Light control by nanostructured metal surfaces and photonic crystals in nanobeams and freestanding membranes

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Front cover image: A modified Scanning Electron Microscope image of several photonic crystal nanocavities standing in a line on InGaAsP substrate.

Back cover image: A modified Scanning Electron Microscope image of suspended InGaAsP nanobeams.
Abstract

Light control by nanostructured metal surfaces and photonic crystals in nanobeams and freestanding membranes

The work presented in this thesis aims at studying the properties of photonic crystals (PhCs) and developing their applications, such as slow light waveguide, superlens, modulator and sensor. PhCs are periodic nanostructures, which affect the motion of photons in a similar way that periodicity of a semiconductor crystal affects the motion of electrons. In this thesis, both simulation and experimental studies are presented. For the simulations, the plane wave expansion and finite difference time domain methods are used to calculate the band structures of PhCs and obtain the field distribution of a finite PhC, respectively. The fabrication is done in the clean room with the state of the art technology. Exploiting the incorporated quantum dots, the optical characterization was performed with a micro-photoluminescence (μPL) experiment.

At terahertz frequencies, tailoring the topography of metal surface allows to localize the evanescent parts of surface waves to a distance significantly smaller than the wavelength. The propagation loss is discussed, when the metal is used as a waveguide. Normally, the loss is large when the group velocity is small. A new type of metal waveguide is designed for slow light with a small propagation loss and small group velocity dispersion by applying two thin metal slabs with subwavelength periodic corrugations on their inner boundaries.

Several dielectric PhC configurations are designed and analyzed for different applications. A PhC superlens is designed with a resolution of 0.164λ which beats the diffraction limit. The effect of disorder in the PhC on the extraction efficiency of a Light Emitting Diode is also studied by modelling the disordered PhC. A PhC waveguide is designed to make a fast modulator as an optical circuit component. A liquid crystal is used to tune the degeneracy of cavity modes of a PhC cavity. The latter design was verified experimentally.

A major part of the thesis is concerned with sensing. Miniaturization of label-free optical sensors is of particular interest for realizing ultracompact lab-on-
a-chip applications with dense arrays of functionalized spots for multiplexed sensing, which may lead to portable, low cost and low power devices. A PhC is very promising as a sensing element. A record high sensitivity PhC nanobeam is realized experimentally with a sensitivity of about 900 nm per refractive index unit. Simulations show that the quality factor can be substantially increased by tapering the two ends. Spectrally encoded PhC nanocavities by independent lithographic mode tuning are experimentally demonstrated for identification.

The PhC nanocavities are taken from the chip to serve as autonomous devices for (bio)sensing. The properties of these free PhC nanocavities are studied by nano-manipulation and µPL experiments. The possibility of attaching one PhC nanocavity to the end of a fibre to make a fibre sensor is shown. The feasibility of an alignment procedure by precise nano-manipulation is demonstrated, which will enable to make three dimensional nanophotonic structures.
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Chapter 1

Introduction

Optical devices based on photonic crystals (PhCs) are discussed in this thesis. A general introduction to the background of integrated photonic chips and sensors is given in section 1.1 and 1.2, respectively. In section 1.3 the theory and properties of PhCs are introduced. In section 1.4 surface plasmon polaritons at THz frequencies are introduced. Finally, the scope of this thesis is shown in section 1.5.

1.1 Integrated photonic chips

As a result of the mid-20th-century technology advancements in semiconductor device fabrication, integrated circuits have been developed. The capabilities of many digital electronic devices are strongly linked to Moore’s law. Moore’s law describes a long-term trend in the history of computing hardware. The number of transistors that can be placed inexpensively on an integrated circuit doubles approximately every two years. This trend has continued for more than half a century and is expected to continue until 2015 or 2020 or later. However, many challenges emerge as we continue to shrink device dimensions further.

The information transmission rate using purely electronic means is fundamentally limited: as the frequency of an electrical signal propagating through a conductor increases, the impedance of the conductor also increases, thus the propagation characteristics of the electrical cable become less favorable. That is the reason why electrical signals with frequencies above 10 MHz must be carried by specially designed conductors, called coaxial cables, in order to minimize the effect of a high attenuation.

Because of the parallel development of optically transparent or active materials, both dielectrics such as polymers, glasses or silica on silicon (SiO₂/Si), and semiconductors such as indium phosphide (InP), gallium arsenide (GaAs) or even silicon (Si), optical
ways of processing or transmitting data have been developed. A wide variety of novel and advanced integrated photonic devices was available to emerge on the market. After the development of the optical fiber, at the beginning of the 1980s, electronic data transmission was slowly supplemented by and even replaced by optical transmission with photons. The use of light for data transmission has many advantages. Light beams can propagate simultaneously with small interaction and low energy dissipation. For most optical materials used in optical communications and photonic devices, the useful frequency window falls in the visible and near-infrared range of the electromagnetic spectrum, which corresponds to light frequency in the range 150-800 THz, $10^6$ times the frequency used in electrical transmission! This high frequency gives the possibility of higher modulation frequency which can lead to higher bit rates.

Integrated photonic devices based on integrated optical circuits take advantage of the relatively short wavelength of the light in this range (0.5-2 µm), which allows the fabrication of miniature components using channel waveguides with the size of microns and smaller. The technology required to fabricate planar lightwave circuit components of such dimensions is common in the well-established micro-electronic technology, using the tools and techniques of the semiconductor industry. The basic concept in optical integrated circuits is the same as that which operates in optical fibres: the confinement of light. A medium that possesses a certain refractive index, surrounded by media with lower refractive indices, can act as a light trap, where the rays cannot escape from the structure due to the phenomena of total internal reflection at the interfaces. This effect confines light within high refractive index media, and can be used to fabricate optical waveguides that transport light from point to point.

Integrated photonic devices are necessary for efficiently processing optical data transmitted through optical fibers. In addition, they will eventually also be embedded in electronic integrated circuits to reduce their energy consumption and enable the continuation of Moore’s law. However, we should also note that the integration of photonics lags behind in comparison with the integration of electronics. The poor integration is mainly caused by the poor confinement capability of optical devices. When the sizes of optical devices are decreased, the light will leak out. In this case, the cross talk between nearby optical devices can be severe. Thus the key point to increase the integration of photonics is to improve the confinement of the optical devices. Photonic crystal (PhC) is one of the candidates to have better confinement of the photons, such as PhC nanocavities, which will be discussed in this thesis.
1.2 Sensors

An optical sensor is a device that measures a physical quantity and converts it into an optical signal, which can then be read by an observer or an instrument. Today, the sensor is an important technical foundation for the new technological revolution and the information society. Almost none of the development and application of science and technology can exist without the support of sensor technology. The 21st century is the century of life sciences. In particular the implementation of the Human Genome Project has greatly accelerated the development of new types of biological sensors, which are needed in multidisciplinary research fields and applications, such as medicine, health, food, chemical analysis and environmental protection. Biosensing is an emerging technology that combines microelectronics, material science and biotechnology.

Miniaturization, integration, multi-functionality, intelligence, wirelessness and portability are the requirements for a successful biosensor. The sensors based on optics can accomplish much in this area. Optical sensors offer various advantages over their electronic and/or mechanical counterparts. Optical sensors have wide dynamic range and lower noise levels. Also, the non-contact nature of the optical measurement avoids all systematic errors that come with tactile techniques. When the measured stimuli change, the corresponding refractive index, absorption, Raman scattering, surface plasmon resonance or fluorescence will change too, which can be measured by optical methods. Optical biosensors can be used to determine the biologically active substances such as enzymes, antibodies and other body fluids, and characterize living matter concentration, composition and other physical quantities. Because of its high sensitivity, short response time and small size, optical biosensors receive widespread interest.

Traditional optical biosensors are mostly based on measuring the fluorescence spectroscopy. This kind of sensor is usually simple and easy to implement, but some preparation before measurement like purifying samples and targeting fluorescent material are needed, while the markers may influence the reaction and contaminate the sample. For the sensors based on fluorescence spectra measurement, the fluorescence signal intensity depends on the amount of the sample. Thus for the ultra-small amount (femto-gram) sample, the signal is often too weak to detect. Integrated optics technology for optical biosensing opened a new realm. It solves the problems with the traditional bulky optical system, such as poor stability, beam alignment and collimation difficulty issues. Integrated optical sensor have the following advantages: (1) without any marker on the sample; (2) detecting the signal is usually not determined by the sample size, only depends on the target concentration for trace detection; (3) by monolithic integration multi-channel simultaneous measurement, miniaturization, multi-function, and low power consumption
1. INTRODUCTION

can be achieved; (4) better stability and reliability, can be useful in harsh environments; (5) can reduce costs by mass production.

The ability of achieving trace detection is an important indicator for a biosensor. Trace has two aspects: first, the amount of sample to be measured (volume or mass) is small, second, the content in the sample is small. This requires maintaining the small sensing area (the small sample size) and at the same time ensuring a high sensitivity (minimal content). Much effort is taken to miniaturize optical sensors and to integrate them into electro-optical chip designs. The above issues can be well resolved by introducing a PhC to the sensor field. PhC sensor based on integrated optics technology has both all the benefits of integrated optical sensor and the characteristics of PhC. The size of its sensing area can be very small, so only a very small amount of sample is needed and even single-molecule detection can be accomplished. Therefore PhC sensor is particularly suited for the trace detection of biological molecules. By integrating a high performance laser, the sensor can be implemented on a single chip. In this thesis, the PhC sensor will be presented.

1.3 Photonic crystals

Figure 1.1: Schematic figures of PhCs in (a) one dimension, (b) two dimensions and (c) three dimensions.

In solid-state physics, the band structure of a crystal describes those ranges of energy that an electron is “forbidden” or “allowed” to have. Band structure derives from the diffraction of the quantum mechanical electron waves in a periodic crystal lattice with a specific crystal system and Bravais lattice. There may be gaps in the energy band structure, meaning that electrons are forbidden to propagate with certain energies. PhCs are periodic nanostructures, which affect the motion of photons in a similar way that periodicity of a semiconductor crystal affects the motion of electrons. Because of the periodic modification of the refractive index of the material, there may exist band gaps. The light with energy within the band gaps is forbidden to propagate. According to
the definition, PhCs can be classified as one dimensional (1D), two dimensional (2D) and three dimensional (3D) PhCs, see Fig. 1.1. 1D PhCs may have band gaps in one direction. 2D PhCs can have band gaps for propagation in plane. 3D PhCs may have band gaps in all the directions. We should note that although the concept of PhCs came out after the publication of S. John [1] and E. Yablonovitch [2] in 1987, the dielectric mirrors which have already been used for a long time are a kind of 1D PhC [3] according to the definition.

The propagation of light in a PhC is governed by the four macroscopic Maxwell’s equations. In SI units, they are

\[ \nabla \cdot \mathbf{B} = 0 \] (1.1)

\[ \nabla \cdot \mathbf{D} = \rho \] (1.2)

\[ \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \] (1.3)

\[ \nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J} \] (1.4)

where \( \mathbf{D} \) and \( \mathbf{B} \) are the displacement and magnetic induction, \( \mathbf{E} \) and \( \mathbf{H} \) are the electric and magnetic fields, \( \rho \) and \( \mathbf{J} \) are the free charge and current densities. Under the assumptions of small electric fields in a homogenous, low-loss medium with a non-dispersive dielectric constant \( \epsilon \), a magnetic permeability \( \mu \) close to 1, no free charges and currents, and harmonically varying fields, the four equations can be incorporated into one,

\[ \nabla \times \left( \frac{1}{\epsilon(r)} \nabla \times \mathbf{H}(r) \right) = \left( \frac{\omega}{c} \right)^2 \mathbf{H}(r) \] (1.5)

where \( r \) is the position vector, \( c \) is the speed of light in vacuum. Eq. 1.5 is the master equation. If we identify the left side of the master equation as on operator \( \hat{\Theta} \) acting on \( \mathbf{H}(r) \) to make it look like a traditional eigenvalue problem, the master equation is often written as

\[ \hat{\Theta} \mathbf{H}(r) = \left( \frac{\omega}{c} \right)^2 \mathbf{H}(r) \] (1.6)

While the solid state equivalent is given by

\[ \hat{H} \Psi = E \Psi, \text{ with } \hat{H} = -\frac{\hbar}{2m} \nabla^2 + V(r) \] (1.7)

where \( \Psi \) is the electron wavefunction, \( E \) is the energy, \( \hbar \) is Plank’s constant divided by \( 2\pi \), \( m \) is the electron mass and \( V(r) \) is the potential.
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For the periodic structure, i.e., $\epsilon(r) = \epsilon(r + R)$ with $R$ a lattice vector, according to the Bloch's theorem the eigenfunction is written as

$$H_k(r) = e^{ikr}u_k(r) \quad (1.8)$$

where $u_k(r)$ is a periodic function on the lattice: $u_k(r) = u_k(r + R)$ for all lattice vector $R$. Because one key factor of Bloch states is that the Bloch state with wave vector $k_r$ and $k_r + mk'$ are identical where $k_r$ is the wave vector in the irreducible Brillouin zone, $m$ is any integer and $k'$ is a reciprocal lattice vector, the master equation can be rewritten in the terms of the Bloch fields $u_k$:

$$\hat{\Theta}_k u_k = \left(\frac{\omega}{c}\right)^2 u_k \quad (1.9)$$

with

$$\hat{\Theta}_k = (ik + \nabla) \times \frac{1}{\epsilon(r)}(ik + \nabla) \times \quad (1.10)$$

The information contained in these functions is called the band structure of the photonic crystal. For each $k$ a discrete set of eigenvalues $\omega_n(k)$ exist, where $n$ is the bandnumber. The frequency of each band $\omega_n(k)$ will vary continuously as $k$ varies.

