temporal resolution of the electric field, even strongly distorted or chirped terahertz pulses can be accurately characterized. Since the bandwidth of our terahertz pulse is much broader than the size of the stop gap, it permits us to extract information over a broad spectral range, giving a complete description of the properties of photonic crystals in the frequency range of interest.

To better illustrate the effects of dispersive propagation, we present the measured signals in both time and frequency domain. We accomplish this using a short-time Fourier transform (STFT) [127, 128]. This procedure is widely used for time-frequency analysis of non-stationary signals. In STFT, the signal is multiplied by a window function, and is then Fourier analyzed to determine the spectral content of the signal within the specified window. By sliding the window along the signal, one obtains the temporal evolution of the frequency content. The spectrogram computed in this way can be represented as:

\[ S(\omega, t) = \int_{-\infty}^{\infty} f(\tau) w(\tau - t) e^{-i\omega \tau} d\tau \]

where \( f(\tau) \) is the measured waveform, and \( w(\tau-t) \) is a Hamming window centered at \( t \).
The duration of the window function determines the time and frequency resolution. Here we choose the duration to be 30 picoseconds, which gives a frequency resolution of 0.03 THz. In order to display the results, we first normalize each spectral component of $S(\omega, t)$ of the photonic crystal data to that of the corresponding frequency in the spectrogram of the waveform taken with an empty waveguide. Then, in order to avoid dynamic range problems in the false color plot for the photonic crystal data, we normalize $S(\omega, t)$ at each frequency by dividing by the maximum value for that frequency. If, for certain values of frequency, the maximum value is smaller than a critical value, which we set as 10% of the maximum value among all those maximum values, this is an indication that this frequency falls within a stop band, and the normalization factor is increased accordingly. The threshold value of 10% is chosen based on the experimental transmission spectra (e.g., figures 4.6 and 4.7). It permits us to clearly distinguish between spectral regions inside and outside of the stop bands.

The spectrograms computed in this way are shown in figure 4.8 for the waveforms along $\Gamma$–$K$ direction. All frequency components in the air signal emerge from the waveguide at almost the same time, indicative of zero dispersion. For the silicon signal, the transit times vary slightly due to the aforementioned multimode excitation of the waveguide. In contrast, both the band gaps and the striking dispersion of the photonic crystal signal become very clear in this false color plot. Similar results for propagation along the $\Gamma$–$M$ direction are shown in figure 4.9. Here, spectrograms are displayed for the three different photonic crystal samples, identical except for the propagation lengths.

We can directly compare these results with the computed band structure. For
light propagating in a given band, the transit time through the photonic crystal can be expressed as:

$$\Delta t(\omega) = \frac{L}{v_g(\omega)}$$

where $L$ is the length of the slab and the group velocity $v_g(t)$ is calculated numerically from the band structure using the Hellman-Feynman theorem [1].

![Figure 4.8](image)

**Figure 4.8** Short-time Fourier transform false-color plots of the three waveforms along Γ-K direction. Here, red indicates high amplitude and blue indicates low amplitude. In the upper plot, the air-filled waveguide is dispersionless, so all of the spectral components of the THz pulse arrive at the same time. In the middle plot, the small dispersive effects arise from multimode excitation of the waveguide. In the lower plot, large dispersion is observed near the edges of the band gaps in the photonic crystal.

The transit times computed in this fashion, for Γ-M, are shown as black curves superimposed on figure 4.9. The computed curves have been shifted along the frequency axis, to account for the finite thickness frequency shift mentioned above, in the context of
figures 4.6 and 4.7. In addition, the calculated results must be shifted along the time axis, since in those measurements the zero of the time is arbitrarily chosen. We determine the absolute time shift by referencing the calculations to the zero of time defined by transmission through an air-filled guide (as in figure 4.8(a)). Thus, aside from the aforementioned finite thickness frequency shift, the black curves in these plots are computed with no adjustable parameters. The correspondence is extremely good, indicating the high quality of the photonic crystals which can be fabricated for THz applications.

![Diagram](image.png)

**Figure 4.9** Short-time Fourier transform false color plots of the THz pulses transmitted through three different samples along the Γ–M direction. In these samples, the thicknesses are 5, 10, and 20 unit cells, from top to bottom respectively. As a result of the increasing propagation distance inside the dispersive medium, both the transit times and the dispersion increase. The solid black lines are calculated as described in the text. These are plotted using only one adjustable parameter: the frequency shift due to the finite thickness of the crystal, mentioned in the context of figures 4.6 and 4.7. This parameter is the same for all three panels.

4.5 Conclusion

In conclusion, we have studied the optical properties of two-dimensional photonic
crystal slabs with copper claddings, using terahertz time-domain spectroscopy. The transmission coefficients in the frequency domain match well to those from transfer matrix calculations, except there is a systematic shift of the band edges due to finite thickness effects. Using short-time Fourier transform, we can display the data in both time and frequency domain, which gives a useful intuitive picture of the propagation characteristics near the band edges. Finally, we note that the long wavelength (compared to visible and near-infrared optics) permits the easy fabrication of photonic crystals which are essentially ideal, with no defects or disorder of any kind. As a result, these experiments are extremely well described by theoretical models, and it may be possible to observe subtle effects which would otherwise be obscured by the disorder present in less perfect samples. These results highlight the power of time-domain spectroscopy for characterizing photonic lattices.
Chapter 5

Defect Modes and Reflection Spectra

Previous chapter describes the in-plane properties of perfect photonic crystal slabs without any defects. Here we introduce defects into the photonic crystal slabs by filling several of the air holes with silicon powders. We observe the signature of a defect mode within the stop band, in both the amplitude and phase spectra. The experimental results are in reasonable agreement with theoretical calculations using transfer matrix method. We have also measured reflection spectra using the photonic crystal as a 90° turning mirror, and in this way demonstrated frequency-selective components for quasi-optic guided wave propagation of terahertz pulses.

Part of this chapter has been published in references [90, 105].

5.1 Introduction

Recent years have seen increasing interest in the use of terahertz radiation for a variety of applications [5]. This trend has led to an increasing need for quasi-optical components which can be used to manipulate terahertz beams. One promising candidate is photonic crystals. Early research in photonic band gap materials used terahertz radiation to probe millimeter and sub-millimeter-scale structures, as a means for understanding the properties of periodic media in a regime where the fabrication was less challenging than at optical frequencies [3, 32, 33, 91, 93-95]. More recently, the motivation has shifted towards the optimization of structures specifically intended for use
at THz frequencies [96, 97, 99-104]. These experiments have primarily focused on
defect-free photonic crystals. Only a few studies of the properties of THz defect modes
have been reported [4, 32, 96, 98]. However, it is clear that, just as at optical frequencies,
the utility of terahertz photonic crystals relies on the incorporation of defect structures to
disrupt the periodicity and thereby introduce propagating modes within the band gap [8].

Here, measurements of a two-dimensional photonic crystal slab are described, in
which functional structures (such as resonant cavities or waveguides) can be incorporated
and removed, reversibly. As with several previous authors, we employ terahertz time-
domain spectroscopy for transmission measurements [93, 94, 100, 101]. This technique
provides a direct measurement of the terahertz electric field, which is generated in the
form of a single-cycle pulse. As a result, both the amplitude and the phase of the
radiation can be determined experimentally.

5.2 Experimental Setup

Our sample is the same as those in the previous chapter. This slab geometry
mimics the most commonly employed configuration used in near-infrared applications, in
which light is confined in two dimensions by the photonic crystal, and in the third by
waveguiding [27]. In our samples, the 305 micron thickness of the slab is large enough
to support not only the fundamental TEM mode but also one set of higher modes (the $E_{10}$
and $H_{10}$ modes [117]), at the highest frequency of interest (the top of the band gap, near
0.4 THz). We have chosen to operate in this multi-mode regime in order to optimize the
coupling efficiency of radiation from free space into the slab waveguide. We note that
undistorted single-mode propagation can still be achieved, even at frequencies above the
cutoff of higher-order modes, if the incident beam is mode-matched to the (dispersionless) TEM mode [129]. In the situation described here, the higher modes are of odd parity [117], and therefore are not efficiently excited by the incident wave.

The experimental setup is the same as described in chapter 4. Broadband single-cycle terahertz pulses are generated and detected using photoconductive antennas [5]. The terahertz radiation is focused into a parallel-plate copper waveguide using a plano-cylindrical lens. The incident field is polarized perpendicular to the plane of the waveguide (TM-polarized). An identical setup is used at the exit facet to collect the transmitted radiation. The photonic crystal slab is sandwiched inside the metal waveguide, which provide a nearly ideal lossless boundary for the guided wave [75]. We have etched the wafer over only half of its area, leaving an unetched portion that we use to collect a reference transmission spectrum.

5.3 Defect Modes

We introduce a defect structure into the otherwise perfect photonic crystal by filling several of the air holes with a finely ground powder of high-resistivity silicon. The grain size of this powder (~10 microns) is much smaller than the shortest wavelength used in our measurement, so it acts as a homogeneous medium with a dielectric somewhat smaller than that of bulk crystalline silicon. Figure 5.1(a) shows the transmission spectrum of the photonic crystal, referenced to that of the unetched silicon slab, in the vicinity of the photonic band gap. The addition of the three-point defect gives rise to an enhanced transmission in the middle of the gap, near 0.28 THz. On removal of the defect, this resonance vanishes.
Figure 5.1 (a) The experimental transmission spectrum for the photonic crystal, relative to a solid silicon slab of equal thickness. Solid squares are for the perfect lattice, and hollow circles are for the same lattice but with three holes filled, in the pattern shown in the inset. A defect mode appears at \(~0.28\) THz. (b) The solid line shows the TMM calculation for a perfect photonic crystal, and the dashed line is for the lattice with a three-point defect. The material filling the holes is assumed to be a uniform dielectric with \(\varepsilon = 5.0\). (c) The difference in the spectral phases of the two measured waveforms which gave the spectra in (a). The signature of the defect mode is evident at 0.28 THz. The shaded area denotes the region of the full photonic band gap, where the transmitted intensity is not large enough for an accurate determination of the phase.

Figure 5.1(b) shows a calculated transmission spectrum for these two experimental situations (with and without defect), using the transfer matrix method (TMM) [113, 114]. For the purposes of the calculation, we assume that the three air holes are uniformly filled, with a dielectric constant of \(\varepsilon = 5.0\). We note that these simulations assume a two-dimensional lattice with infinite extent in the third dimension. So, we do not expect a perfect correspondence with the experimental results. However, we note that the metal cladding in our structures eliminates the light cone states, extending perpendicular to the slab [27]. As a result, one might expect these 2D
simulations to be more accurate than in the case of dielectric-clad slabs. We also note that the dielectric of the composite material filling the slabs is not known with any precision. We use a representative value of $\varepsilon = 5.0$ for these illustrative calculations.

The TMM spectra contain many features similar to those observed in the data. We observe a systematic shift between the experimental and computed locations of the band edges, of about 0.025 THz. This shift has been previously attributed to the finite thickness of the photonic crystal slab [27, 121], an effect which is not accounted for in the TMM simulation. The calculation also predicts narrow enhanced transmission peaks, similar to the one observed in the data. Several defect modes, near the upper and lower edges of the complete gap, are not observed in the experiment. Finally, we note that the high frequency portion of the stop band corresponds to the full 2D gap for TM polarization, whereas the lower portion corresponds only to a pseudo-gap, in which the bands support anti-symmetric mode patterns that do not couple strongly to the incident radiation [3, 4]. As a result, the transmission coefficient is somewhat higher in this low-frequency region, a result echoed in our experimental findings.

We take advantage of this somewhat larger transmission to obtain the dispersion associated with the defect mode. The time-domain spectroscopy technique provides a direct measure of the spectral phase of the terahertz wave. Ordinarily, obtaining this spectrum would be quite challenging for radiation inside the stop band, since the transmitted intensity is so small. However, the combination of the slightly higher transmission (due to the fact that the defect mode lies in a pseudo-gap rather than inside the complete gap) with the excellent dynamic range of the measurement permits us to extract phase information across the defect mode. Figure 5.1(c) shows the phase.
difference \((\phi_{\text{defect}} - \phi_{\text{no defect}})\) obtained from the measured waveforms. Because the defect mode introduces both amplitude and phase changes for propagation near the resonance frequency, we expect to see a signature of the defect at \(~0.28\) THz in this difference spectrum. This feature is indicated by an arrow in figure 5.1(c).

5.4 Reflection Spectra

Using terahertz time-domain techniques, it is also generally possible to measure reflection spectra. However, in the present case, this presents a special challenge. Because we are coupling terahertz waves from free space into the waveguide, it is difficult to couple 100% of the input beam into the waveguide. Part of the beam is inevitably reflected from the copper plates above or below the dielectric slab. This reflected beam can be significant compared with the reflection from the thin photonic crystal slab. Because the two reflections overlap in the time domain, it can be difficult to experimentally distinguish them from each other. So, instead of measuring the reflected beam at normal incidence, we employ a 90 degree setup, as shown in the inset of figure 5.2. Here, the photonic crystal is used inside the metal waveguide as a quasi-optic turning mirror [89]. We obtain a reference signal by replacing the photonic crystal with a silicon slab of the same thickness. Typical detected waveforms are shown in Figure 5.2(a), where the reference signal keeps its single-cycle property while the signal reflected by the photonic crystal slab is significantly extended in duration. We then calculate the power spectra via Fourier transform of the two measured signals. The results are shown in figure 5.2(b). We observe that, in certain spectral regions near the complete band gap, the reflection from the photonic crystal is significantly enhanced
relative to that from the un-patterned silicon wafer. This result demonstrates that photonic crystals can be used in combination with quasi-optics for a variety of functions such as frequency selection and pulse shaping.

![Waveform graphs](image)

Figure 5.2 Upper: Time-domain waveforms reflected from an un-patterned silicon reference slab (solid) and a photonic crystal (dotted). The inset shows a schematic of the reflection geometry. In these measurements, \( \Gamma-M \) direction is perpendicular to the incident surface of the photonic crystal. Lower: The power spectra of the two waveforms shown in the upper plot, on a log scale. The photonic crystal result (squares) exhibits enhanced reflection in certain spectral regions (indicated by arrows), due to the high reflectivity of band gap regions.

5.5 Conclusion

In conclusion, we have studied transmission properties of two-dimensional photonic crystal slab with metal cladding using terahertz time-domain spectroscopy. By filling several holes with a fine powder, defect modes are reversibly introduced to the photonic crystal lattice. These modes can be characterized in both amplitude and phase. The amplitude transmission spectra are in reasonable agreement with TMM calculations.
We can also measure reflection spectra, and in this way construct frequency-selective components for quasi-optic guided wave propagation of terahertz pulses. Such components are in principle tunable by varying the angle of the photonic crystal slab. These results highlight the possibility of making optical components for terahertz waves with photonic crystals, and the power of time-domain spectroscopy for characterizing photonic lattices.
Chapter 6

In-Plane and Out-of-Plane Dispersion and Homogenization

Here we discuss the in-plane and out-of-plane dispersion in two-dimensional photonic crystal slabs. Using terahertz time-domain spectroscopy, we obtain the complex transmission coefficient over a broad spectrum. We find that the effective in-plane index is equal to the square-root of the volume-weighted average dielectric constant, precisely the result predicted by homogenization theory. Despite the absence of a band gap, the out-of-plane dispersion is significant and in addition exhibits a complicated spectral dependence. Calculations of the effective refractive index which assume translational invariance in the direction perpendicular to the slab are in only approximate agreement with the measured homogeneous effective index and dispersion. In contrast, numerical simulations which accurately account for the finite slab thickness give much more accurate predictions.

Part of this chapter is published in our paper [130].

6.1 Introduction

The propagation of electromagnetic waves in periodic dielectric structures has become an important area of research. In particular, photonic crystal slabs, with periodicity in two dimensions and finite thickness in the third dimension, are of special interest [27]. In the plane of the periodicity, such structures can exhibit a complete photonic band gap, which can be exploited for a variety of applications [8]. Recently the
propagation of light along the direction perpendicular to the plane of periodicity has also attracted much attention. Consideration of out-of-plane propagation is relevant in the coupling between guided and lossy or defect modes [26, 131-134]. In addition, guided resonances, which couple to freely propagating out-of-plane modes, have recently been the subject of intense study [28, 135]. Such resonances may be used as the basis for novel mirrors or filters [136-138] or as sensitive displacement sensors [9]. Despite the significance of the out-of-plane propagation, only a few studies have reported experimental measurements of transmission or reflection spectra [26, 131, 134, 138-140], and we are aware of no reports of spectral phase measurements. Theories based on plane wave expansion methods have been used to predict the effective refractive index perpendicular to the plane [1, 141], but experimental confirmation of these predictions is lacking.

Here, we describe measurements of the complex transmission coefficient perpendicular to a photonic crystal slab. Our data span the spectral range from the homogeneous (long wavelength) limit to beyond the first few guided resonances. We find that predictions of the phase of the transmitted radiation, computed using plane wave expansion methods, provide only a qualitative description of the homogeneous limit and the low-frequency dispersion. In contrast, numerical simulations which accurately account for the finite thickness of the slab [142] give better agreement with the measurements. These experimental results emphasize the difficulties in using plane wave expansion methods to describe propagation perpendicular to the slab.

6.2 Experimental Setup
For broadband characterization of photonic crystals, we employ terahertz time-domain spectroscopy to determine both the transmission amplitude and phase over a wide spectral range [90, 91, 93, 100, 101, 105]. Because of the low frequency of the radiation (100 – 1000 GHz), photonic crystals can be fabricated which are nearly perfect on the scale of the wavelength, with essentially zero positional or size disorder and negligible interface roughness. We have used deep reactive ion etching to form an array of circular air holes, penetrating all the way through a 305 μm-thick high-resistivity (>10 kΩ•cm) silicon wafer [90, 103, 105]. This material exhibits extremely low absorption and a frequency-independent refractive index of $n_{Si} = 3.418$ throughout the THz range [115]. The holes, with diameters of 360 μm, are arranged on a hexagonal lattice with spacing $a = 400$ μm. The in-plane band structure of this sample, computed using a plane wave expansion method, may be found in reference [90] or chapter 4 of this thesis.

For in-plane measurement, because the thickness of the slab is less than the longest free-space wavelength of our THz pulse, we perform these measurements in a waveguide geometry, with the photonic crystal slab placed inside a parallel plate copper waveguide, as we have done in chapter 4 and 5. Since the lowest-order E-polarized (TM) mode of this waveguide exhibits no cutoff wavelength [75, 117], all of the measured dispersion can be attributed to the effects of the photonic crystal. This geometry has proven to be a powerful tool for broadband waveguide THz spectroscopy [88, 90, 105].