![Figure 1.2: PhCs found in nature. (a) peacock feather, (b) butterfly and (c) opal.](image)

PhCs also exist in nature. The natural PhCs are responsible for the iridescent color of peacock feathers [4], butterfly wings [5] and opal [6], see Fig. 1.2.

The 3D PhCs fabrication is still significantly challenging, and this issue will be addressed in Chapter 9. In the present work 1D PhCs and 2D PhC slabs are studied. The band structure of a 1D PhC made of air ($n_1 = 1$) and GaAs ($n_2 = 3.45$) is shown in Fig. 1.3(a). There are three band gaps in the plotted frequency range. The light with the frequency within the band gaps is prohibited to propagate inside this structure.

2D PhC slabs retain most of the important features of full 3D PhCs [7]. Their appreciated advantage comes from an easy fabrication procedure, which is compatible with
1.3 Photonic crystals

Figure 1.3: (a) Band structure of 1D PhCs with air \((n_1 = 1)\) and GaAs \((n_2 = 3.45)\). The thickness of air and GaAs layers is 0.5\(a\). (b) Band structure of 2D PhC InP \((n = 3.37)\) slab with triangular lattice of air holes. The thickness of the slab is 0.44\(a\). The diameter of the hole is 0.6\(a\).

Figure 1.4: (a) Top view of the triangular lattice. The lattice constant is \(a\), the hole radius is \(r\) and the high symmetry directions are \(\Gamma K\) and \(\Gamma M\). (b) Brillouin zone of the triangular lattice, in which the irreducible Brillouin zone is highlighted. The high symmetry points are marked by \(\Gamma\), \(M\) and \(K\).

standard planar technology used to make electronic circuits. In PhC slabs, the localization of light in the vertical direction is controlled by the total internal reflection (TIR) resulting from the high index contrast between the high-index slab and the low-index
1. INTRODUCTION

environment. On the other hand, the confinement in the lateral direction is controlled by the band structure resulting from the 2D PhCs. In the 2D case, the modes can be classified as TM modes (magnetic field in plane) and TE modes (electric field in plane).

In this thesis, a triangular lattice of air holes in a semiconductor layer is studied. The top view of the lattice is given in Fig. 1.4(a). The triangular lattice has six fold rotational symmetry, the important directions in the lattice are marked by the vectors $\Gamma K$ and $\Gamma M$ according to the direction in reciprocal space. Fig. 1.4(b) shows the Brillouin zone of the triangular lattice. The high symmetry points are indicated by $\Gamma$, $M$ and $K$, which exist at all edges and corners. The eigenmodes can be subject to any symmetry transformation that does not change the distribution of the refractive index. Hence, the triangles made by the adjacent symmetry points are the so called irreducible zones, into which all the possible wavevectors can be transformed by using periodicity and symmetry transformations. In consequence, the analysis of the Bloch modes of any PhC can be limited to this irreducible zone. In order to determine the band-gap, it is even sufficient to compute the frequencies for the wavevectors at the edges of this zone [8]. The band structure of a 2D PhC InP slab with air holes is displayed in Fig. 1.3(b). For this structure, there exists a band gap for TE modes.

![Figure 1.4(a)](image1)

![Figure 1.4(b)](image2)

Figure 1.5: (a) Cavity formed by two missing holes in a PhC lattice. (b) Waveguide formed by omitting a row holes in a PhC lattice.

Today there are two kinds of photonic devices studied thoroughly, i.e., cavities and waveguides. The introduction of intentional defects in the PhC creates confined states, where the field is allowed but exponentially decreases away from the defect. This property is used to created cavities and waveguides, see Fig. 1.5. The ratio of the energy stored inside the cavity with respect to the energy that is lost per cycle can be very high and is defined as the quality (Q) factor. Nowadays, high Q factors in small volumes make cavities useful in quantum electrodynamics (QED) [9–12]. Record Q factors have been reported as high as $10^6$ for cavities which have been modified by shifting the surrounding holes [13]. Even higher Q factors have been reported in heterostructure cavities [14]. PhC cavities and waveguides have been used in many applications, such as lasers [15–19], sensors [20–26], bends [27–30], filters [31–33], slow light propagation [34–37] and nonlinear effect enhancement [38–40].

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Except the bandgap effect, another property which receives lots of attention is the abnormal behavior in PhC [42, 43]. When the frequency of light is around the PhC band edges, the refraction becomes abnormal. Even a negative refraction can be achieved for some PhC, see Fig. 1.6. The earliest theoretical analysis of negative refraction inside PhC was done by Notomi [41]. By analyzing the equal frequency curves (EFC), he finds the effective refractive index (ERI) is negative and ERI can be considered as isotropic within some frequency range (i.e., EFCs are almost circles), see Fig. 1.7. In this frequency range the PhC can be considered as to an isotropic negative material. After that, Luo et al. proposed a PhC which has the negative refraction phenomenon, without having an isotropic negative index [44]. Based on the abnormal behavior in PhC, some basic elements, like open cavites [45], superlens [46, 47], polarization beam splitters [48] and superprism [49], have been reported.

1.4 Surface plasmon polaritons at THz frequencies

Surface plasmon polariton (SPP) is a collective oscillation of the electrons at the interface between a metal and a dielectric. One of the major driving forces in the field of plasmonics is the ability of spatially confining electromagnetic energy at visible frequencies over a distance significantly shorter than the wavelength. It is known that the in-plane wavevector of SPPs on a planar interface is

\[ \beta(\omega) = k_0 \sqrt{\varepsilon_d \varepsilon_m(\omega)/(\varepsilon_d + \varepsilon_m(\omega))} \]  

(1.11)
where $\varepsilon_d$ and $\varepsilon_m$ are, respectively, the complex permittivity of the dielectric and metal, and $k_0$ is the vacuum wavevector. While $\varepsilon_d$ is, in general, weakly dependent on $\omega$, $\varepsilon_m$ is strongly dispersive. As such, the in-plane wavevector $\beta$ departs from $k_0\sqrt{\varepsilon_d}$ as $\omega$ increases and the deviation reaches a maximum when the real part of $\varepsilon_m$ is negative and has an absolute value equal to $\varepsilon_d$ (i.e. the absolute value of the denominator in Eq. 1.11 is minimized), leading to evanescent decay of the fields perpendicular to the interface. The frequency at which this condition is satisfied is called the asymptotic SPP frequency.

In dealing with terahertz (THz) or even lower frequency radiation, the following question arises: are there surface plasmons (having the key property of strong (i.e. subwavelength) confinement typical of surface plasmons at visible and near-infrared frequencies) at such long wavelengths? At THz frequencies, however, the real part of $\varepsilon_m$ is at least two to three orders of magnitude greater than that of $\varepsilon_d$ so that the SPP dispersion curve is well approximated by the light line: $\beta(\omega) \approx k_0\sqrt{\varepsilon_d}$. As a result, the out-of-plane wavevector (i.e. the decay rate normal to the interface)

$$|\kappa| = \sqrt{\beta^2 - k_0^2\varepsilon_d}$$

is very small, corresponding to poorly confined surface waves, known as Sommerfeld or Zenneck waves. In this regard, there are no surface plasmons in the real sense at THz frequencies. More recently, the idea of tailoring the topography of a perfect conductor to allow localized surface waves similar to optical SPPs was discussed in the context of one-dimensional groove arrays and two-dimensional hole lattices [50, 51]. This kind of

Figure 1.7: (a) PhC structure and EFCs. (b) ERI and bandstructure of PhC. The PhC is a triangular lattice with GaAs ($n=3.6$) pillar. The diameter of the pillar is $0.7a$. Adopted from Ref. [41].
artificial SPP on a structured metal surface has been experimentally verified recently in the microwave regime, where a metal can be treated as a perfect conductor \[ 52 \]. Since then, many efforts have been devoted to this kind of artificial SPPs (also called spoof SPPs) \[ 53 - 58 \].

1.5 Outline of this thesis

The main topic of this thesis is light control by nanostructured metal/dielectric surfaces and PhCs in InGaAsP nanobeams and freestanding membranes. To this end, several nanostructured metal/dielectric surfaces are designed, a PhC waveguide is designed, PhC nanobeams and PhC cavities are designed, fabricated, measured and analyzed.

Chapter 2 deals with the simulation method and the fabrication process. The simulation methods include the plane wave expansion (PWE) and the finite difference time domain (FDTD) method, which are used to calculate the band structure and the mode profiles. The fabrication process and the testing method are also introduced, respectively.

Two kinds of nanostructured metal surfaces are discussed in chapter 3. The propagation loss of light at THz frequency is calculated in section 3.1. The relation between the propagation loss and the topography of the grooves are discussed in this section. One metal waveguide consisting of two thin metal slabs for slow light propagation at THz frequency is proposed in section 3.2. The origin of slow light is analyzed. Advantages over the propagation with surface plasmon polaritions are verified by comparing the group dispersion and propagation loss of both mode types.

In chapter 4, 5 and 6 the optical properties of 1D PhC (chapter 4 and 5) and 2D PhC waveguide are explored. The negative refraction achieved by 1D PhC is proposed in chapter 4. The effect of PhC on the extraction efficiency of a light-emitting diode is discussed in chapter 5. A silicon on insulator (SOI) 2D PhC waveguide is optimized to make it suitable for a modulator (chapter 6).

Chapter 7 covers the results of the PhC slot nanobeam waveguides. A structure with high sensitivity is shown. Both the simulation result and the experimental result is given. Then a new structure with improved quality factor is proposed.

The optical properties of PhC nanocavites are shown in chapter 8 and 9. In chapter 8 the controlling mode degeneracy in a PhC nanocavity with infiltrated liquid crystal is shown. The mechanism behind is given. In chapter 9 the free PhC nanocavities taken from the chip are described. The properties of these free PhC nanocavities are studied by nano-manipulation and micro-photoluminescent (µPL) experiments. The possibility of attaching one PhC nanocavity to the end of a fibre to make a fibre sensor is shown.
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Chapter 2
Methods

This chapter covers the simulation, fabrication and characterization methods which were used to obtain the results that will be presented in the following chapters. Section 2.1 deals with the simulation methods, including Plane Wave Expansion and Finite Difference Time Domain. Section 2.2 describes the fabrication process. In section 2.3, the experimental setup is introduced.

2.1 Simulation methods

Although the optical behavior of the photonic crystals (PhCs) is completely described by Maxwell’s equations, the complicated structures make the analytical analysis almost impossible. Therefore, numerical calculations are used widely to make designs and analyze the properties. Here we only list the most common methods that are used. The most used method to get the PhC band structure is the Plane Wave Expansion (PWE) method using a basis of plane waves. Finite Difference Time Domain (FDTD) is the most common method to get the transmission and reflection spectra, resonant frequencies and field patterns. However other methods are also used widely. The Multiple Multipole method uses a basis of spatial Bessel/Hankel functions for performing electrodynamic field calculations in the frequency domain. In systems that are composed of a small number of easily-analyzed pieces, such as a sequence of constant-cross-section waveguides, a collection of cylinders, or a multi-layer film, transfer-matrix/scattering-matrix methods may be especially attractive. These methods treat the individual simple elements in some analytic or semi-analytic fashion, enabling the entire structure to be simulated with great speed and accuracy. One useful free tool that can handle a wide variety of structures is CAMFR [59]. The finite element method is a numerical technique for finding approximate solutions of partial differential equations as well as of integral equations which is also used
2. METHODS

to solve Maxwells equation. In this thesis, PWE and FDTD are used. A more detailed discussion of those two methods is given below.

2.1.1 Plane wave expansion

Plane waves are solutions to the master equation 1.9, and form a basis to represent fields in the periodic media. The electric or magnetic fields are expanded for each field component in terms of the fourier series components along the reciprocal lattice vector. Similarly, the dielectric permittivity is also expanded through Fourier series components. In order to solve the equation numerically one needs to truncate the series to a finite number N of plane waves. Under assumptions of a source free, linear, and non-dispersive region we obtain the eigen value relations which can be solved.

The bandstructure for the dielectric PhC in this thesis is calculated with a free MIT program called MPB [60]. This program computes definite-frequency eigenstates (harmonic modes) of Maxwell’s equations in periodic dielectric structures for arbitrary wavevectors, using fully-vectorial and three-dimensional methods. Besides the uniform PhC, it’s also possible to simulate structures with simple defects using the supercell approach. For calculating the band structure with a dispersive material, we use FDTD method.

2.1.2 Finite difference time domain

The FDTD method is a powerful numerical algorithm for directly solving Maxwell’s equations in the time domain, and it can be used to investigate the interaction of light fields with virtually arbitrary structures. It is a very accurate numerical method, since there is no approximation adopted, except the discretization for the space and time domains. For the same reason, it is quite memory and time consuming, especially in three-dimensional (3D) cases. Nowadays personal computers are capable of performing most FDTD calculations for photonic components, but in the cases of large computational domains or very fine structures, parallel computer cluster might be needed. There also exist some free software packages for FDTD calculations. In this thesis, we use a MIT package called meep [61] to calculate the band structure of silver nanostructured surfaces, the resonant peaks of PhC cavities and mode profiles. The calculation were performed on a cluster at Zhejiang University, which has a 128 GB memory and 32 CPUs.
2.2 Fabrication method

The wafer is grown by Metal Organic Chemical Vapor Deposition (MOCVD). First, a 1 µm InP buffer layer is grown directly onto the InP substrate. Then followed by a 110 nm InGaAsP layer, a quantum dot layer (InAs QDs) and again a 110 nm InGaAsP layer, the wafer is completed see Fig. 2.1(a). Second, 400 nm SiNx is deposited as a hard mask by using Plasma Enhanced Chemical Vapor Deposition (PECVD). Third, an electron beam resist, ZEP 520A solution in anisole (the organic compound with the formula CH₃OC₆H₅), is spin coated onto the sample using a rotation speed of 5000 rpm for 60 seconds, see Fig. 2.1(b). The wafer with the resist was baked at 200 °C. This procedure results in a resist layer of approximately 350 nm. By means of electron beam lithography
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(EBL), the photonic crystal patterns were defined into the resist layer, see Fig. 2.1(c). For the EBL, we use Raith 150I and II with 30 kV electron energy and 10 \( \mu \)m aperture. After the exposure with the electron beam, the pattern was developed by immersing the sample into n-amyl acetate for 60 seconds. The n-amyl acetate acts as an solvent for the exposed regions. The development is stopped by rinsing the sample for 40 seconds with a 9:1 mixture of methylisobutylketone and isopropanol. Next the patterns are transferred from the resist layer to SiN\(_x\) by Reactive Ion Etching (RIE) with CHF\(_3\) see Fig. 2.1(d). Before transferring the patterns to the InP/InGaAsP/InP stack layer, the left resist layer needs to be removed by oxygen plasma for 30 minutes. Then the InP/InGaAsP/InP stack is opened by Inductively Coupled Plasma (ICP) etching with Cl\(_2\), Ar and H\(_2\) see Fig. 2.1(e). The SiN\(_x\) layer can be removed by a 10 % HF. The final step is a selective wet etching using a 4:1 mixture of HCl and H\(_2\)O for 15 minutes at 2 °C. The remains is a free standing InGaAsP membrane Fig. 2.1(f).

2.3 Photoluminescence

![Figure 2.2: PL spectra of (a) un-patterned InGaAsP membrane, (b) PhC cavity.](image)

By incorporating QDs into a III/V structure, an active material is created. QDs are artificial atoms with discrete energy levels. As a consequence, they can be excited by absorbing a photon and relax again by emitting one. Because the PhC structures discussed in this thesis are different kinds of cavities, using the active material is a huge advantage compared to passive semiconductor materials like silicon for which transmission or reflection set-ups need to be built. Thus the experiments performed in this thesis to obtain the resonance spectra are quite easy and quick: by shining the laser spot onto
the membrane, the QDs are excited and their emitted light is detected. This process is called photoluminescence (PL). The PL spectrum of an un-patterned surface is shown in Fig. 2.2(a). This is a very broad spectrum which is caused by the size dispersion of the InAs QDs. They are self-assembled and therefore they have different size, resulting in different quantization energy and a wide emission spectrum. By patterning the PhC structures into the membrane, most wavelengths between 1300 nm and 1600 nm will be forbidden, because they are in the band gap of the PhC. The PL spectrum will have a few very sharp peaks at the resonance wavelengths of the PhC cavity modes which are inside the PhC band gap. This is shown in Fig. 2.2(b).

Figure 2.3: A schematic configuration of \( \mu \)-PL set-up.

Room temperature micro-PL (\( \mu \)-PL) experiments are conducted using a continuous wave diode laser with wavelength \( \lambda = 660 \) nm. This set-up allows the focusing of the laser spot to an area of a few \( \mu \)m\(^2\), which is why it is called \( \mu \)-PL. Low powers are used to avoid heating and to avoid rapid evaporation when the PhC structures are infiltrated. Fig. 2.3 shows the entire \( \mu \)-PL set-up. The set-up is placed on a shock-absorbent optical table to prevent mechanical noise from interfering with the experiments. The sample is placed on a stage for which the \( x \) - and \( y \) -position can be controlled on a nanometer scale by means of piezo-positioning so that the focus of position of the laser light by the microscope objective can be accurately controlled.

During a PL experiment, first, the laser light goes to a beam splitter that reflects light to sample. The laser is focused onto the PhC structure by an objective with a magnification of 50\( \times \) and a numerical aperture of 0.5. The light from laser excites the QDs inside the PhC structures and they will emit light around between 1300 nm and
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1600 nm. The same objective will be used to collect the emitted light. Afterwards the light enters the 50 cm monochromator. The light is dispersed and detected by an InGaAs diode array which is cooled by liquid nitrogen. The resolution of the spectrometer is 0.31 nm with a 300/mm grating and 0.13 nm with a 600/mm grating.
Chapter 3

Light propagation on a periodically structured Ag surface at THz frequency

The terahertz (THz) region occupies a large portion of the electromagnetic spectrum located between the microwave and optical frequencies and is normally defined as the band from 0.1 to 10 THz (30–3000 µm). In recent years, this intermediate THz radiation band has attracted much interest as it offers significant scientific and technological potentials for applications in many fields, such as sensing [62], imaging [63], and spectroscopy [64]. There are many conventional guiding structures in THz region, such as metal tubes [65, 66], plastic ribbons [67], dielectric fibers [68] and photonic crystal fibers [69]. In these works, the usefulness of the guiding structures for transport of THz waves is limited by the group velocity dispersion of the guided waves. Dispersionless propagation can be achieved in parallel metal plate waveguides [70–72], but in this case the attenuation is high as the cross-section of the waveguide is larger than that of a cylindrical metal wire for THz pulses [73–75]. These waves are known as Sommerfeld-Zenneck waves, which are weakly guided and this limits its applications. To confine these waves on a surface, engineered surface plasmon waveguides were designed [54]. Note that similar corrugated waveguides have already been studied in microwave and millimeter regions around 1950 [76, 79]. Later these modes are called “spoof SPPs” (surface plasmon polaritons) because they mimic SPPs even on perfect conductors (with an infinitely large imaginary part of the refractive index), on which SPPs cannot exist. Note that although the properties of corrugated waveguides in the millimeter region have been studied, these corrugated waveguides behave differently in THz region and need to be studied further (such as how to reduce the loss). This chapter deals with the propagation at terahertz frequency in two different situations. The propagation on a periodically structured Ag surface will be discussed in...
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section 3.1. The propagation as slow wave in a corrupted Ag waveguide will be presented in section 3.2.

3.1 Propagation on a periodically structured Ag surface

In this section, the characteristics, including the dispersion curve and the propagation loss, of terahertz SPPs on a periodically structured Ag surface are studied numerically by using a two-dimensional (2D) finite-difference time-domain (FDTD) method [80]. The effects of the groove width, the period, the groove depth, and the shape of the groove corners on the dispersion relation and the propagation loss are analyzed.

Fig. 3.1 shows schematically the structure we study in the present section. An Ag surface is drilled with periodic grooves, where air is assumed for the ambient and in the groove regions. Parameters $a$ and $h$ are the width and depth of the grooves, respectively, $d$ is the period of the array, and $r$ is the radius of the corner. Instead of perfect conductor, here we use the following lossy Drude model to describe the permittivity of the metal,

$$\varepsilon_m = 1 - \frac{\omega_p^2}{\omega \times (\omega + \gamma \times i)} \quad (3.1)$$

where $\omega_p$ is the plasma frequency and $\gamma$ is the damping constant. Here we adopt $\omega_p = 1.44 \times 10^{16}$ rad/s and $\gamma = 4 \times 10^{13}$ for Ag in THz regime [81]. The computational domain covers one unit cell of the periodic structure, where the standard boundary treatment of perfectly matched layer is used in $\pm y$ directions, and the Bloch boundary condition is used in $\pm x$ directions. A uniform rectangular mesh with a step size of 25 nm is adopted, and the numerical convergence of the FDTD results has been checked. We excite eigenmodes by some pulse point sources and compute the frequency spectrum of the time-domain response, where each peak in the spectrum corresponds to an eigenfrequency. The propagation loss per period can then be calculated with [82].

$$loss = \exp\left(-\frac{d \times \Re(\omega)}{Q \times v_g}\right) \quad (3.2)$$

where $v_g$ denotes the group velocity (calculated from the derivative of the dispersion relation). The quality factor ($Q$) of the fundamental SPP mode in the periodical structure is calculated by $Q = \frac{\Re(\omega)}{2\Im(\omega)}$ [61].
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Figure 3.1: Schematic sketch of the SPP waveguide structure in two dimensions. A unit cell is marked by the two dashed lines.

3.1.1 Grooves with different air gap/period ratios

Throughout the section 3.1 the height $H$ of the structure is fixed to 30 $\mu$m, which is large enough as compared to the penetration depth of the field into the metal. In Fig. 3.2 the red curve shows the calculated dispersion relation of the SPP mode in a structure with $h = 10$ $\mu$m, $d = 10$ $\mu$m, $a = 2$ $\mu$m, and $r = 0$ (i.e., a rectangular corner). The surface mode asymptotically approaches the light line in the ambient (air) at low frequency, and approaches $\omega = 0.208 \cdot 2\pi c/d$ at the Brillouin zone edge. We then study the field distributions of the fundamental SPP modes with different Bloch wave vectors ($k_x$). The inset of Fig. 3.2 shows, from left to right, the distributions of field $E_y$ for $k_x = 0.2(2\pi/d)$, $0.3(2\pi/d)$, and $0.5(2\pi/d)$, respectively. One can find that the field extends to a large distance in the air for $k_x = 0.2(2\pi/d)$, while it is strongly confined at the air-Ag interface near the Brillouin zone edge ($k_x = 0.5(2\pi/d)$). This is consistent with the corresponding dispersion relations shown in Fig. 3.2.

To study the effect of groove width $a$, the dispersive relations when $a = 0.1d$, $a = 0.3d$, $a = 0.5d$, and $a = 0.8d$ are calculated and also shown in Fig. 3.2. Generally speaking, the fundamental SPP mode always exists in all these cases, although the dispersion curves asymptotically reach lower values at the Brillouin zone edge as the groove width increases, which is similar to the results presented in ref. [58]. Furthermore, we focus on one specific frequency, i.e., $\omega = 0.17 \cdot 2\pi c/d$ (corresponding to $f=5.1$ THz), which is within the THz regime. Fig. 3.3 shows the distribution of the electric field intensity ($|E_x|^2 + |E_y|^2$) for this fundamental SPP mode with different $a$. Increasing the groove width results in a more localized field at the air-Ag interface, especially around the metal bump between two grooves. This can be explained as the strong field enhancement near a sharp edge [83].

The frequency-dependence of the propagation loss is also an important characteristic of the SPP surface waves. In Fig. 3.4 we plot the loss per unit length as the frequency varies from 4.5 THz (corresponding to $\omega = 0.15 \cdot 2\pi c/d$) to 6.3 THz (corresponding
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Figure 3.2: Dispersion relations of spoof SPPs for $d = 10 \, \mu m$ and five different groove width $a = 0.1d$, $0.2d$, $0.3d$, $0.5d$, and $0.8d$. The dashed gray line is the light line in air. The inset shows, from left to right, the distributions of field $E_y$ for $k_x = 0.2(2\pi/d)$, $0.3(2\pi/d)$, and $0.5(2\pi/d)$, respectively.