To obtain the transmission coefficient for propagation perpendicular to the plane of the slab, we compare the transmitted THz pulse with the sample in the collimated THz beam to that measured with no sample in the beam path. A schematic of the out-of-plane experimental setup is shown in figure 6.1. The photonic crystal slab is illuminated at
normal incidence to the plane of the periodicity. The THz beam spot size is large enough
to illuminate many holes.

![Diagram](image)

Figure 6.1 A schematic of the out-of-plane experimental arrangement. The photonic crystal slab is
illuminated at normal incidence to the plane of the periodicity. The THz beam spot size is large
enough to illuminate many holes.

6.3 In-Plane Dispersion and Effective Refractive Index

Shown in figure 6.2 (a) is power transmission spectrum for photonic crystals
along the \( \Gamma - M \) direction. A gap is denoted by the two vertical dashed lines. The relative
phase spectrum, \( \Delta \phi = \phi_{pc} - \phi_{air} \), is obtained by subtracting phase of air signal from that of
photonic crystal signal and is shown in figure 6.2(b). We observe that \( \Delta \phi \) is nearly linear
up to a frequency close to that of the lower edge of the first (partial) photonic band gap, a
result which is consistent with previous in-plane dispersion measurements on similar
samples [119, 125, 143].

We can then examine the effective index using the thickness \( L \) of the samples and
the phase difference \( \Delta \phi(\omega) \) between the sample signals and the reference air signals:
$$\phi_{pc} - \phi_{air} = \Delta \phi = -\frac{\omega[n(\omega) - 1]}{c}$$

$$n(\omega) = -\frac{c \times \Delta \phi(\omega)}{L \times \omega} + 1$$

where $c$ is the light speed in vacuum, and $\omega$ is the circular frequency. The as-calculated effective index is shown in figure 6.2(c), with the solid line from theoretical prediction. At low frequencies, the effective index is equal to the square-root of the volume-weighted average dielectric constant, which is precisely the result predicted by homogenization theory [141]. Deviations from this value occur only for $f>0.205\text{THz}$, which is the lower edge of the band gap.

Figure 6.2 (a) The transmission and (b) relative phase for in-plane propagation (TM polarization), along the $\Gamma$-M direction. The vertical dashed lines indicate the edges of the first (partial) photonic band gap. The slanted dashed line in (b) is a guide to the eye to indicate the linearity (and the zero intercept) of the in-plane phase at low frequencies. (c) Effective refractive index versus frequency, for propagation in the plane of the slab. The predicted homogeneous value of $n_{hom} = 1.9585$ (horizontal solid line) is precisely consistent with the measurement at low frequencies, $n_{meas} = 1.958\pm0.011$. Deviations are observed only as the frequency approaches that of the band gap (vertical dashed lines).
6.4 Out-of-Plane Dispersion and Effective Refractive Index

Fig. 6.3 shows a typical set of out-of-plane results. The transmission amplitude, shown in Fig. 6.3(a), exhibits Fabry-Perot oscillations at low frequency and shows evidence of three guided resonances at higher frequency [28]. The solid curve is the result of a simulation using the finite element method (FEM), which reproduces all of these features. Fig. 6.3(b) shows the transmitted phase measured relative to that of no sample in the beam path, $\Delta \phi = \phi_{\text{slab}} - \phi_{\text{air}}$. The phase exhibits a marked nonlinearity, and also shows abrupt jumps due to the guided resonances. Here, the solid curve is the result of a finite-difference time-domain (FDTD) simulation.

The above out-of-plane data were obtained with the input polarization oriented along the $\Gamma$–M axis of the hexagonal lattice. However, as expected [141], we observe no polarization dependence. Crystals with three-fold rotational symmetry (such as ours) are uniaxial in the homogeneous limit, possessing only two distinct effective dielectric constants, one for in-plane and one for out-of-plane propagation.

We can obtain the out-of-plane dielectric constant from the data of figure 6.3(b). However, the oscillatory structure at low frequencies in fig. 6.3(a) highlights the need for care in processing data. These Fabry-Perot fringes cannot be removed by a simple windowing procedure in the time domain, because here the sample is too thin. Instead, we obtain the effective refractive index using a numerical error minimization procedure described previously [144]. In our case, because the attenuation (due to guided resonances) is relatively small below $\sim$0.5 THz, this procedure leads to only a small modification, but still effectively eliminates Fabry-Perot effects from the extracted index. We note that this procedure is not required to obtain $n_{\text{eff}}(\omega)$ for in-plane propagation,
since in that case the sample is thick enough (20 periods) that the Fabry-Perot effects can be removed by time-domain filtering, as what we have done in the in-plane case.

![Power transmission coefficient and relative phase](image)

**Figure 6.3** (a) Power transmission coefficient and (b) relative phase $\Delta \phi$ for transmission perpendicular to the photonic crystal slab. The phase is measured relative to the case of no sample in the THz beam path. In (a), the solid line is the result of a finite element method (FEM) simulation, while in (b), the solid line is a finite-difference time-domain (FDTD) simulation. Both simulations account for the finite thickness of the sample along the propagation direction, and both reproduce the frequency-dependent features of the data.

Fig. 6.4 shows the effective refractive index for out-of-plane propagation, obtained from $\Delta \phi(\omega)$. Despite the absence of a band gap for propagation perpendicular to the slab, the effective out-of-plane index exhibits large dispersion in the frequency range below the first guided resonance. Moreover, the frequency dependence is not simply a smooth increase or a constant (as in the case of the in-plane effective index). Finally, the measured low-frequency limiting value, $n_{\text{meas}} = 1.73 \pm 0.07$, is notably larger than the calculated homogeneous limit of $n_{\text{hom}} = 1.6448$.

In figure 6.4, we also show computations of both the homogeneous limit (dashed
line) and the dispersion (dotted curve), obtained using analytic theories based on plane wave expansion of the spatially varying dielectric for our photonic crystal but with infinite thickness [1, 2, 141, 145]. Such theories rely on the assumption of translational invariance along the direction perpendicular to the slab; in other words, the finite thickness of the slab is not considered. As a result, the agreement with experiment is only qualitative [142]. In contrast, a finite-difference time-domain (FDTD) simulation (solid curve), which includes a realistic representation of the sample, accurately reproduces both the frequency-dependent dispersion and the low-frequency limit of the out-of-plane effective index.

Figure 6.4 Effective refractive index versus frequency, for propagation normal to the plane of the photonic crystal slab, for the frequency range below the first guided resonance. The horizontal dashed line indicates the predicted homogeneous limit of $n_{\text{hom}} = 1.6448$, which is smaller than the measured low-frequency value of $n_{\text{meas}} = 1.73 \pm 0.07$. The dotted curve shows the dispersion predicted by a band structure calculation for out-of-plane propagation in an infinite-thick photonic crystal, based on a plane wave method [2]. The solid curve is the FDTD simulation from figure 6.3(b), which is in excellent agreement with experimental results.

To understand why the effective index increases with frequency, we can examine
the power distribution at a cross section of our photonic crystal slabs in a steady state. We solve the Maxwell's equations for the structure in FEMLAB, and the computed power distribution is shown in figure 6.5. At low frequencies such 0.1THz, most of the power concentrates in the air holes; with the increase of the frequency, more power moves to the silicon part. Since silicon has a larger refractive index than that of air, the net result is an increase of the effective index of refraction.

![Diagram](image.png)

**Figure 6.5** Top: a schematic of a unit cell in our photonic crystal. Bottom: power distribution at the region denoted by the bold-line area, calculated with FEMLAB. With the increase of frequency, power moves to the silicon region, making the effective index increases with frequency.

6.5 Finite Element Method Simulation

Here we discuss how to simulate the photonic crystal slab for out-of-plane propagation perpendicular to the slab using FEMLAB. As discussed earlier, there are five steps in FEMLAB to simulate a device. They are geometry modeling, physics settings to setup boundary conditions and subdomain settings, mesh generation,
computing the solution, and postprocessing and visualization. Here I detail each of those steps in the simulation of the photonic crystal slab.

First step is to define modeling geometry. Choosing the right geometry is a very important step. The geometry must first catch the characteristics of the devices to be modeled, which is a necessary condition to generate correct simulation results. In the meantime, the modeling area should be as small as possible, as the larger the area modeled, the longer it takes to get the computation done and the more computation resources it takes. To reduce the size of geometry, several techniques could be utilized, such as symmetry properties.

In the photonic crystal slab, the holes form a periodic structure. Considering the symmetry property, there is no need to simulate the whole structure. Instead, modeling a unit cell is enough. At the first sight, one might tend to model a hexagonal unit cell. However, careful examination shows that a rectangle is also a unit cell for the lattice, as shown by the magenta rectangle in figure 6.6. If we consider the symmetry of this rectangle, we will find this is a highly symmetric shape and one quarter of the rectangle is enough to describe it. As a result, we choose the rectangle in red as the area that needs to be modeled. One might also wonder the red rectangle is a symmetric shape and one half of it, which is a triangle, is enough to describe it. That is true. However, configuring the boundary conditions for that triangle area is much more challenging than for the red rectangle area. Thus, here we go with the rectangle area.

With the chosen modeling area, we can set up the geometry and it is shown in figure 6.7. Here the center part is the device area needs to be modeled, with its thickness 300 microns. It is put in waveguide geometry, and waves are propagating inside the
waveguide along the direction perpendicular to the slab.

![Diagram](image)

**Figure 6.6** A schematic to show how to choose the minimal modeling area in FEMLAB. As the holes are periodically arranged, a unit cell such as the hexagon in yellow represents the whole pattern. However, according to symmetry properties, we do not need to model such a big area; instead, it is enough to modeling the rectangle in red.

The second step is to configure physics settings such as materials properties and boundary conditions. The index of silicon is 3.418, and that of air is 1. We can put those numbers into each subdomain. At the both ends of the waveguide, we use low-reflecting boundary condition, which means no waves are reflected by those boundaries. The waves are excited at the left end with electric field only along the up-down direction, which is set to 1 and along other directions they are set to 0. Then perfect magnetic conductor and perfect electric conductor boundary conditions are assigned to proper walls of the waveguide to satisfy the boundary condition requirement.

The third step is to generate mesh. This can be done automatically by FEMLAB. However, care must be taken in choosing the maximum size of meshing elements to get right simulation results. One rule of thumb is that the maximum meshing element size should be at most 1/10 of the wavelength in a material, in order to get the right simulation
results for the waves with the wavelength. This indicates that with the increase of the frequency, one needs to have more meshing elements. Also, more meshing elements should be put to where there are fine structures. A meshed geometry is shown in figure 6.7 (b). More meshing elements can be seen in the center part where the structures are fine.

![Figure 6.7](image)

(a)

(b)

Figure 6.7 (a) the geometry of modeling area. The center part is the red area shown in figure 6.6. The two sides are needed to simulate the propagation of waves perpendicular to the slab. (b) meshed geometry. The center part has more meshing elements, as it has finer structure.

The fourth step is to compute the solution. This is done by FEMLAB automatically.

The final step is to do postprocessing and visualization. Various physical quantities can be extracted, such as electric field and magnetic field. Shown in figure 6.8 is the power distribution at different planes along the propagation direction. At the two sides power distribution is more uniform than those in the center part. This is because the center part has a more complex structure than two sides, where there is only air. If we integrate power at the output plane, and divide that by the integrated power at the input
plane, we can then get the transmission coefficients as shown in figure 6.3.

Figure 6.8 A solved model, with power distribution shown at different planes along the wave propagation direction. The distribution is more uniform at two sides than at the center, as the center part has a more complex structure.

6.6 Conclusion

In conclusion, we have described an experimental measurement of the in-plane and out-of-plane dispersion and homogenization of photonic crystal slabs. We find excellent agreement between experiment and homogenization theory in the in-plane case, but there are notable discrepancies with existing theoretical treatments in the out-of-plane measurement. Because numerical simulations (which account for the finite thickness of the slab) give better agreement with measurements, the discrepancies would seem to be a consequence of the lack of translational symmetry along the propagation direction, which is not considered in many theoretical treatments. This highlights the unique challenge of describing propagation perpendicular to the slab, even in the long wavelength limit. This
configuration is not particularly amenable to homogenization, because the wave does not sample a large number of unit cells [141]. For the case of a slab of finite thickness, this difficulty is not limited strictly to normal incidence propagation – indeed, for all incident angles $\theta < \theta_0$, the propagating wave samples less than one unit cell before exiting the medium. Here, $\theta_0$ is a critical angle determined by the effective index and the ratio of the slab thickness to the lattice period. For the sample described here ($n_{\text{hom}} \sim 1.73$, $d/a = 0.763$), we find $\sin\theta_0 > 1$, which implies that no out-of-plane incident wave, arriving from any external angle, samples the homogeneous infinite-slab limit. For slabs of finite thickness, a more sophisticated theoretical treatment is required to accurately describe the out-of-plane dispersion and homogenization.
Chapter 7

Broadband Group Velocity Anomaly in Photonic Crystal Slabs

At higher frequencies, we observe a broadband group velocity anomaly for out-of-plane propagation perpendicular to the slab. The group delay is equal to that of empty space despite the fact that the volume-weighted average dielectric of the slab is $\varepsilon_{\text{ave}} \sim 3.8$. In contrast to most other examples of anomalous group delay effects, this unusual phase transparency persists over a very broad spectral bandwidth, demonstrating that such anomalies do not require the presence of a nearby isolated resonance. Our results are consistent with finite-difference time-domain (FDTD) simulations.

Part of this chapter is published in our paper [146].

7.1 Introduction

Observations of unusual behavior in the group velocity of propagating light waves are of considerable interest. The possibility of a superluminal group velocity near a resonance has been recognized for many years [147]. Numerous approaches have been described for observing pulse propagation in a regime of superluminal or negative group velocity, including operation near a resonant gain line [148, 149], penetration through a tunnel barrier [150], and propagation in the transparent regime between two closely spaced absorption resonances [151]. Similar effects can be observed in photonic crystal devices [152, 153], as well as in the propagation of electronic signals [154]. Such effects generally rely on the rapid variation of the refractive index with frequency which occurs
near a resonance or when the wavelength is close to a characteristic length scale of the medium. As a result, the regime of anomalous group velocity is confined to a fairly narrow portion of the spectrum. One consequence of this practical bandwidth limit is that the duration of optical or electrical pulses used to study these effects is generally much larger than the shift in transit time being observed [151, 154].

Here we report an observation of a broadband group velocity anomaly in the transmission of a picosecond terahertz pulse through a photonic crystal slab. For wavelengths shorter than the lattice parameter of the periodic structure, we find an abrupt transition to a regime of zero phase dispersion. This anomaly persists for at least hundreds of GHz, occupying a fractional bandwidth greater than 50%. In this spectral range the group velocity \( v_G \) is equal to the vacuum speed of light, despite the fact that the volume-weighted average dielectric constant of the sample is \( \varepsilon_{\text{ave}} \sim 3.8 \). Furthermore, because of the lack of spectral dispersion and the presence of guided resonances at lower frequencies, it is very difficult to uniquely determine the phase velocity in this range.

To understand this behavior, we consider a medium which can be described, within a certain spectral bandwidth \( \Delta \omega \), by an effective refractive index, \( n_{\text{eff}}(\omega) = 1 + \eta \Omega_0 / \omega \), where \( \eta \) is a dimensionless positive constant and \( \Omega_0 \) is a fixed frequency parameter which is characteristic of the medium. Clearly, the phase velocity depends on the parameter \( \eta \), as \( v_p(\omega) / c = 1 / n_{\text{eff}} = (1 + \eta \Omega_0 / \omega)^{-1} \). In contrast, the group velocity is given as [147]:

\[
 v_G(\omega) / c = \left[ n_{\text{eff}}(\omega) + \omega \frac{dn_{\text{eff}}}{d\omega} \right]^{-1} = \left[ 1 + \eta \frac{\Omega_0}{\omega} - \omega \frac{\eta \Omega_0}{\omega^2} \right]^{-1} = 1 \tag{1}
\]

In other words, the group delay for propagation through a slab of thickness \( L \), \( \tau_g = d\phi / d\omega \),
is given by $L/c$, equivalent to the group delay for propagation through a distance $L$ of vacuum. The pulse envelope of an optical pulse propagating in this medium traverses the slab as rapidly as if the slab were removed from the optical beam, regardless of the value of $\eta$.

Since the group velocity in a medium of this type is independent of the parameter $\eta$, it is reasonable to consider how one might determine the effective index of this material. In a coherent spectroscopic technique such as terahertz time-domain spectroscopy (THz-TDS), one measures the real electric field of the wave transmitted through a sample $E_S(t)$, and compares to a reference measurement $E_R(t)$, typically one in which the sample has been removed from the beam [5]. It is generally presumed that, with complete access to both $E_S(t)$ and $E_R(t)$, one can uniquely determine the phase velocity of light in the sample [80, 144]. In the case under consideration here, the measured phase difference, $\Delta\phi = \phi_S - \phi_R$, is given by:

$$\Delta\phi = \left(n_{\text{eff}}(\omega) - 1\right) \frac{\omega L}{c} = \eta \frac{\Omega_0 L}{c},$$

which is a frequency-independent constant. However, it is important to note that this constant is only determined up to an additive multiple of $2\pi$. This ambiguity implies that $\eta$ cannot be uniquely determined from a single experiment.

This phase ambiguity is of course well known [155, 156], and in many situations can be avoided. One can apply a Kramers-Kronig analysis, if the measured bandwidth is sufficiently large. More practically, one can often appeal to a continuity condition, such as the fact that the phase must extrapolate continuously to zero as $\omega \to 0$. However, this condition may be difficult to apply if the sample exhibits sharp resonances at frequencies
below the range of interest. In this case, it may not be possible to determine the phase velocity, even with complete information about both $E_S(t)$ and $E_R(t)$.

7.2 Experimental Setup

As an example of a physical system which manifests this behavior, we consider propagation of radiation through a photonic crystal slab, in a direction perpendicular to the plane of the slab. Recently, out-of-plane propagation has attracted a great deal of attention in the photonic crystal community, due to the significance of out-of-plane loss mechanisms [26, 131-134]. For propagation perpendicular to the slab, calculations of the long-wave (homogeneous) limit pose special challenges [141]. In addition, guided resonances, which couple to freely propagating out-of-plane modes, have recently been the subject of intense study [28, 135-138]. Despite the significance of out-of-plane propagation, there have been only a few experimental reports of transmission or reflection spectra [26, 131, 134, 138-140], and none with sensitivity to spectral phase.