Figure 3.3: Electric field intensity distribution at $\omega = 0.17 \times 2\pi c/d$ with (a) $a = 0.1d$, (b) $a = 0.2d$, (c) $a = 0.3d$, (d) $a = 0.5d$, and (e) $a = 0.8d$. The surface of the metal is marked by the white lines. The other parameters are the same as those for Fig. 3.2.

to $\omega = 0.21 \cdot 2\pi c/d$). In general, the propagation loss increases monotonically as $\omega$ increases, due to better confinement of the field. It is worthwhile to note that there exists a “threshold frequency” for each of the propagation loss curves. Above this “threshold frequency”, the loss increases dramatically, and a larger groove width $a$ gives a larger propagation loss. This is because the asymptotical frequency at the Brillouin zone edge
3.1 Propagation on a periodically structured Ag surface

is lower for a larger $a$ (see Fig. 3.2). At low frequencies, especially below the lowest “threshold frequency”, the propagation losses are very small and thus these three curves are very close to each other. This is due to the fact that at a low frequency the SPPs penetrate very little into Ag and the grooves and propagate mainly on the air-Ag interface (cf. the inset of Fig. 3.2). On the other hand, there exist multiple crosspoints between these loss curves. No simple relation can be drawn between the propagation loss and the groove width in this regime.

Figure 3.4: Propagation loss per unit length as a function of $\omega$ for three different groove width $a = 0.2d$, $0.5d$, and $0.8d$. Here $h = 10 \mu m$ and $r = 0$.

To investigate this phenomenon, we plot the quality factor $Q$ and the group velocity $v_g$, as shown in Fig. 3.5, since these two quantities are directly related to the propagation loss (cf. Eq. 3.1). As expected, both $Q$ and $v_g$ are monotonically decreasing functions of the frequency. The group velocity $v_g$ also deceases as the groove width $a$ increases at all frequencies. However, the quality factor $Q$ exhibits a rather complicated relation with $a$. From Fig. 3.5(a) we can find that $Q$ is more sensitive to the change of the frequency for a narrower groove. At a high frequency, a larger $a$ gives a higher $Q$, while an opposite trend is found at a low frequency. As a result, the product of $Q$ and $v_g$, which is inversely proportional to the propagation loss, can have several crosspoints in e.g. the curves of $a = 0.5d$ and $a = 0.8d$ in Fig. 3.5(c).
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Figure 3.5: (a) The Q factor, (b) group velocity \( v_g \), and (c) the product of Q and \( v_g \), as a function of \( \omega \) when \( a = 0.2d, 0.5d, \) and \( 0.8d \). The other parameters are the same as those for Fig. 3.2.

3.1.2 Grooves with fixed air gap/period ratio but different periods

In the limit of \( \lambda_0 \gg d \) and \( \lambda_0 \gg a \), the following approximate dispersion relation can be obtained by replacing the array of grooves with a single homogeneous but anisotropic
layer of thickness $h$ on top of the surface of a perfect conductor \cite{51},

\[ \sqrt{k_x^2 - k_0^2} = \frac{a}{d} \times \tan(k_0 \times h), -\frac{2\pi}{d} < k_x < \frac{2\pi}{d} \] (3.3)

where $k_0$ and $\lambda_0$ are wavenumber and wavelength in vacuum, respectively. From this equation one can see that if both $a/d$ and $h$ are fixed the effective media are the same regardless of the specific value for $a$ or $d$. In this case, the dispersion curves for different $d$ should overlap with each other under this low-frequency approximation. While for a minimal propagation loss the period $d$ still needs to be optimized. Thus, the propagation losses per unit length are studied for structures with different period $d$ while having the same filling factor (namely, $a = 0.2d$, $h = 10 \mu m$, and $r = 0$). The results for $d = 10 \mu m$, $5 \mu m$, and $2 \mu m$ are shown in Fig. 3.6(a), from which we can see that the dispersion curves for all these cases are almost overlapped (three dispersion curves overlap with each other at low frequencies and the two dispersion curves for $d = 5 \mu m$ and $2 \mu m$ overlap almost entirely inside the whole overlapped Brillouin zone, as $\lambda_0 \gg d$ and $\lambda_0 \gg a$ are satisfied). Note that these curves end at different $k_x$ values, which is simply due to different sizes of the Brillouin zones. We also found that the asymptotical frequency at the Brillouin zone edge increases as $d$ decreases. The corresponding propagation losses per unit length for these three structures are shown in Fig. 3.6(b). From Fig. 3.6(b) one sees that the period $d$ imposes a significant impact on the propagation loss even at low frequencies, which is different from the case when the relative groove width varies (cf. Fig. 3.2).

The corresponding quality factor $Q$ and group velocity $v_g$ for different $a$ are shown in Fig. 3.7, from which one can see that the quality factor decreases as $d$ decreases at all frequencies. Like the dispersion relation, the group velocity curves are also close to each other. There exists one crosspoint between each two of the group velocity curves. As a result, each two of the corresponding propagation loss curves also have a crosspoint (the crosspoints between curve $d = 2 \mu m$ and the other two curves are outside the plotting range of Fig. 3.6(b)).

### 3.1.3 Grooves with different radius at the corners

The influences of the groove depth $h$, as well as the shape of the corner with a certain radius $r$, on the dispersion relations and the propagation losses are also calculated. In all these cases, the period $d$ and the groove width $a$ are fixed to $10 \mu m$ and $2 \mu m$, respectively. The results for five cases with $(h = d, r = 0)$, $(h = d, r = 0.05d)$, $(h = d, r = 0.1d)$, $(h = 0.9d, r = 0)$, and $(h = 0.8d, r = 0)$ are shown in Fig. 3.8, where we can see that the asymptotical frequency increases and the loss decreases when $h$ decreases or the corner becomes less sharp.
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Figure 3.6: (a) Dispersion relations of spoof SPPs (with \( a = 0.2d \)) for \( d = 10 \, \mu \text{m}, 5 \, \mu \text{m}, \) and \( 2 \, \mu \text{m} \). The gray light is the light line in air. (b) Propagation loss per unit length as a function of \( \omega \) for the corresponding structures. Here \( h = 10 \, \mu \text{m} \) and \( r = 0 \)

Figure 3.7: (a) The Q factor and (b) group velocity \( v_g \), as a function of \( \omega \) when \( d = 10, 5, \) and \( 2 \, \mu \text{m} \). Here \( a = 0.2d \).
3.1 Propagation on a periodically structured Ag surface

Figure 3.8: (a) Dispersion relations of spoof SPPs for cases \((h = d, r = 0)\), \((h = d, r = 0.05d)\), \((h = d, r = 0.1d)\), \((h = 0.9d, r = 0)\), and \((h = 0.8d, r = 0)\). The gray light is the light line in air. (b) Propagation loss per unit length as a function of \(\omega\) for the corresponding structures.

3.1.4 Discussion

We have studied the effects of the structural parameters including the groove width \(a\), the period \(d\), the shape of the corner (i.e., the radius \(r\) of the corner), and the groove depth \(h\) on the dispersion relation and the propagation loss. The dispersion curves asymptotically reach higher values at the Brillouin zone edge as \(a\), \(d\), and \(h\) decrease or \(r\) increases, as shown in Figs. 3.2, 3.6(a), and 3.8(a). Around this asymptotical frequency a tightly confined electromagnetic field can be achieved, which could support applications in, e.g., bio-sensing [84]. However, the propagation loss in this case is very high. Far below this asymptotical frequency, the loss is low, which is desirable for transporting THz waves. The structural parameters still have to be carefully designed in order to minimize the propagation loss in this regime. As we have discussed before, the variation of the groove width does not impose a significant influence on the propagation loss at low frequencies, while the period does. From here, we can already conclude that the loss is highly related to the number of grooves included in a unit length. However, the loss in one groove can also arise from the cavity walls inside the groove as well as the sharp corners at the surface, since significant field enhancement is expected there (cf., Fig. 3.3). As we can see in Fig. 3.8(b), the sharpness of the corners is less important for the propagation loss as...
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compared to the groove depth. From the above analysis, we can finally conclude that the propagation loss is mainly influenced by the total area of the side-walls of the grooves in a unit length.

3.2 Propagation as slow wave in a corrugated Ag waveguide

Low group velocity has been utilized in e.g. low power switches and modulators owing to the enhanced light-matter interaction [35]. A slow guided wave should also have very small group velocity dispersion (GVD) for distortionless signal propagation. In near infrared frequency, two-dimensional (2D) photonic crystal waveguides are used widely to achieve slow light [35, 34]. 2D photonic crystal waveguides have also been used to guide waves in THz region [85–87], and thus they can be designed to achieve slow light in THz region. However, large group velocity dispersion and complicated fabrication are their main obstacles [42]. Many periods should be used in both sides of the line defect in order to make sure that the electromagnetic distribution is weak outside the line defect (i.e., to confine light in a line defect). Engineered surface plasmon waveguides can also be used to obtain slow light, but large GVD and high propagation loss at the Brillouin boundary are then unavoidable. In this section, we introduce a subwavelength metal waveguide which can be used to slow down the speed of light at terahertz frequencies. The proposed waveguide consists of two thin metal slabs with subwavelength periodic corrugations on their inner boundaries, and can give some very flat bands (indicating low group velocity). Compared with structures based on engineered surface plasmons, the structure discussed in this section has small GVD and relatively low propagation loss. Since this structure is made of metal, light can be well confined in a subwavelength region and the whole structure is very small (the width of the present structure is only 70 µm).

3.2.1 Design and calculation

Fig. 3.9(a) shows the schematic diagram of the proposed THz waveguide. Two thin metal slabs with thickness \( d \) are put very close to each other in air (the distance between their inner surfaces is \( g \)). The inner surfaces of the two metal slabs are corrugated with a period of \( a \). The depth and width of the grooves are \( h \) and \( l \), respectively. The structure in \( z \) dimension is assumed infinite and the magnetic field is assumed along \( z \) axis everywhere in all our simulation. This structure is called structure A hereafter. We assume that the magnetic field is along the transversal \( z \) axis and the harmonic time factor is \( \exp(-i\omega t) \). For a Gaussian beam of finite spot size propagating along \( x \) direction, the effects of
the finite $z$ dimension on the field in the central region can be small or negligible, and the present 2D model can be used as an approximation for the field propagation in the central region. The permittivity of the metal is described by the following well-known Drude model, Eq. (3.1). After some optimization, we choose $g = 10 \, \mu m$, $d = 30 \, \mu m$, $l = 45 \, \mu m$, $h = 20 \, \mu m$ and $a = 50 \, \mu m$. The finite-difference time-domain method is used to calculate the dispersion curves, propagation loss and modal profiles. We excite eigenmodes by pulse point sources and compute the frequency spectrum of the time-domain response, where each peak in the spectrum corresponds to an eigenfrequency. The mesh size is uniform and 25 nm in our calculation.

![Waveguide structure](image)

Figure 3.9: (a) The proposed waveguide structure (structure A) for slow light at THz. (b) Structure B (based on engineered surface plasmons) for comparison.

Dispersion curves of the waveguide are shown in Fig. 3.10(a), where the antisymmetric bands (with the magnetic fields antisymmetric with respect to the axis of the waveguide) are marked by red triangles. Note that the difference between the dispersion curves obtained from a lossy Drude model and those obtained from a lossless Drude model are negligible (the dispersion curves obtained from a lossless Drude model are not shown here). In Fig. 3.10(a) one can see that some bands are very flat, especially the antisymmetric bands.

The fourth antisymmetric band is very flat but not extremely flat compared with the first three antisymmetric bands. A flatter band corresponds to a lower group velocity but narrower bandwidth. When material loss exists (metal Ag is lossy), too small group velocity will give high propagation loss. Therefore, we choose the fourth antisymmetric band, which possesses simultaneously a low group velocity and a certain bandwidth, to investigate the characteristics of the slow light waveguide at THz. Fig. 3.10(c) gives an enlarged view for the central part (corresponding to a wavelength range from 9.05 THz
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Figure 3.10: (a) Band structure of structure A. Antisymmetric bands are given by curves with red triangles. (b) Band structure of structure B (for comparison). (c) The enlarged band structure of the fourth antisymmetric band of structure A in the wavelength range between 9.05 THz and 9.085 THz.

to 9.085 THz) of the fourth antisymmetric band. The group velocity is defined by

\[ v_g = \frac{d\omega}{dk_x} \]  \hspace{1cm} (3.4)

The group velocity of the fourth antisymmetric band is shown in Fig. 3.10(a). In
3.2 Propagation as slow wave in a corrugated Ag waveguide

Fig. 3.11(a), one can see that the group velocity reaches the maximal value \( v_g = 0.03c \) (\( c \) is the light velocity in air) at 9.066 THz. The group velocity decreases slowly around this maximum group velocity and a small GVD can be expected. GVD parameter \( D \) is obtained by

\[
D = \frac{1}{c} \frac{dn_g}{d\lambda}
\]

where \( n_g \) is the group index defined as \( n_g = c/v_g \). \( D \) is shown in Fig. 3.11(b) for the fourth antisymmetric band. The absolute value of \( D \) is less than 1ps/mm/nm in the wavelength range between 9.05 THz and 9.085 THz, and is almost zero around 9.066 THz. Thus, the wavelength range between 9.05 THz and 9.085 THz is our slow light region of interest. Propagation loss is a very important factor in practical situations, and the propagation loss per period is given by Eq. 3.2. The quality factor \( Q \) increases smoothly and almost linearly with frequency, which is clearly shown in Fig. 3.11(c). The product of the quality factor \( Q \) and \( v_g \) is shown in Fig. 3.11(d), where one can see clearly that the maximum of the product is achieved around 9.066 THz. The propagation loss per period is shown in Fig. 3.11(e). The propagation loss varies very slowly, and is about 1 dB/\( \lambda \) in the wavelength range of interest, and reaches the minimum at 9.066 THz. Because the frequency changes little in this region, the position for minimal propagation loss and the position for the maximal product of the quality factor \( Q \) and \( v_g \) almost overlap with each other according to Eq. 3.2. Note that the proposed waveguide is demonstrated to be able to slow down electromagnetic waves at frequencies around 9 THz, but the structure can be scaled up to make it work at around 1 THz. The basic properties of group velocity and group velocity dispersion will be similar, while the propagation loss will be smaller.

3.2.2 Origin of slow wave

In order to find the origin of slow wave, a unit cell of structure A is isolated and put in air (i.e., an isolated cavity in air is considered). The resonant modes of this cavity are calculated. We found that in the low frequency range every band corresponds to an eigen frequency of the cavity except the first band. Since the wavelength of the first band is very long, electromagnetic wave can not “see” the microstructure of the grooves inside the waveguide and structure A can be treated as an effectively homogeneous waveguide. Two resonant modes of the isolated cavity are used as examples to demonstrate the connection between the resonant modes and corresponding waveguide modes of slow light. First, we compare the resonant mode of the isolated cavity at 9.074 THz and the corresponding waveguide mode at 9.055 THz (on the fourth antisymmetric band in Fig. 3.10(a)). The quality factor \( Q \) of the resonant mode at 9.074 THz is about 680. The permittivity \( \epsilon_m \) of
3. LIGHT PROPAGATION ON A PERIODICALLY STRUCTURED AG SURFACE AT THZ FREQUENCY

Figure 3.11: (a) Group velocity $v_g$. (b) Group velocity dispersion parameter $D$. (c) The quality factor $Q$. (d) The product of the quality factor $Q$ and group velocity $v_g$. (e) Propagation loss per period ($a = 50 \, \mu m$). Curve with red triangles is for the fourth antisymmetric band of structure A and curve with blue circles is for the second band of structure B.

Ag at 9.076 THz is about $-4.27 \times 10^4 + 3 \times 10^4 i$ according to Eq. 3.1. The imaginary
3.2 Propagation as slow wave in a corrugated Ag waveguide

Figure 3.12: Distribution of $|H_z|$ and time average Poynting vector (marked by black arrows) of (a) a unit cell of structure A at 9.055 THz, (b) a single isolated metal cavity at 9.074 THz, (c) a unit cell of structure A at 6.120 THz and (d) a single isolated metal cavity at 6.144 THz. The white boundaries indicate the profile of Ag structures. The units for the magnitude of magnetic field in (a), (b), (c) and (d) are arbitrary.

part of $\epsilon_m$ is large, but the absolute value of the negative real part is also very large. Consequently, high reflection occurs on the Ag surface, and little wave can enter the Ag slab. Thus, the absorption loss is small and the Q factor of the resonant mode may be
large. When the damping factor $\gamma$ in Eq. 3.1 is omitted, the Q factor becomes 1180. The energy loss of the resonant mode is caused by energy leak from the two slits of the isolated cavity and the absorption loss (both are not large). The distributions of the absolute amplitude of $H_z$ and time average Poynting vector (marked by black arrows) of the waveguide mode and resonant mode are shown in Fig. 3.12(a) and 3.12(b) respectively. Comparing Fig. 3.12(a) and 3.12(b) one can see that the distributions of the mode profiles and Poynting vectors are almost the same. When such isolated cavities are connected to form the waveguide, the interaction between them is weak. Weak coupling deviates the mode pattern of the waveguide mode a bit from that of the isolated cavity. We also compare the resonant mode of the isolated cavity at 6.144 THz and the corresponding waveguide mode at 6.120 THz (on the third symmetric band in Fig. 3.10(a)). The Q factor of the resonant mode at 6.144 THz is about 50. The permittivity $\epsilon_m$ of Ag at 6.144 THz is about $-6.71 \times 10^4 + 6.95 \times 10^4 i$, whose absolute value of the real part is larger than that at 9.074 THz and this means larger reflection. The distributions of the absolute amplitude of $H_z$ and time average Poynting vectors (marked by black arrows) of the waveguide mode and resonant mode are shown in Fig. 3.12(c) and 3.12(d) respectively. When lossless Drude model is used, the Q factor varies little (still about 50), which means the energy loss of the resonant mode is mainly caused by the energy leak from the slits (the Poynting vectors around the slits in Fig. 3.12(d) are larger and denser than those in Fig. 3.12(c)). Thus, lower Q indicates that energy runs away quicker from the isolated cavity. Large energy leak gives strong coupling of the connected cavities when forming a waveguide. The strong coupling disturbs the corresponding waveguide mode from the resonant mode. That is why the distributions in Fig. 3.12(c) and 3.12(d) are quite different.

From Fig. 3.10(a) one sees that the third symmetric band is not as flat as the fourth antisymmetric band. This indicates that when the energy leak for a resonant mode of the isolated cavity is smaller the band for the corresponding guided mode of the waveguide is flatter. This is also verified by studying various slow wave bands in Fig. 3.10(a). We can conclude that structure A can be considered as a coupled cavity waveguide, with each face-to-face pair of grooves forming a cavity (these cavities are coupled through the narrow slits). It is the weakly coupled resonance that makes some dispersion bands rather flat [89]. The distributions of $|E_x|^2$ and $|E_y|^2$ of a unit cell of structure A at 9.055 THz are shown in Fig. 3.13(a) and 3.13(b) respectively. From this figure one sees that the $E_x$ field of the guided mode is distributed in the whole air hole while the $E_y$ field localizes at the corners of the hole and is weak inside the air region.

Efficient coupling between the slow waveguide and free space or a conventional waveguide (with a normal value of group velocity) is also important. As the present slow wave is achieved by weak coupling between the cavities, we can change the physical parameters
3.2 Propagation as slow wave in a corrugated Ag waveguide

Figure 3.13: Distribution of (a) $|E_x|^2$ and (b) $|E_y|^2$ of a unit cell of structure A at 9.055 THz. The white lines give the profile of Ag structures. The units for the intensity of electric field in (a) and (b) are arbitrary.

of the structure so that the coupling between the cavities becomes larger and the group velocity increases. To obtain high coupling efficiency, we can change the period $a$, the depth $h$ and width $l$ of the grooves near the input and output smoothly so that the tapered input/output can be coupled efficiently to free space or a conventional waveguide (with a normal value of group velocity).

3.2.3 Comparison

When the upper metal slab is removed, the remaining metal slab (called structure B as shown in Fig. 3.9(b)) can still support surface waves guided on the corrugated surface (as engineered surface plasmons). To show fairly that the function of slow wave for this reduced structure is not as good as that for structure A, we have optimized the geometrical parameters of structure B and finally chosen $d = 30 \, \mu m$, $l = 9 \, \mu m$, $h = 21.8 \, \mu m$ and $a = 10 \, \mu m$. The band structure is shown in Fig. 3.10(b) and the region above the light line in air is filled in grey. The second band is within the terahertz frequency range and thus studied. Group velocity $v_g$, GVD parameter $D$, the quality factor $Q$, the product of $Q$ and $v_g$, and propagation loss of this band are shown by curves with blue circles in Fig. 3.11(a)-3.11(e), respectively. The group velocity changes linearly. The absolute values of $D$ for structure B are large compared with those for structure A. As shown in Fig. 3.11(c) the
Q factor for structure B changes little and is very small (compared with that for structure A). This is because the $E$ field has good confinement when the corresponding frequency is near Brillioun zone edge. However, the $E$ field is mainly distributed in air for structure A, and thus the Q factor is large. Although $v_g$ of structure B is larger than that of structure A in some cases, the Q factor of structure B is much smaller than that of structure A in all cases (see Fig. 3.11(b) and 3.11(c)). Thus, the product of Q and $v_g$ for structure B is smaller than that for structure A, as shown in Fig. 3.11(d). According to Eq. 3.2, the propagation loss per period (50 µm) for structure B is larger compared with those for structure A, as shown in Fig. 3.11(e). When the group velocity is low, the absolute value of $D$ is large and the propagation loss is high. Compromise should be made for structure B in order to get small absolute value of GVD and low propagation loss, whereas structure A does not need such compromise as shown in the previous sections.

### 3.3 Summary

We have studied the characteristics of the terahertz SPP propagation on a periodically structured Ag surface with a FDTD method. The dispersion relations and the propagation losses of the SPP mode have been calculated. This numerical method is more straightforward, and eventually can be applied to more complex structures other than rectangular grooves. The influence of the groove width, the period, the sharpness of the groove corners, and the groove height, has been analyzed. We have found that the total area of the side-walls of the grooves in a unit length has a major effect on the propagation loss. For a typical structure with a groove width of 2 µm, a groove depth of 10 µm, and a period of 10 µm, the propagation loss is less than 0.2 dB/10 µm below 5.67 THz, while increases dramatically beyond this frequency. Although our study is for a two-dimensional structure, the present method can be readily extended to a three-dimensional structure.

To slow down the speed of light at THz, we have introduced a metal waveguide consisting of two parallel thin metal slabs with subwavelength periodic corrugations on their inner boundaries. Within a bandwidth of 35 GHz around 9.066 THz, the group index is above 33, the absolute value of GVD parameter $D$ is less than 1ps/mm/nm and the propagation loss is about 1 dB per period (50 µm). Compared with another metal waveguide based on engineered surface plasmons, our structure has obviously smaller absolute value of $D$ and lower propagation loss. As the waveguide is made of metal, the light can be confined tightly in a subwavelength region (the width of the present structure is only 70 µm), which can not be realized with a 2D photonic crystal-based waveguide. The physical mechanism of the slow light for the proposed structure is that a portion of the field re-circulates back and forth through a number of directly coupled optical cavities. The
coupling of light between the slow waveguide and free space or a conventional waveguide can be done by tapering some structural parameters at the input and output smoothly. Although our bandwidth is not so wide, we think our structure can be used for some applications in THz range, such as compact optical delay lines, buffers, enhancement of nonlinear effects. In addition, the bandwidth can be narrow for a modulator [90], and the size of the modulator can be reduced by slowing down the group velocity in the modulator [91]. We thus hope that our structure may also be used to make a compact modulator in THz range.
3. LIGHT PROPAGATION ON A PERIODICALLY STRUCTURED AG SURFACE AT THZ FREQUENCY
Chapter 4

Superlens formed by a one-dimensional dielectric photonic crystal

Left hand materials (LHM) were first theoretically discussed by Veselago in 1967 [92]. He studied the abnormal behavior in materials having simultaneous negative permittivity \( \epsilon \) and permeability \( \mu \). In that materials \( \mathbf{k}, \mathbf{E} \) and \( \mathbf{H} \) form a left-handed set of vectors (i.e., \( \mathbf{S} \cdot \mathbf{k} < 0 \), where \( \mathbf{S} \) is the Poynting vector.) and, therefore, are called LHM. The refraction at the interface of the normal material and LHM will be at the same side of the normal, which is called negative refraction. Because the materials having simultaneous negative permittivity \( \epsilon \) and permeability \( \mu \) don’t exist in nature, his study didn’t attract much attention at that time.

LHM have attracted great interest since the publication of the perfect/superlens [93] of subwavelength focusing and the first experimental confirmation of negative refraction [94]. Later on, it was also found that a slab of some two- or three-dimensional (2D or 3D) photonic crystals (PhCs) can also give negative refraction and/or subwavelength focusing [41, 44, 95, 96].