The experimental setup is the same as in the out-of-plane measurement in Chapter 6. We employ THz-TDS to determine the complex transmission coefficient of a photonic crystal over a broad spectral bandwidth [90, 91, 93, 100, 101, 105]. The sample is a slab (305 $\mu$m thick) of high-resistivity ($\rho > 10^4 \Omega\text{-cm}$) silicon ($n = 3.42$), with an array of circular holes etched all the way through, using deep reactive ion etching. The holes have diameters of 360 $\mu$m, and are arranged on a hexagonal lattice with a pitch of $a = 400$ $\mu$m. The remaining dielectric occupies $\sim$26% of the slab, so the volume-weighted average dielectric is $\varepsilon \sim 3.8$. In order to confirm that the bandwidth of the incident pulse is broad enough to extract useful spectroscopic information up to 1.5 THz, we also
measure a silicon slab of equal thickness but with no holes.

7.3 Group Delay

We have recently described the first measurements of the dispersion in photonic crystal slabs for the case of propagation perpendicular to the plane of the slab. At relatively low frequencies, we observed a strong variation in the phase [130], superimposed on phase jumps associated with guided resonances [28, 135]. However, as shown in figure 7.1, at higher frequencies there is a fairly abrupt transition at ~0.9 THz to a nearly frequency-independent plateau.

Figure 7.1 The measured relative phase, $\Delta \phi = \phi_s - \phi_R$, for (a) a solid silicon slab and (b) a photonic crystal slab. In (a), the solid curve is a calculation of the Fabry-Perot phase, using the known thickness and refractive index. This shows that the measured results are reliable up to at least 1.5 THz. In (b) the solid curve is a finite-difference time-domain (FDTD) simulation. Above 0.9 THz, the relative phase is nearly constant, indicating a group velocity equal to the vacuum speed of light in this broad spectral range.

This region of constant $\Delta \phi$ persists over a wide spectral range, extending beyond 1.5 THz, the high-frequency limit of our measurement. If we define the scale frequency
\( \Omega_0 \) as \( 2\pi c/a \approx 2\pi \times 0.75 \text{ THz} \), then we can extract from the value of \( \Delta \phi \) in this region (using equation 2) the value \( \eta \approx 1.2 + 1.3p \), where \( p = 0, 1, 2, \ldots \), reflecting the phase ambiguity.

![Graph](image)

**Figure 7.2** Time-domain waveforms after propagating through air, a solid silicon slab, and the photonic crystal slab. These have been filtered to remove all spectral content below 0.9 THz, as described in the text. The solid curves show the pulse envelopes, while the dashed curves show the real electric field. The group delay (transit time) through the photonic crystal slab is identical to that of air, whereas the middle (solid silicon) waveform is delayed by \( \Delta t = (n_{si} - 1)L/c \) relative to the other two. Curves vertically offset for clarity.

This effect is even more dramatic when viewed in the time domain. We first apply a frequency-domain window to the measured THz pulses in order to remove all spectral content below 0.9 THz, where the propagation is strongly dispersive. We then inverse Fourier transform, and show the resulting filtered waveforms in the time domain (see figure 7.2). Of course, the spectral windowing introduces distortions in the waveforms, but since the same window is used for all three cases it is reasonable to make comparisons among them. In these time-domain data, it is clear that the group delay for transmission through the photonic crystal is the same as for air, and quite distinct from
that of a solid silicon slab of equal thickness. In essence, the radiation above 0.9 THz acts as if it propagates only through the holes and not through the solid dielectric, despite the fact that the dielectric occupies about one fourth of the illuminated area.

This phase transparency is likely an indication of a feature in the out-of-plane band structure of the photonic crystal slab. In particular, we would expect that at least one strongly coupled band lies parallel to the light line in a broad spectral range. For normal incidence \( k_\parallel = 0 \), such band structures are difficult to compute because the wave experiences no periodicity along the propagation direction. Furthermore, the surfaces of constant phase inside the material are not planar, but rather are corrugated with the periodicity of the lattice \([141]\). Finally, accurately accounting for the finite thickness of the slab poses serious computational challenges \([157]\). So, we rely on finite-difference time-domain (FDTD) calculations for comparisons. The solid curve in figure 7.1(b) shows an FDTD simulation which accurately reproduces all of the significant features of the data, in particular the abrupt transition to zero dispersion at 0.9 THz.

Of course, using THz-TDS one also obtains a measurement of the amplitude transmission coefficient. This result is shown in figure 7.3. The transmission coefficient resembles a Fabry-Perot spectrum at very low frequencies, then exhibits signatures of guided resonances starting at \( \sim 0.5 \) THz. It is interesting to note that there are no abrupt changes in the qualitative features of this spectrum near 0.9 THz. We interpret the structures in the amplitude spectrum as being due to the onset of coherent diffraction. At frequencies near and above \( \Omega_0 \), the two-dimensional periodic structure can act as a diffraction grating, giving rise to beams propagating at large angles to the normal. These diffracted beams, which do not reach the detector, deplete the transmitted beam and give
rise to a complicated transmission spectrum such as shown in figure 7.3. We note that, at lower frequencies (between 0.5 and 0.9 THz), the dips in the spectrum arising from guided resonances align precisely with abrupt jumps in the phase spectrum, as expected. These discontinuities make it difficult to extrapolate the high frequency phase towards \( \omega = 0 \).

![Graph](image)

Figure 7.3 The amplitude transmission coefficient, \( |E_S(\omega)/E_R(\omega)| \), for (a) a solid silicon slab and (b) a photonic crystal slab, corresponding to the two phase measurements shown in figure 7.1. As in figure 7.1, the solid curve in (a) is computed from the Fabry-Perot effect, demonstrating the reliability of the measurement up to at least 1.5 THz. The spectrum in (b) shows no obvious signatures corresponding to the abrupt change in the phase spectrum at 0.9 THz.

7.4 Conclusion

In conclusion, we report what is to our knowledge the first example of an anomalous group delay which extends over a broad fractional bandwidth, \( \Delta \omega/\omega > 50\% \). This striking behavior is observable only in the phase of the transmitted light, with no
obvious signatures in the amplitude spectrum. The broad bandwidth indicates that the effect is not related to the dispersion in the vicinity of a single resonance, but rather is a consequence of the characteristics of the out-of-plane photonic band structure. Further work will be required to understand if this is a general feature of high contrast photonic crystal slabs, or if it is specific to a particular set of structural parameters.
Chapter 8

Guided Resonance Modes in Photonic Crystal Slabs

In chapter 6 and 7 we discuss the out-of-plane dispersion at low and high frequencies. The middle-frequencies part between the two is also interesting. Here we describe guided resonance modes observed at the middle frequency range. In the time domain, we observe two stages of guided resonance modes: an initial transmission pulse and a long decaying tail. In the frequency domain, signatures of guided resonances are observed to be superimposed on a large dispersive effect. Those results are in good agreement with Finite Element Method simulation.

8.1 Introduction

Photonic crystals are materials that exhibit periodicity in the dielectric function in one or more dimensions [6-8]. They have been intensively investigated theoretically and experimentally to control the radiation fields and optical properties of materials. Although a three-dimensional photonic crystal is desired to completely confine the radiation fields, it is difficult to fabricate such kind of structures. Much attention, therefore, has been turned to photonic crystal slabs, which can be fabricated more easily and accurately.

Photonic crystal slabs are dielectric slabs with two-dimensional in-plane periodicity of refractive index. They control in-plane radiation fields by two-dimensional periodic dielectric structure, and in the third direction, light is confined in the structure
due to the refractive index difference [27]. This third-direction confinement is, therefore, not complete and some modes can couple to external radiations, resulting in so-called guided resonances or leaky modes [28, 131, 137-139, 158-162]. Those resonances are not stable modes and they can decay out of the slab. Vice versa, external radiations can couple to and excite those resonances.

In the band structure diagram, the guided and leaky modes are separated by the light line, below which the modes are guided and cannot couple to external radiations, and above which modes have finite lifetimes and slowly couple to external radiations [27]. This coupling provides a way to excite these resonance modes using external waves. However, it is found later that some modes above the light line are also not leaky, because coupling between them and external radiations are prohibited by the mismatching of spatial symmetries [160-162]. This provides the possibility of a complete confinement of certain radiation using photonic crystal slabs. Although there have been quite a few theoretical and experimental investigation on those resonances, almost all focus on their power transmission properties, and there are very few reports on their dynamics and phase properties.

Here we present study of photonic crystal slabs using terahertz time-domain spectroscopy [5]. This permits direct time-resolved measurement of the electric field with sub-cycle temporal resolution. The dynamical properties can be directly characterized, and the power spectra and phase spectra can be obtained independently at the same time. Our photonic crystal slab consists of a hexagonal array of holes etched all the way through a 305µm thick high-resistivity silicon wafer (>10⁴ Ω•cm) using deep reactive ion etching method. The holes have diameters of 360 µm, and they are arranged
on a 400 \( \mu m \) lattice. Silicon has a frequency-independent refractive index of 3.42 in our interested frequencies, and the volume-weighted refractive index of the photonic crystal slab is calculated to be 1.96. Rather than studying the slab's in-plane properties, which we have done before in waveguide geometry [90, 105], here we employ an out-of-plane excitation geometry to study the slab sandwiched between air claddings. Generated by photoconducting antennas, broadband and linearly polarized pulses are collimated by a lens and then transmit through the sample, along the direction parallel to the axes of the cylindrical holes. Waves of the same polarization are then detected by the photoconducting-antenna detector. For comparison, we have measured transmission through an un-etched silicon wafer of the same thickness. A reference measurement is taken when there is no any sample present.