Recently, some efforts have been made to achieve negative refraction and/or slab focusing with a one-dimensional (1D) PhC [98, 99]. However, all these 1D structures contain metal and thus loss is inevitable. In this chapter, we design a pure dielectric 1D PhC to achieve slab-focusing and study their subwavelength focusing properties. Since our structure is one-dimensional, the fabrication is much easier and the position of surface termination has no effect on the image quality (different from the higher-dimensional case [97], in which the image quality can change a lot [Fig. 4.1]. The image quality can also be improved greatly as we do not use any metal here. Off-axis subwavelength focusing is achieved (similar to the off-axis focusing by a slab of 2D PhC with elliptical
4. SUPERLENS FORMED BY A ONE-DIMENSIONAL DIELECTRIC PHOTONIC CRYSTAL

Figure 4.1: (a) Schematic diagram for an imaging system formed by a PhC slab. The position of the surface termination is denoted by $\delta x$. The snapshots of the electric field of a point source and its image formed by a PhC slab with surface termination of (b) $\delta x = 0$ (c) $\delta x = 0.2a$. Adopted from Ref. [97].

inclusions [100] and its physical mechanism is explained in Section 4.1. On-axis subwavelength focusing achieved by the combination of two such slabs of 1D PhC is also studied in Section 4.2.

4.1 Off-axis focusing with a slab of 1D dielectric photonic crystal

Consider a 1D PhC consisting of Si and SiO$_2$ layers stacked alternately with a period of $a$ along the $y$ direction, as shown in the inset of Fig. 4.2(a). The refractive indices of Si and SiO$_2$ are 3.5 and 1.45, respectively. The Si and SiO$_2$ layers are assumed to have the thickness of $0.5707a$ and $0.4293a$, respectively. Here we only consider the TE polarization (the electric field $E$ is parallel to the $z$ axis, i.e., perpendicular to the plane of incidence). Since the structure is uniform in the $x$ direction and periodic only in the $y$ direction, $k_x$ (the $x$ component of the wave vector) is allowed to take an arbitrary value while the $y$ component $k_y$ is limited to the first Brillouin zone, i.e., $-\pi/a < k_y < \pi/a$. The plane wave expansion method is used to calculate the band structure for such a simple 1D PhC, and the calculated results are shown in Fig. 4.2(a) (the band structure is projected onto the $x$ direction). In all the numerical simulations in this chapter we choose the normalized
4.1 Off-axis focusing with a slab of 1D dielectric photonic crystal

Figure 4.2: (a) Projected band structure (TE polarization) for a 1D PhC. The dashed line corresponds to the normalized frequency of 0.221. The inset shows the structure of the 1D PhC; (b) Equi-frequency contours (EFCs) of the 1D PhC at the normalized frequency of 0.221; (c) Part of EFCs of band 1.

frequency of $0.221$ (in unit of $2\pi c/a$) corresponding to the gray line (a bit over the bottom of the second band) in Fig. 4.2(a).

The equi-frequency contours (EFCs) can be obtained by drawing the bands in contour lines in Brillouin zone. EFC of normalized frequency $0.221$ in the first Brillouin zone are shown in Fig. 4.2(b), from which we see that both band 1 and band 2 contain this frequency. However, band 2 has no influence in all our numerical examples (the construction line associated to any wavevector of propagating wave in air will have some intersections with band 1 but not with band 2 of EFC, as shown in Fig. 4.2(b) below). Part of the
4. SUPERLENS FORMED BY A ONE-DIMENSIONAL DIELECTRIC PHOTONIC CRYSTAL

EFCs of band 1 is shown in Fig. 4.2(c).

Figure 4.3: (a) The superlensing slab formed by terminating a 1D dielectric PhC; (b) Negatively (associated with point A') and positively (associated with point B) refracted beams constructed from EFCs and conservation of $k_y$. Red arrows indicate group-velocity directions; (c) Diagram for the principle of the present off-axis focusing.

The above analysis of band structure is for 1D PhC of infinite extension in both $x$ and $y$ directions. To form a focusing lens, we need to terminate the 1D PhC into a slab. The geometry of the PhC slab for focusing is depicted in Fig. 4.3(a). The angle between the normal (defined as the $x$-axis hereafter) of the termination surface and the layers is denoted by $\phi$. Note that the $xy$ coordinate system in Fig. 4.2 has been rotated by an angle of $\phi$ in the $xy$ coordinate system in Fig. 4.3 (and the rest of this chapter). In order to study the wave transmission through a slab of this 1D PhC with arbitrarily surface termination, it is necessary to use a diagram of EFCs in some repeated Brillouin zones. The propagation direction inside PhCs is the direction of group velocity vector, while the group velocity vector is the gradient of EFC. Fig. 4.3(b) shows the wave vector diagram for the EFCs of the normalized frequency 0.221. The black dashed lines in Fig. 4.3(b) represent the construction lines for this case representing $k_i = \omega/c sin\theta_{inc}$, which are normal to the interfaces of our PhC slab. They intersect with the EFCs at point B in the first Brillouin zone and point A in a higher-order zone. Point A corresponds to point A' in the first Brillouin zone. From Fig. 4.3(b) one sees that points A' and B correspond to negative and positive refraction, respectively. Therefore, we would expect an appropriate design for such a 1D PhC slab can give an off-axis focusing as shown in Fig. 4.3(c). Note that both positive refraction and negative refraction occur in the present subwavelength focusing (while only negative refraction occurs in subwavelength focusing by a slab of some high-dimensional PhC of negative refraction).
4.1 Off-axis focusing with a slab of 1D dielectric photonic crystal

Figure 4.4: (a) The snapshots of the electric field \(E_z\) for the PhC lens (indicated by the black solid lines) of thickness 2\(a\), 4\(a\) and 8\(a\) when the point source is placed at \(x = -2a, -3a, -5a\) in (a), (b), and (c), respectively.

To demonstrate the off-axis superlensing property, we perform some finite-difference time-domain (FDTD) simulations with the boundary treatment of perfectly matched layer [80]. The size of the FDTD discretization grid is fixed to \(a/30\) in each direction. The point source is placed on the left-hand side of the PhC slab with \(y = 0\). The slab is always centered at the origin of the coordinate system and its interfaces make an angle...
4. SUPERLENS FORMED BY A ONE-DIMENSIONAL DIELECTRIC PHOTONIC CRYSTAL

with the medium layers of the PhC. The snapshots of the electric field ($E_z$) for PhC slabs (with fixed surface termination angle $\phi = 45^\circ$) with thickness $w = 2a$, $4a$, and $8a$ are shown in Figs. 4.4(a)-4.4(c), respectively, where the point source is located at $x = -2a$, $-3a$, $-5a$, respectively. The length of the PC slab is $50a$ in all the simulations in this section.

From Fig. 4.4 we see that a point-like off-axis image is formed on the right-hand side of the PC slab in all the three cases. The best image occurs for the case of $w = 4a$ (see Fig. 4.4(b)). Our simulations indicate that when the slab thickness increases further, the image becomes obscure and aberrations become serious.

Figure 4.5: (a)The distribution of the electric field intensity at the transversal image plane when the surface termination angle $\phi$ varies. The thickness of the PhC slab is $4a$ and the point source is located at $x = -3a$, $y = 0$; (b)The distribution of the electric field intensity at the transversal image plane. The inset shows the on-axis superlens consisting of two slabs of the 1D PhC.

Fig. 4.5(a) shows the electric field intensity $|E_z|^2$ at the image plane when $\phi$ varies. The PhC slab is $4a$ thick and the point source is located at $x = -3a$, $y = 0$. When $\phi$ is set to $44^\circ$, $45^\circ$ and $46^\circ$, the position of the image is at $(x, y) = (3.8a, 4.8a)$, $(4.3a, 5.2a)$, $(4.6a, 5.6a)$ and the full width half maximum (FWHM) is $0.164\lambda$, $0.189\lambda$ and $0.206\lambda$, respectively. Thus, subwavelength focusing can be achieved easily. When $\phi$ increases further, the off-axis image moves farther and downward with its imaging quality degraded. These results show that the orientation of the surface termination influences the quality of subwavelength focusing (though the position of the surface termination does not). For
4.2 On-axis focusing with combination of two slabs of the 1D photonic crystal

This example, $\phi = 44^\circ$ gives the best quality of subwavelength focusing (with a FWHM of 0.164\(\lambda\) whose spot size is much smaller than that of a 2D or 3D PhC slab (typically 0.3\(\lambda\)).

The image point will be at the back surface when $\phi$ is 43\(^\circ\). Thus, $\phi$ should be larger than 43\(^\circ\) for slab-focusing. Note that the distance between the object and the front surface should not be too large (as compared with the width of the PhC slab) in order to obtain a focusing image. One advantage of the present superlensing structure is that its thickness can be much thinner as compared with 2D or 3D PhC slabs for subwavelength focusing.

4.2 On-axis focusing with combination of two slabs of the 1D photonic crystal

Finally we study some on-axis focusing with the combination of two slabs of the 1D PhC. Both slabs have the same thickness of 4\(a\) but different angles for surface termination. Here we choose $\phi = 43^\circ$ for the left side slab and $\phi = -43^\circ$ for the right side slab. The structure is shown in the inset of Fig. 4.5(b).

The snapshots of the electric field ($E_z$) are shown in Figs. 4.6(a)-4.6(c), where the point source are located at $x = -6a$, $-8a$ and $-10a$, respectively. In Figs. 4.6(a)-4.6(c) the distance between the object and the image remains roughly the same (16.2\(a\), 16.2\(a\) and 16.3\(a\), respectively). Fig. 4.5(b) shows the electric field intensity $|E_z|^2$ at the image plane when the source is at $x = -6a$ and FWHM is 0.201. From Figs. 4.6(a)-4.6(c) one sees that the image is roughly symmetrical and is on the $x$ axis. The case when the point source is located at $x = -20a$ and $y = 0$ is show in Fig. 4.6(d), from which one sees that the image is sort of imaginary image (located at the left side of the back surface) when the object is quite far away. These properties usually exist only when the PhC has an isotropic effective refractive index. Note that the present 1D PhC does not have any isotropic effective refractive index since its EFCs are not of circular shape.

4.3 Conclusion

We have introduced a simple superlens formed by a 1D dielectric PhC. Off-axis subwavelength focusing has been achieved and explained with some EFCs analysis. Unlike in subwavelength focusing by a slab of some high-dimensional PhC of negative refraction, both positive refraction and negative refraction occur in the present subwavelength focusing. The present 1D PhC lens is easy to fabricate, and the spot size can be much smaller than that for a 2D or 3D PhC slab. The superlens properties including the influence of the orientation of the surface termination to the image quality have been studied with the
4. SUPERLENS FORMED BY A ONE-DIMENSIONAL DIELECTRIC PHOTONIC CRYSTAL

Figure 4.6: The snapshots of the electric field ($E_z$) for a point source placed at $x = -6a$, $-8a$, $-10a$ and $-20a$ in (a), (b), (c) and (d), respectively. The slab surfaces are indicated by the black solid lines and the interface of the two slabs is marked by the dash-dotted line.

Figure 4.6: The snapshots of the electric field ($E_z$) for a point source placed at $x = -6a$, $-8a$, $-10a$ and $-20a$ in (a), (b), (c) and (d), respectively. The slab surfaces are indicated by the black solid lines and the interface of the two slabs is marked by the dash-dotted line.
FDTD simulation. Later on, the off-axis focusing structure was verified by Savo et al experimentally [101]. The present superlensing structure can be much thinner than existing 2D or 3D PhC slabs for subwavelength focusing. The properties of on-axis image achieved by the combination of two such slabs of 1D PhC have also been studied. Although the present 1D PhC does not have any isotropic effective refractive index, the combination of two such slabs of 1D PhC can give some properties which usually exist only for some 2D or 3D PhC with an isotropic effective refractive index.
4. SUPERLENS FORMED BY A ONE-DIMENSIONAL DIELECTRIC PHOTONIC CRYSTAL
Chapter 5

The effect of a photonic crystal on the extraction efficiency of a light-emitting diode

Semiconductor light-emitting diodes (LEDs) have great potential as low-cost and long lifetime solid-state lighting sources for various applications from room lighting to flat panel displays [102,103]. LEDs are also used in short-range communication systems and may be desirable for optical interconnects in computers [104]. A limiting factor to achieving high efficiency is that without some special light extraction technique only a small percentage of the light can go out from the LED (1/4n^2 per surface) because of the total internal reflection [103]. Various methods have been employed to increase extraction efficiency (\(P_{\text{out}}/P_{\text{tot}}\), where \(P_{\text{out}}\) and \(P_{\text{tot}}\) are the optical power emitted into free space and optical power emitted from the active region, respectively.), such as surface roughening [105] and geometrical modification [106]; however, these methods rely on random light redirecting events.

In 1997, Fan et al, proposed a photonic crystal (PhC) slab to get a high extraction efficiency of spontaneous emission [107]. There are two mechanisms to get the high extraction efficiency, bandgap effect and leaky mode effect. The schematic figure of the PhC slab is shown in Fig. 5.1(a). The corresponding band diagram is shown in Fig. 5.1(b). The attention is focused on the TE guided modes since light emitted from a quantum well “sandwiched” between two dielectric layers would have a similar polarization. The extraction efficiency is shown in Fig. 5.1(c) as a function of frequency. At the band edge of the lowest band, the extraction efficiency jumps sharply from less than 15% to more than 70%. The efficiency remains close to 70% inside the entire gap region. A dip occurs around 0.55 (c/a), which coincides with the upper edge of the gap. Above the second band, there are no TE-like guided modes. The efficiency oscillates around an average
5. THE EFFECT OF A PHOTONIC CRYSTAL ON THE EXTRACTION EFFICIENCY OF A LIGHT-EMITTING DIODE

Figure 5.1: (a) Schematic diagram of the computational cell containing a finite number of air holes inside a dielectric slab on a triangular lattice. (b) Dispersion relation of the structure shown in (a) for the case of an infinite number of air holes. The gray area corresponds to the continuum of leak modes. The solid circles correspond to TE-like guided modes, while the open circles correspond to TM-like guided modes. (c) Output efficiency as a function of frequency, for the case shown in (a). Spatial distribution of the electric-field power density radiating from a dipole in the triangular lattice. The power density is shown for frequencies (d) \( f = 0.44 \frac{c}{a} \) and (e) \( f = 0.76 \frac{c}{a} \). Adopted from Ref. [107].

value of 70% with the occasional peak close to 90%. In Figs. 5.1(d) and 5.1(e) the power distribution of the electric field radiating from the dipole is shown. The power is shown for two different frequencies, namely, 0.44 (c/a) which lies inside the gap [Fig. 5.1(b)] and 0.76 (c/a), which falls inside the continuum of leaky modes [Fig. 5.1(b)]. In both cases, a large fraction of the power is radiated into free space. He suggests to use this way to
improve the extraction efficiency of LED.

Since then, PhCs have been studied as an effective means of controllably extracting guided light from LEDs [108–112]. However, the effect of disorder, which is inevitably introduced in the fabrication process, on the extraction efficiency of the ordered PhC LED (EEOPL) was seldom reported except Ref. [113], where the influence of the disorder of a PhC on the leaky mode contribution to the extraction efficiency of a LED was briefly discussed. In this section, the effects of disorder in a PhC on the extraction efficiency of an LED are studied numerically. The difference between the EEOPL and the extraction efficiency of the disordered PhC LED (EEDPL) is studied and the physical mechanism is explained.

Fig. 5.2(a) shows schematically the LED structure studied in this chapter. The LED structure consists of two layers. The first layer is a perfect electric conductor (PEC) and the second layer is a dielectric layer with some nano-structures on its top (containing many air grooves). In some realistic cases the first layer is an omnidirectional reflector whose reflective efficiency is very high [114], and therefore can be approximated to a PEC to get a simple and reliable model in our simulation. The period of the unit cell, the width of the air grooves, the depth of the air grooves and the thickness of the dielectric layer are $a$, $d$, $h$ and $H$, respectively. Note that every unit cell contains one air groove. The center of the air groove always coincides with the center of unit cell for the ordered PhC LED, while this is not the case for the disordered PhC LED.

The FDTD method is used to calculate the dispersion curves of the PhC structure. The computational domain covers one unit cell of the periodic structure, where the standard boundary treatment of perfectly matched layer (PML) is used in ±$y$ directions and the Bloch boundary condition is used in ±$x$ directions. The size of the FDTD discretization grid is fixed to $a/50$ in each direction to make the results reliable. We excite eigenmodes by some pulse point sources and compute the frequency spectrum of the time-domain response, where each peak in the spectrum corresponds to an eigenfrequency.

To get the extraction efficiency of the LED, a finite size of structure is used. Forty thousand point sources are located randomly on a plane which is marked by the red line in Fig. 5.2(a) to approximate the practical active layer. The width of the LED (and the active plane) is $L$. The distance between the plane and the top surface of PEC is $D$. A two-dimensional model based on the FDTD by solving Maxwell’s equations with PML is employed to calculate the light field distribution. The position of each point source ($p$) is described by a random number $ran_1$ in a uniform distribution between 0 and 1 generated by a computer and the relation are described by

\[
p = (ran_1 - 0.5) \times L
\]
5. THE EFFECT OF A PHOTONIC CRYSTAL ON THE EXTRACTION EFFICIENCY OF A LIGHT-EMITTING DIODE

![Schematic sketch of the LED model in our simulation.](image)

**Figure 5.2:** (a) Schematic sketch of the LED model in our simulation. (b) The dispersion relation of the PhC, the red line is the light line of air and the four gray dashed lines correspond to the four normalized emission frequencies which are analyzed in the following part. The inset shows the unit cell.

For the disordered PhC LED, the deviation of the position of each air groove is generated randomly and the width of each air groove kept equal to \(d\). The position disorder parameter \(\delta\) is described by another random number \(\text{ran}_2\) in a uniform distribution between 0 and 1 generated by computer and the relation are described by

\[
\delta = \text{ran}_2 \times (a - d) \tag{5.2}
\]

The realistic cases are three-dimensional, whose simulation needs huge memory and is time consuming. Here we use two-dimensional simulation to study the physical mechanism for the difference between the EEOPL and EEDPL. The final conclusion is independent of the specific sources and structures, and thus can be extended to three-dimensional cases.
\(\omega(2\pi c/a)\) & Average \(E_{\text{normal}}\) % & Average \(E_{\text{ordered}}\) % & Average \(E_{\text{disordered}}\) % \\
0.2(\omega_1) & 4.345 & 9.826 & 20.203 \\
0.3846 (\omega_2) & 43.843 & 67.764 & 81.364 \\
0.4545 (\omega_3) & 30.461 & 84.404 & 83.674 \\
0.5556 (\omega_4) & 37.997 & 66.685 & 63.578 \\

Table 5.1: The extraction efficiency of the normal LED, the ordered PhC LED and the disordered PhC LED.

We set \(d = 0.5a\), \(h = 0.2a\), \(H = 0.8a\) and \(L = 87a\). The refractive index of the dielectric layer is 2.67. The sources are set to excite transverse-electric (TE) modes. Fig. 5.2(b) shows the dispersion curves of the PC and the inset shows the unit cell. Four special normalized emission frequencies NEFs), namely, \(\omega_1 = 0.2 \times 2\pi c/a\), \(\omega_2 = 0.3846 \times 2\pi c/a\), \(\omega_3 = 0.4545 \times 2\pi c/a\) and \(\omega_4 = 0.5556 \times 2\pi c/a\) which are marked as gray dashed lines in Fig. 5.2(b) are chosen to investigate the extraction efficiencies of the LED. In Fig. 5.2(b) one can see clearly that at each of these four NEFs there is a mode which is very close to the light line of air (called critical mode in this chapter). Besides the critical mode, other modes also exist for light with \(\omega_1\) (guided mode), \(\omega_2\) (guided mode and leaky mode) and \(\omega_3\) (leaky mode). Light in the PhC can only propagate as one of these four modes, namely, sum mode \((\omega_1)\) of critical mode and guided mode, sum mode \((\omega_2)\) of critical mode, guided mode and leaky mode, sum mode \((\omega_3)\) of critical mode and leaky mode, and sum mode only \((\omega_4)\). Light at these four NEFs represents all kinds of light which can exist in the PhC. Thus the EEOPL and EEDPL at these NEFs are calculated in order to compare the extraction efficiency under different extraction principles.

The EEOPL and EEDPL are denoted by \(E_{\text{ordered}}\) and \(E_{\text{disordered}}\), respectively. The extraction efficiency of the normal LED (which has no nanostructures on the top surface) denoted by \(E_{\text{normal}}\) is also calculated for comparison. The extraction efficiency is defined as the fraction of emitted flux through the top surface of the LED to the total emitted flux generated by the point sources. For each of the four NEFs, ten simulation cases with different random numbers generated by a computer are carried out and the results are averaged to ensure the numerical convergence of the extraction efficiency within 2%. The final averages are shown in Table 5.1.

In Table 5.1 one sees that the difference between the EEOPL and EEDPL is large at \(\omega_1\) and \(\omega_2\), while the difference is small at \(\omega_3\) and \(\omega_4\), (both the EEOPL and EEDPL are always higher than that of the normal LED). Fan et al pointed out that an efficient light extraction from an LED can be achieved by eliminating guided modes through designing the emission wavelength inside the bandgap region or leaky mode region of the PhC [107].
5. THE EFFECT OF A PHOTONIC CRYSTAL ON THE EXTRACTION EFFICIENCY OF A LIGHT-EMITTING DIODE

In our cases, if more part of the light propagates as leaky mode, more part of the light will be scattered out of the LED (i.e., less part of the light propagates as guided mode), and consequently higher extraction efficiency can be achieved. Thus we put a line monitor on the top of the disordered PhC LED to study the effect of the disorder on the modes generated by the PhC. The average of the square of the amplitude of the fast Fourier transformation (FFT) of the complex-amplitude distribution on the monitor is obtained and given by the red curves in Fig. 5.3, while that for the ordered PhC LED is given by the blue curves for comparison. Note that the total emitted flux generated by the point sources is normalized by a constant. The relation between the output power and the square of the amplitude of the FFT on the monitor can be described as

\[ P \propto \int FFT(k_x)^2 \times \cos(k_x/k_0 \times \pi/2) dk_x \]  

(5.3)

where \( k_0 \) is the propagation constant in vacuum and \( k_x \) should obey \(-k_0 < k_x < k_0\). The output power increases as the average of the square of the amplitude of the FFT within \((-k_0, k_0)\) becomes larger.

In Fig. 5.3(a) there are some peaks around \( k_x = \pm 0.2(2\pi/a) \), \( k_x = \pm 0.41(2\pi/a) \) and \( k_x = \pm 0.59(2\pi/a) \) for the ordered PhC LED at \( \omega_1 \), which correspond to a critical mode, the fundamental guided mode, and a guided mode with a larger propagation constant. The peak around \( k_x = \pm 0.41(2\pi/a) \) is much higher than the others. Since higher peak means more part of the light propagates as the corresponding mode, light scattered out of the LED is much less than light propagating inside the LED in this case, which causes the low extraction efficiency. For the disordered PhC LED, one still sees the peaks around \( k_x = \pm 0.2(2\pi/a) \), \( k_x = \pm 0.41(2\pi/a) \) and \( k_x = \pm 0.59(2\pi/a) \), which means the bandstructure of the PhC influences the disordered PhC LED to some extent. While the peaks around \( k_x = \pm 0.59(2\pi/a) \) become lower, the peaks around \( k_x = \pm 0.41(2\pi/a) \) are nearly unchanged because the corresponding guided mode is the fundamental mode and can not be influenced easily by such a small disorder. The red curve within \(-0.2(2\pi/a) < k_x < 0.2(2\pi/a)\) is always above the blue curve. The distributions of the absolute amplitude of \( H_z \) and the time average Poynting vectors (marked by white arrows) with a single point source (with frequency \( \omega_1 \)) in the ordered PhC LED and disordered PhC LED are shown in Fig. 5.4(a) and 5.4(b), respectively. The Poynting vectors in air have little vertical values in Fig. 5.4(a) while they have a bit larger values in Fig. 5.4(b) Thus some part of the guided mode with a larger propagation constant is influenced by the disorder and scattered out of the LED so that the EEDPL (20.203\%) is higher than the EEOPL (9.826\%).

In Fig. 5.3(b) there are some peaks around \( k_x = \pm 0.04(2\pi/a) \), \( k_x = \pm 0.44(2\pi/a) \) and \( k_x = \pm 0.56(2\pi/a) \) for the PhC LED at \( \omega_2 \), which correspond to a leaky mode, a
Figure 5.3: The average of the square of the FFT amplitude on the line monitor with normalized emission frequencies at (a) $\omega_1 = 0.2 \times 2\pi c/a$, (b) $\omega_2 = 0.3846 \times 2\pi c/a$, (c) $\omega_3 = 0.4545 \times 2\pi c/a$ and (d) $\omega_4 = 0.5556 \times 2\pi c/a$. For graphic clarity, a logarithmic scale is used. Light between two gray dotted lines $k_x = \pm k_0$ can get out of the LED and contributes to the output power.

guided mode, and a guided mode with a larger propagation constant. One sees clearly that these peaks are lower for the disordered PhC LED. Between the two dotted gray lines $k_x = \pm k_0$, the red curve is nearly always above the blue curve except the peaks around
5. THE EFFECT OF A PHOTONIC CRYSTAL ON THE EXTRACTION EFFICIENCY OF A LIGHT-EMITTING DIODE

Figure 5.4: The distributions of the absolute amplitude of \( H_z \) and the time average Poynting vectors (marked by the white arrows) with a single point source (with \( \omega_1 = 0.2 \times 2\pi c/a \)) inside (a) the ordered PhC LED and (b) the disordered PhC LED. The outline of the structures is marked by the black lines.

\[ k_x = \pm 0.04(2\pi/a). \] Then the output power of the disordered PhC LED is larger than that of the ordered PhC LED [cf. Eq. 5.3]. Thus the disorder in the PC damages the leaky mode and scatters some part of the fundamental guided mode and the guided mode with a larger propagation constant out of the LED. This not only compensates the reduction of the emitted light from the leaky mode but also increases the total output power (from 67.764\% to 81.364\%; cf. Table 5.1).