8.2 Temporal Behavior of Guided Resonances

Typical measured waveforms are shown in figure 8.1. Air reference signal is a single-cycle pulse of \(~1\) picosecond duration and a broad bandwidth from 0.05 to 1.2 THz. The solid silicon wafer shows pronounced echoes in the time domain due to multiple reflections. These oscillations are also present in the waveform transmitted through the photonic crystal slab, but in this case there are also pronounced decaying oscillations, persisting for tens of picoseconds. To distinguish features from the interaction of the radiation with the samples and those intrinsic to the THz system, here we employ a Fourier and wavelet based scheme to simultaneously deconvolve and denoise the air reference signal from the sample signals [163]. The results are shown as the bottom two curves in figure 8.1, with both being shifted the same value along the time
axis for a better comparison. Three reflected pulses can be clearly observed for solid silicon wafer, as denoted by those small arrows. The time difference and amplitude ratio between any pulses are in good match with theoretical predictions and it demonstrates the soundness of the deconvolution technique. When the incident pulse transmits through the photonic crystal slab, two distinct stages are observed: an initial pulse and a following decaying tail. The decaying tail comes from part of the incident waves that excite the guided resonances. Since guided resonances are modes not supported inside the crystal, they decay out of the slab with various speeds depending on their individual lifetimes and then form the decaying tail. This phenomenon was predicted before by Fan et al. using Finite-Difference Time-Domain (FDTD) simulation [28], but it is the first time in our knowledge to observe it experimentally. The other part of the incident wave goes straight through the slab and forms the initial pulse, and in this initial pulse, different frequency components arrive at different times, which manifests the effective refractive index is frequency dependent.

![Waveform Diagram]

Figure 8.1 Typical time domain waveforms. From top to bottom, the top three signals are for air, un-etched silicon wafer, and photonic crystal slab, respectively. The bottom two curves illustrate the deconvolution of the air signal from the silicon wafer and photonic crystal slab signals, respectively. These deconvolved signals highlight the interaction of the radiation with the samples under study.
8.3 Transmission Spectra of Guided Resonances

To quantify this dispersive effect and the guided resonance effect, we can study them in the frequency domain. Since we are detecting the electric fields directly, we can perform Fourier transformation to get spectra information. Figure 8.2 shows the power transmission spectra, calculated relative to air reference.

![Power transmission spectrum](image)

**Figure 8.2** Power transmission spectrum, computed using the Fourier transforms of the time-domain waveforms, with the air signal as a reference. Upper: Results for the silicon wafer from measurement (square) and theoretical calculation considering only the Fabry-Perot effect (solid). Lower: Circle line shows the experimental results for the photonic crystal slab. Finite Element Method is used for simulation and it (solid line) agrees very well with the experimental results. Limited by our computation power, we can only reach frequencies up to about 0.75THz at this moment.

Many oscillations can be observed in the measured solid silicon wafer curve, which can be well explained by taking into account only the Fabry-Perot effect, as shown by the solid line, calculated assuming a real and wavelength-independent refractive index 3.418. Numerous transmission minima, which are manifestations of guided resonances modes, can be observed in the photonic crystal slab for frequencies larger than 0.5 THz. To explain what we observed, here we use Finite Element Method to calculate the
transmission spectra. In the calculation, the slab is assumed to be losses, and the refractive index of the silicon 3.418 is considered to be wavelength independent. The result is shown as the thick solid curve in the plot, which matches well with the experimental results, especially the positions of guided resonances modes.

Different dispersions result in not only different power transmission coefficients, but also, more distinctly, different phase spectra. It is therefore more instructive to investigate the phase spectra to determine the effective refractive index. Here we extract directly the phase information from the measured amplitude of electric fields. The net phase shift $\Delta \varphi(\omega)$ between sample signals and the reference signal are show in figure 8.3.

![Graphs showing phase spectra](image)

**Figure 8.3** Upper: phase spectra of the silicon wafer, subtracted by that of the air reference signal, from experiments (gray) and theoretical calculations (solid line). Lower: phase spectra of the photonic crystal slab, subtracted by that of the air reference signal. Results from the experiments are shown as square and those from FDTD are shown as the solid line. Excellent agreement is obtained between the two. The thin black arrows denote the positions of guided resonances.

Induced by the silicon wafer are many regular oscillations superimposed on a straight line. These are signatures of the Fabry-Perot effect, which is calculated and
shown as the solid line in upper part of figure 8.3, and excellent agreement is obtained between the two. In the calculation the refractive index of silicon slab is set again to be 3.418. The effect of photonic crystal slab on the phase, on the other hand, is much more complex, and two components can be observed here: a smooth profile and jumps superimposed on the profile. Those jumps, indicated by the thin black arrows, are resulting from the guided resonances. With the increase of the frequencies, the slope of the phase curve increases, and this represents increasing effective refractive index. Using FDTD simulation, with refractive index of silicon being a frequency independent number 3.418 and that of air holes being 1, we obtain the solid line, which matches the experimental results almost perfectly.

8.4 Dispersion Relation

We can then examine the dispersion relation using the thickness $L$ of the samples and the phase difference $\Delta \phi(\omega)$ between the sample signals and the reference signal:

$$k = \frac{\omega}{c} n(\omega) = \frac{\omega}{c} \left[ \frac{c \times \Delta \phi(\omega)}{L \times \omega} + 1 \right] = \frac{\Delta \phi(\omega)}{L} + \frac{\omega}{c}$$

where $k$ is the out-of-plane wave vector, $n(\omega)$ is the frequency-dependent refractive index and $c$ is the light speed in vacuum. The as-calculated dispersion relation is shown in figure 8.4, with solid lines from theoretical predictions. With the increase of the out-of-plane wave vector, the frequency increases with varying slopes, which manifest the existence of the unusual dispersion. The agreement between measured data and simulation is excellent. The effect of guided resonances is also present and denoted by the blank area. Phase jumps resulting from the resonances make it hard to get an accurate determination of the dispersion for this region.
Figure 8.4 The dispersion relation from photonic crystal slab. Triangle shows the experimental results and solid line shows the FDTD simulation. The blank area between the two dashed lines denotes the region where there are phase jumps resulting from guided resonances, so an accurate determination of the dispersion for this region is not available.

As a final note, all of above results are for normal incidence. We have observed very similar dispersive effects when changing the incident angles for up to 30° away from the slab normal. But for in-plane excitation, there are no these effects. It would be interesting to look into when and how the transition between the two cases happens.

8.5 Short-Time Fourier Transform

To better illustrate what we observed, similar to what we did in chapter 4, here we present the measured signals in both time and frequency domain using Short-Time Fourier Transform (STFT). We choose the duration of the sliding window to be 4 picoseconds in STFT. To avoid dynamic range problems in the false color plot data, we normalize $S(\omega, t)$ at each frequency by dividing by the maximum value for that frequency.
The results are shown in figure 8.5. Following the initial pulse, there is a second pulse in the silicon signal. The time difference between the initial pulse and the second pulse is exactly the time needed to travel back and forth in the silicon slab, which indicates the second pulse is a reflected pulse and this demonstrates the Fabry-Perot effect.

![Figure 8.5](image)

**Figure 8.5** Short-time Fourier transform false color plots of the THz pulses transmitted through silicon (top) and photonic crystal slab (bottom). The Fabry-Perot effect in the silicon sample is manifested by the reflected pulse following the main input pulse. In the PC signal, at low frequencies, the arrival time increases with frequency, indicating the increase of effective index. At the middle frequencies, at many picoseconds later, there are still components. At high frequencies, almost all frequency components arrive at the same time, indicating the broadband group delay anomaly discussed in chapter 7.

In the photonic crystal plot, all of the phenomena observed in chapter 6, 7 and 8 are shown in this single figure. At low frequencies, the arrival time increases with frequency, indicating the increase of effective index, which is discussed in chapter 6. At the middle-range frequencies, at many picoseconds later, there are still components. This is resulting from the guided resonance modes which decay out of the slab with varying
speeds. At high frequencies, almost all frequency components arrive at the same time, indicating the broadband group delay anomaly discussed in chapter 7.

8.6 Conclusion

In summary, we have studied photonic crystal slabs using out-of-plane excitation with terahertz time domain spectroscopy. Together with the properties of the dispersive effects, those of the guided resonances are examined in the time domain waveforms, in the transmission spectra, and in the phase spectra. Our experimental results are in remarkably good agreement with simulation results. These results highlight the value of pulsed terahertz techniques in studies of guided resonances in photonic crystal slabs, since it permits a complete characterization of these resonant phenomena.
Chapter 9

Angled Incidence and Displacement Sensitive Structures

In previous chapters we discuss the out-of-plane properties of photonic crystal slab for normal incidence waves. Here we consider the angled incidence situation. We observed strong dispersive effects, guided resonance modes and broadband group delay anomaly for non-normal incidence of waves. By putting two photonic crystal slabs next to each other, we observe similar effects. The two-slab structure can be a sensor structure, as we change the spacing between the two slabs, the transmission spectra change accordingly.

9.1 Introduction

In previous chapters we investigate the out-of-plane properties of photonic crystal slab and we observe large dispersion effects at low frequencies [130], guided resonance modes most prominent at middle frequencies, and broadband group delay anomaly at high frequencies [146]. All those are observed for the waves propagating perpendicular to the slab. One might ask if there are similar effects for non-normal incidence waves. Also, in those experiments only one single slab is used, thus, another question would be if there are similar effects when there is more than one photonic crystal slab. Here we will address those questions both experimentally and theoretically.

The radiation source and detectors are still terahertz time-domain spectroscopy, which generates terahertz waves with a broadband frequency range from 0.1 up to about
1.6 THz. The samples we use here are the same as before, which is a high-resistivity silicon slab with a thickness of 305 microns. Many circular holes are etched in the slab using deep reactive ion etching method, with the diameter of the circular holes being 360 microns. These holes form a hexagonal lattice with a pitch of a=400 microns. For reference, we have taken the measurement where is no any sample, which we refer to as air signal.

9.2 Angled Incidence

Instead of perpendicular to the slab, here waves are illuminated onto the slab with an angle $\theta$ with respect to the slab normal. A schematic of the experimental setup is shown in figure 9.1, with the black arrow representing the incident direction of waves and the dashed line being the slab normal.

![Figure 9.1 A schematic of the out-of-plane experimental arrangement. The photonic crystal slab is illuminated at normal incidence to the plane of the periodicity. The THz beam spot size is large enough to illuminate many holes.](image)

With this experiment setup, we can fix the positions of the terahertz wave transmitter and detector, and get different incident angles by rotating the slab with respect
to the slab normal. We have measured waveforms at a number of different angles, ranging from $\theta=0$ up to $\theta = 30$ degrees, with a step of 5 degrees.

Figure 9.2 shows the deconvolved signals for typical detected time-domain waveforms, using the same deconvolution and denoise scheme described in chapter 8. Signals detected at the different angles have similar profiles, which consists of two components: an initial pulse and a long decaying tail. This suggests that there are still guided resonance modes in non-normal incident cases. However, those modes may exist at different frequencies, and have different lifetimes, judging from the different shapes of the decaying tail. This will be more obvious in the transmission spectra. The initial pulse exists in all the signals, suggesting the existence of the group anomalies, which we will see more in the phase spectra. The amplitude of the initial pulse decreases with the incident angle. This may result from the fact that with the increase of the angle, the incident waves see smaller area of the holes in the slab, therefore the amplitude of the group anomaly part decrease.

Figure 9.2 The deconvolution of the air signal from photonic crystal slab signals measured at different incident angles, ranging from 0 up to 30 degrees, respectively. Although measured at different angles, these signals have similar profile, while changes also exist, such as the amplitude of the initial pulse decreases with the increase of the angle.
Starting from the measured electric fields for air reference and photonic crystal slab, we can Fourier transform both and get the ratio, which is the transmission spectra and the results are shown in figure 9.3. Once again, all signals have similar profiles. At the low frequency part, there are Fabry-Perot like oscillations, and at frequencies higher than 0.5 THz, there are numerous transmission minima, which are manifestations of guided resonance modes. With the change of the incident angle, new transmission minima emerge, as denoted in the black dashed line area. These are new guided resonance modes, which are excited because of the change of the incident angle. Many other new guided resonance modes can be observed in the figure.

![Figure 9.3 Gray lines are experimental power transmission spectra for waves detected at different incident angles, computed using the Fourier transforms of the time-domain electric waveforms with the air signal as a reference. They are offset for clarity. The black dashed line shows new guided resonance modes emerge with the change of the incident angle.](image)
Almost all the unusual features observed in the previous have their prominent signatures in the phase spectra. Here we also examine the phase spectra by directly extracting the phase information from the measured amplitude of electric fields for different incident angles, then obtaining the net phase $\Delta \varphi(\omega)$ between sample signals and the corresponding reference signal. The results are show in figure 9.4. These curves are almost the same, indicating there are almost same dispersive effects at frequency below 0.5 THz, guided resonance modes between 0.5 and 0.9 THz and group delay anomaly above 0.9 THz.

![Figure 9.4 Phase spectra of the photonic crystal slab, subtracted by that of the air reference for four representative incident angle $\theta$=5, 10, 20 and 30 degrees, from top to bottom, respectively. These curves are offset for clarity. They are almost the same, indicating there are almost same dispersive effects, guided resonance modes and group delay anomalies no matter what is the incident angle.](image)

Changes, of course, exist in the different incident-angle curves. Shown in figure 9.5 is a small portion of the figure 9.4. As denoted by the gray dashed circle, different guided resonance modes emerge with the increase of the angle. This echoes the results in
the transmission spectra shown in figure 9.3, where at the same frequencies, there exist extra transmission minima at larger incident angles.

Figure 9.5 Phase spectra of the photonic crystal slab, subtracted by that of the air reference signal for different incident angles. An extra guided resonance modes is highlighted in the gray circle. This result echoes what we obtained in the transmission spectra.

9.3 Two-Slab Structure

In this section we study a two-slab structure. This structure is first proposed by Suh et al [9] as a displacement sensitive structure, with the possibility of being an all-pass transmission or flat-top reflection filter [136]. The operation of these devices is based on the coupling of guided resonance modes between the two slabs. In this study, we study this structure experimentally, and compare experimental results with simulations. We not only investigate transmission spectra, but also phase spectra, and compare them with those of a single slab.

Figure 9.6 shows a schematic of the two-slab structure, which consists of two of our photonic crystal slabs, as described above, with the longitudinal spacing $t$ and lateral
shift $s$ between the two slabs. Incident waves illuminate the structure along the direction perpendicular to the slab. Changing $t$ and $s$ can result in tuning of the transmission and reflection spectra of the structure.

![Diagram of the two-slab structure experiment](image)

Figure 9.6 Schematic of the two-slab structure experiment. The black arrows denote the direction of the incident waves. The transmission spectra depend significantly on the separation $t$ and the lateral shift $s$ between the two slabs.

As an example, here we show the transmission spectra of the structure with longitudinal shift $t = 390$, and 610 microns, respectively and of no lateral shift ($s=0$). The results are shown in figure 9.7, where the solid lines are from experiment, which are in excellent agreement with Finite Element Method simulation. In the simulation the dielectric constant of the silicon is considered to be a frequency-independent constant 3.418. The transmission spectra depend strongly on the spacing $t$, with transmission and reflection peaks appearing at different positions for different spacings. A transmission minimum can be observed at 0.41 THz. As we increase the spacing from 390 to 610 microns, the minimum moves to 0.37 THz. This suggests that by changing the spacing
between the two slabs, we can manipulate the properties of the structure. We can take advantage of this to make frequency-select filters to pass or block arbitrary frequencies.

![Transmission spectra](image)

**Figure 9.7 Transmission spectra through a two-slab structure, with the spacing of 390 and 610 microns, respectively. Solid lines are experimental results, which agree well with the FEM simulation results shown in gray dashed lines.**

Since we are directly detecting the electric fields of the waves transmitted through the structure, we can examine its phase spectra in addition to the transmission spectra. Figure 9.8 shows the phase spectra of the two-slab structure of different spacing \( t \), subtracted by that of the air reference signal, as indicated by the black squares and gray triangles. The gray circles show the 2 times of the phase of a single slab. Although some small changes can be found among those three curves, they all have three stages: the huge dispersive effects at low frequencies, the guided resonance modes most prominently at middle frequencies, and the broadband group delay anomalies at high frequencies.

The inset shows the difference between the phase from the two-slab structure of \( t=0 \) micron and the two times of the phase of a single slab. The difference is quite small
at frequency smaller than 0.5 THz. This means the dispersive effects of a two-slab structure are twice that of a single slab, no matter what is the spacing. That is, those slabs just behave as the other one does not exist, and there is no coupling between the two slabs at those low frequencies. This can be understood as the wavelengths of those low-frequency waves are longer than the slab thickness; they therefore transmit straight through the slabs without much interaction with the slabs. At frequencies higher than 0.5 THz, however, exist many oscillations around the mean value zero. These oscillations come from the near-field and evanescent coupling, which then introduces splitting of guided resonance modes at different frequencies [9] and causes these oscillations.

Figure 9.8 Phase spectra of photonic crystal slabs, subtracted by that of the air reference signal. The gray circles are from a single slab, and multiplied by two. The black squares are from a two-slab structure with the spacing t=0 microns. The triangles are for two-slab structure whose spacing t is 80 microns. These curves are offset for clarity. There are only minor differences between those curves, as indicated by the inset which is the difference between the top two curves.
Other than the longitudinal spacing, there could also be lateral shift, where s is not zero. Figure 9.9 shows the phase spectra of two-slab structures with fixed longitudinal spacing t and different lateral shift s. Once again, the phase spectra are the same at low frequency part, and changes begin from frequency higher than 0.5 THz. At high frequencies, the phase spectra are still straight, and they start from almost the same frequencies, indicating the existence of the same broadband group delay anomalies as in a single slab.

![Phase spectra of two-slab structures](image)

Figure 9.9 Phase spectra of two-slab structures with spacing t=80 microns, subtracted by that of the air reference signal. From top to bottom, the black circles, the gray square, the black diamonds, and the gray triangles correspond to lateral shift of 0, 80, 160, and 305 microns, respectively. These curves are offset for clarity. These curves are more or less the same, and all have dispersive effects, guided resonance modes and group delay anomaly from low to high frequencies.

9.4 Conclusion

In summary, comparing to normal incidence situation, we observed similar and the same order dispersive effects at low frequencies for angled incidence, and new guided
resonances modes appear with the change of the incident angle, in time waveforms, transmission spectra and phase spectra. At high frequencies, there are still broadband group delay anomalies. In two-slab structures, we observed the transmission spectra are displacement sensitive, and the results are in good match with FEM simulation results. The phase spectra of two PCs also have the same features as those of a single slab, and the dispersive effects are twice big as those of single slab, no matter what are the longitudinal and lateral shifts.
Chapter 10

Summary of Results and Future Prospects

In this chapter, a summary of what have been studied will be given. Following that, I will talk about more experiments for further study.

10.1 Summary of Results

This thesis describes the study of two-dimensional photonic crystals slabs with terahertz time domain spectroscopy. In the study we first demonstrate the realization of planar photonic components to manipulate terahertz waves, and then characterize photonic crystal slabs, especially their out-of-plane properties, using terahertz pulses.

In the effort to construct planar photonic crystal devices, we have showed it is possible to use photonic crystals to manipulate the flow of terahertz waves inside two metal-plate waveguide. We have successfully demonstrated transmission filters, reflections filters, defect modes and superprisms. To make integrated terahertz photonics possible, more photonic components would be needed. Photonic crystals can be used to make many such components to satisfy the development of field. Here in this chapter I will introduce some devices that would be interesting to fabricate and test.

In the out-of-plane studies of photonic crystal slabs, we have found many interesting effects. At low frequencies, we found very strong dispersion that is not amenable to homogenization theory; at medium frequencies, we found many signatures of guided resonance modes; and at high frequencies, we observed a surprising group
velocity anomaly. All those effects are worthy of further investigation to elucidate their origins by studying samples with a variety of different parameters. In this chapter I will discuss more about this.

What we have studied in this thesis is two-dimensional photonic crystal slab. As pulsed terahertz technology has many unique properties, it would be also interesting to use it to study other more complex photonic crystal structures, such as three dimensional photonic crystals, especially given that there are many interesting photonic crystal properties that have not been touched in this thesis, such as negative refraction, slow light, and quantum information processing.

10.2 Planar Photonic Crystal Devices

With photonic crystals, we have demonstrated planar terahertz devices such as transmission filters, reflection filters, and defect modes. More devices can be constructed by using photonic crystals to manipulate terahertz waves, through introducing defects into photonic crystals or using certain special photonic bands.

By introducing defects into photonic crystals, waves whose frequencies are in the band gap will have nowhere else to go but to flow along the defects. This principle makes it possible to construct many devices, such as a waveguide bend, which can steer light around sharp corners with small loss [37]; and a waveguide branch, in which light will flow with the defect linear waveguides [38].

As an example, Figure 10.1 shows some devices made from two-dimensional photonic crystals that can be put into the terahertz parallel-metal-plate waveguide. Those circles represent one kind of material that stands in another kind of material with different
dielectric function. Figure 10.1(a) shows a perpendicular waveguide bend, where waves whose frequencies inside a band gap will flow along direction indicated by the arrows. (b) shows waveguide splitter, where waves of the frequencies in a band will be split into two beams. (c) shows a channel add-drop filter, where waves can couple from the input linear waveguide to the output linear waveguide through the two defects which act as coupling elements [39]. (d) shows a waveguide branch, with the same working principle as in (b).

![Figure 10.1 Schematics of two-dimensional photonic devices made from photonic crystals. (a): a waveguide bend. (b): a waveguide splitter. (c) a channel add-drop filter. (d) a waveguide branch. Here those circles can be considered as the air holes etched in a solid slab, or as solid rods standing in air, even more generally, as one material standing in another material of different dielectric function.](image)

Of course, those are just examples of photonic devices that can be made from photonic crystals by manipulating the shape of defects. One can make more of those
devices by fiddling with the shape of defects, the lattice structure, the size of those circles, the dielectric functions of those circles and surrounding materials. Other than two-dimensional photonic crystals, one may also consider devices made from one or three dimensional photonic crystals.

10.3 Superprism Effects

Other than introducing defects to photonic crystals to control the flow of light, one can also use photonic bands to reach the same goal. For example, certain photonic bands can have very strong curvature, and that can be used as a prism. Comparing with conventional gratings and prisms, this effect is orders of magnitude stronger, therefore it is called superprism.

The superprism effect was first found by Kosaka and coworkers [42]. They reported that a single-frequency light beam swings inside a photonic crystal when the incident angle changes. Later they found the output direction also changes when the frequency of the input wave is changed [43]. The effect is also polarization dependent; waves with different polarization have different output angles [44].

To understand this superprism effect, we can calculate the band structure in the whole first Brillouin zone, instead of just along some high symmetric points in a typical band structure plot. Figure 10.2 (a) shows the band structure of our photonic crystal. The bottom is in-plane wave vector, and the vertical axis is frequency. A band gap can be clearly seen from the plot, where there are no any bands.
Figure 10.2 (a) Band structure of our photonic crystals with infinite thickness. The horizontal axes are in-plane wave vectors. A band gap can be clearly seen from the surface. (b) Equi-Frequency contour. The red dotted line is the projection of the mode that has its frequency of 0.67 c/a onto the bottom plane, and the solid line is the projection of the mode which has its frequency of 0.06 c/a. The solid line is a circle, which is symmetric, while the red dotted line is highly asymmetric. This asymmetry is where the super prism comes from.

If we project some modes onto the bottom plane, we get the equi-frequency contour shown in figure 10.2(b). The gray lines show the first Brillouin zone, and those black dots are high symmetric points in the first Brillouin zone. The contour for some modes is a circle, while for others it is highly asymmetric. As the wave propagation direction is determined by group velocity direction dω/dk, for those modes that have circular contour, the propagation direction in the photonic crystal will be always the same as the input direction in the input material. However, they could be different for modes with asymmetric contours. For example, as indicated by the red arrow, those waves have their incident direction along Gamma-M direction. The output wave is still along that direction, because dω/dk is along that direction. But if the incident angle changes a little, such as shown by the blue line starting from Γ point, then the output wave in the photonic crystal will be along a totally different direction, as shown by the blue line starting from a
point on the red line. This is the origin of the superprism effect.

As our calculation results show there is superprism effect in our photonic crystal, we can do experiments to verify those results. In the experiment, photonic crystals are put between two copper plates which will act as a terahertz waveguide. When the propagation direction of the incident terahertz waves is not perpendicular to the crystal normal, waves of different frequencies will exit the photonic crystal at different positions. One can also cut the photonic crystal, and the output angles of waves with different frequencies will be different.

Other than the superprism effect, photonic bands can also have other properties. For example, a band at certain region could be quite flat, that is, $d\omega/dk$ is small. This indicates the group velocity is small for relevant frequencies. This phenomenon could be used to study slow light or construct optical delay lines [164]. A band could also decrease with increasing wave vector $k$, that is, $d\omega/dk$ is negative. This indicates a negative refraction [10], and it can be used to make superlens which would make perfect images without any physical resolution limitations [57].

10.4 Group Velocity Anomaly

In the out-of-plane study of photonic crystal slab, we have found several interesting things, such as the group velocity anomaly at high frequencies. To have a more complete understanding the observed phenomena, one needs to study the effects of many different things, such as the effect of hole sizes, lattice structure, lattice pitch, slab thickness, hole shapes, and slab material. Here I will explore them one by one.

The first one we want to do is to keep everything else unchanged, and only
change the diameter of holes. This would allow us to investigate the role of hole sizes on the anomalous effect. By varying the hole diameter, we essentially change the band structures and modes that can be supported. As an example, we can make two such devices: one with hole diameter of 300 microns, and the other of 250 microns. In terms of frequency in vacuum, those dimensions are 1 THz and 1.2 THz, respectively. They are distinctly different from each other so we can resolve them in frequency with our terahertz time domain spectroscopy. That would make the explanation of data easier.

The second thing we want to do is to investigate the role of lattice structure on the anomalous effect, and we do that by changing the lattice structure while keeping everything else unchanged. One of the most widely used lattice structures is square lattice. Here we can make two such devices: one square lattice with hole diameter of 360 microns, and the other square lattice with hole diameter of 300 microns. This would provide opportunities for us to compare results from square lattice to those of hexagonal lattice.

The lattice pitch might play an important role on the anomalous effect, just like the plasmonic effect which results in the extraordinary transmission of waves through periodic holes in a metallic slab [165]. We can look into this by changing the lattice pitch. We propose to make two such devices: one with a pitch of 480 microns and the other whose pitch is 576 microns. We choose numbers because for one thing, we want to know if the results would be changed by changing the pitch; and for the other, we can compare results from those samples with those of hole sizes: because the ratio of 360 to 480 is equal to that of 300 to 400, and 360 to 576 is the same as that of 250 to 400.

We can also investigate the role of slab thickness on the anomalous effect, by
keeping everything else unchanged and just change the slab thickness. For example, we can make two such devices: one with thickness of 200 microns and the other 150 microns.

Other factors such as hole shapes slab material might also have different effects on the anomalous effect. Instead of circular holes, we may also study rectangle, square or other shapes. Changing the slab material is essentially changing the dielectric function of the photonic crystal, which will result in the change of band structures and it might also play an important role on the anomalous effect.

In a word, there are many unsolved issues in the fields of terahertz technology and photonic crystals. More research is wanted to explore new frontiers in those fields. With this, I end my thesis here.
Bibliography