For the ordered PhC LED at \( \omega_3 \), there are peaks around \( k_x = \pm 0.15(2\pi/a) \) and \( k_x = \pm 0.35(2\pi/a) \) in Fig. 5.3(c) which all correspond to leaky modes. For the disordered PhC LED, these peaks are affected and become lower. The corresponding energy is converted to other scattered part which corresponds to some tiny peaks between the two gray dotted lines \( k_x = \pm k_0 \) and can be scattered out of the LED directly. Because both the leaky mode and the scattered part are between the two gray dotted lines, they contribute to the extraction efficiency. Thus the disorder in the PhC converts some part of the leaky mode to scattered part, which is scattered out of the LED directly, and keeps the extraction efficiency nearly unchanged (cf. Table 1). In many practical cases, the emission wavelength of the PhC LED is in leaky mode, and thus this property can give some interesting conclusion and will be discussed later.

In Fig. 5.3(d), there are peaks around \( k_x = \pm 0.5556(2\pi/a) \) for both the ordered PhC LED and the disordered PhC LED at \( \omega_4 \). In this case, only critical mode can exist in the photonic crystal (see Fig. 5.2(b)), and thus the critical mode is excited strongly in this
case. However, the critical mode propagates with \( k_y = 0 \) and thus has no contribution to the extraction efficiency. The output power is all from the scattered part, which has no relation with the bandstructure effect, and the disorder does not give any effect. Thus although the NEF is in the leaky mode region, the leaky mode is not excited at all and this leads to a comparatively low extraction efficiency (below 70%; see Table 1).

In the previous analysis, we have found that disorder always harms the PhC modes. When light can propagate as a guided mode, the disorder can extract some part of guided mode light and scatter it out of the LED, which increase the extraction efficiency. When most of the light propagates as a leaky mode, the disorder will cause part of the leaky mode scattered out of the LED, while keeping the total output power nearly unchanged. Note that some part of light will propagate as a critical mode because of the weak bandstructure effect, which still exists in two-dimensional PhC slab. We have also found that the extraction efficiency in leaky modes region will not be high when most of light propagates as a critical mode which will not contribute to the output power as it propagates with \( k_y = 0 \), such as the case with \( \omega_4 \), which should be avoided.

In conclusion, the effects of disorder in a PhC on the extraction efficiency of the LED have been investigated by using a full-vectorial FDTD method. The EEOPL and EEDPL at several NEFs are calculated to compare the extraction efficiency with different extraction mechanisms. The EEOPL and EEDPL are comparable when the frequency is in leaky modes region. Other kinds of disorder have also been simulated (such as other kinds of random distribution, air grooves of half circle shape and triangles), but not shown here. These simulations show that a similar conclusion can be expected for other kinds of disordered PhC LEDs in which the effect of the PhC band structure still exists. Thus when the emission frequency is in a leaky modes region, the functionality of the PhC LED can be sustained even if the disorder exists in the fabrication process and the Purcell enhancement of the ordered PhC LED and the disordered PhC LED are more or less the same. Our calculation shows that the ratio of the Purcell enhancement factor for the ordered PhC LED over that for the disordered PhC LED is 0.93 at \( \omega_3 \). The Purcell enhancement can even be neglected when the distance between the active layer and the nanostructures on the top surface is larger. Although our simulation is two-dimensional, the method and similar conclusion can be extended to three-dimensional cases.
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Chapter 6

A compact electro-optic modulator based on photonic crystal

With the advantages of the compatibility with the mature silicon IC manufacturing and the availability of low cost silicon-on-insulator (SOI) wafers, silicon photonics has been a spectacular technology to implement monolithic integration of microelectronic and photonic components [115, 116]. One of the key photonic components is a high speed and compact electro-optic modulator. Though silicon has excellent material properties including high thermal conductivity, high optical damage threshold, high third-order optical nonlinearities and low transmission loss for near-infrared communication band, it is not an ideal material for electro-optic modulation because of the very weak linear electro-optic effect, the so-called Pockels effect, which is the basis for the most commercial modulators nowadays [115]. Although the optical refractive index in silicon can be obviously changed by temperature variation, it is not suitable for high speed application due to the very slow thermo-optic transient response.

Feasible high speed modulation based on silicon medium can be achieved by the plasma dispersion effect [117], which describes the relation between the density change of free carriers in a semiconductor and the modification of real refractive index and optical absorption coefficient. The free carrier density in silicon can be varied by charge carrier injection, accumulation or depletion. Recently, some great breakthroughs utilizing plasma dispersion effect have been reported with the structures based on a MOS capacitor [118], a p-i-n diode [90, 119] or a pn junction [120]. However, the plasma dispersion effect is still very weak for efficient electro-optic modulation and it usually leads to a device with a large footprint. For example, with a case of uniform carrier injection of electrons and holes of $3 \times 10^{17} \text{ cm}^{-3}$ throughout the whole intrinsic region, the change of the real index is only 0.001, going with an absorption coefficient variation of $\Delta \alpha = 4.35 \text{ cm}^{-1}$ [121]. Consequently, in order to achieve a $\pi$ phase shift for a Mach-Zender Interferometer (MZI)
6. A COMPACT ELECTRO-OPTIC MODULATOR BASED ON PHOTONIC CRYSTAL

configuration, an interaction length of more than 800 µm is required.

![Dispersion relation of a guided mode of a photonic crystal waveguide.](a)
![Schematic diagram of the silicon Mach-Zehnder PhC modulator.](b)

Figure 6.1: (a) Dispersion relation of a guided mode of a photonic crystal waveguide. (b) Schematic diagram of the silicon Mach-Zehnder PhC modulator. Adopted from [91].

An ultra-compact implementation of a silicon modulator is reported by a structure based on a micron-sized ring resonator with a high quality factor Q=39,350 [119]. The high Q nature of the ring resonator increases the sensitivity of the device to small index change. But it also enhances the sensitivity to the environmental fluctuations and fabrication tolerances simultaneously, which greatly limits its practical applications. A promising way is to use photonic crystal waveguides (PhCW). The extraordinary dispersion of PhCWs offers an unprecedented opportunity for developing ultracompact MZI modulators, where slow light effect could keep the device’s effective modulator optical path length whereas reduce the actual modulator length by several orders of magnitude [91].

Consider a typical dispersion relation for a PhC waveguide mode shown in Fig. 6.1. If the refractive index of the waveguide core material i.e., silicon varies by an amount \( \Delta n \), the dispersion curve will shift vertically by an amount \( \Delta \omega_0 \). As theoretically explained by Soljacic et al. [38], for a fixed frequency of light, the propagation constant \( \beta_{PhC} \) of PhC waveguide changes as \( \Delta \beta_{PhC} = (d\beta_{PhC}/d\omega)\Delta \omega \), which grows significantly whenever the group velocity \( v_g = (d\beta_{PhC}/d\omega)^{-1} \) approaches zero, e.g., on the rightmost segment of the dispersion curve. Such an extraordinary growth of \( \Delta \beta_{PhC} \) directly leads to a significant enhancement of phase modulation efficiency because the phase change is related to the change of propagation constant and waveguide length \( L \) as \( \Delta \phi_{PhC} = \Delta \beta \times L \). The length of a fabricated silicon PhCW modulator reported by Gu et al has been scaled down to 80 µm, while keeping a large 3 dB bandwidth [122]. There is a great room to further improve the device’s performance by optimizing the device design and fabrication. One effective method is to replace the normal single line-defect PhCW by a width-reduced line-defect PhCW, where the much stronger capability in optical confinement could allow
6.1 Proposed structure

In this chapter, we investigate the electronic and optical characteristics of a width-reduced line-defect photonic crystal waveguide within a lateral p-i-n structure. The schematic structures are shown in Fig. 6.2. Section 6.1 presents the proposed structure. Section 6.2 describes the optical characteristics of the proposal. Improvement in optical confinement could be obviously observed by the results obtained by three dimensional (3D) plane wave expansion analyses. Conclusions are followed in Section 6.3.

6.1 Proposed structure

![Figure 6.2](image)

Figure 6.2: (a) Schematic view of a width-reduced line-defect PhCW embedded in a lateral p-i-n structure on a silicon on insulate substrate; Schematic diagrams of the electrical model based on (b) cross section and (c) longitudinal section for the active PhCW device.

A schematic 3D view of the proposed configuration is depicted in Fig. 6.2(a). It consists of a line-defect waveguide embedded in a silicon photonic crystal slab with two-dimensional (2D) triangle lattice of air holes (lattice constant is $a$ and hole diameter is $d$). The line-defect waveguide is introduced by removing a row of air holes along the $\Gamma K$ direction. The waveguide width ($w_d$) is defined as the distance between the centers of the holes nearest to the waveguide, where $w_d$ for a single line-defect waveguide is defined by $W = \sqrt{3}a$ [123]. Shifting the PhC regions towards the waveguide will lead to a width-reduced PhCW. Theoretical and experimental investigations have proved that the width-reduced PhCW has a broad lossless propagation band when its $w_d$ is in the range of $0.6 \sim 0.7W$ [123] [124]. It should be noted that this PhC slab, with the SiO$_2$ cladding in the bottom and the air cladding above, exhibits an asymmetric refractive-index distribution along the vertical direction. Although the vertical optical confinement
6. A COMPACT ELECTRO-OPTIC MODULATOR BASED ON PHOTONIC CRYSTAL

is not as good as an air-bridge type, it is more preferable when the practical applications and the fabrication process are taken into consideration. In order to form a p-i-n diode structure, Ion implantation should be applied to the PhC slab, which usually has a light background doping concentration (e.g. $10^{15}$ cm$^{-3}$) of n-type. Heavy p and n doped regions are formed and located in the two sides of the PhCW. A concentration of $5 \times 10^{19}$ cm$^{-3}$ is assumed for both the p+ and n+ regions in the following simulation. The width of the intrinsic region is denoted as $w_i$, which plays an important role on the device’s electrical response.

In the following simulation and analysis, we choose a width-reduced PhCW structure defined on an SOI platform with a silicon slab thickness of 0.6a, an air-hole diameter of 0.5a and a waveguide width of 0.66W, which is called W0.66 PhCW in the following parts. The lattice constant a of the photonic crystal is set to 380 nm to tune the dispersive curve having a group index of about 10 at 1550 nm, which is similar to that of the device in [122].

The electric analysis was performed by Tang [125], and showed that the response time was decreased as the intrinsic layer width was reduced. In this chapter we showed how the optical mode width can be correspondingly decreased, so that the mode doesn’t overlap with the highly doped regions.

6.2 Optical analysis

We calculate the dispersion relation and modes profile by using three dimensional (3D) plane wave expansion (PWE) method. The bandstructure is shown in Fig. 6.3, where the black line is the light line of SiO$_2$ and the shaded region represents the projection of the TM-like (the magnetic field $H$ is in-plane) and TE-like (the electric field $E$ is in-plane) slab modes. Note that the perfect photonic crystal has a band gap for the TE-like slab modes, but not for the TM-like slab modes. Thus, light that propagates in the waveguide with a frequency within the band gap of the crystal for the TE-like slab modes can be propagated along the line-defect. However, optical coupling between transverse-electric (TE)-like waveguide modes and transverse-magnetic (TM)-like slab modes occurs in an asymmetrically cladded SOI 2D PhC slab which causes large propagation losses when the in-plane direction wave-vector conservation is satisfied between both modes [123]. Thus, the region outside the projection of both the TM-like and within the band gap for the TE-like slab modes is in our consideration.

Fig. 6.3(a) shows the relation between the normalized frequency ($c/a$) and the group index. Here we choose the lower band of W1 and higher band of W0.66 for comparison, because both are around the center of band gap and flatter than the other. For both cases,
6.2 Optical analysis

Figure 6.3: (a) Dispersion curves of W0.66 (blue) and W1 (red). The shaded region represents the projection of the TM-like and TE-like slab modes. The relation between the normalized frequency and the group index for (b) W0.66 and (c) W1.

we make the group index equal 10, which corresponds a normalized frequency of 0.2452 (W0.66) [Fig. 6.3(b)] and 0.2562 (W1) [Fig. 6.3(c)], respectively. The lattice constant $a$ of the PhC is set to 380 nm to tune the dispersive curve having a group index of about 10 at 1550 nm as we mentioned before. We calculated the optical field distribution of the

Figure 6.4: (a) Top view of the W1 PhCW and W0.66 PhCW. The white dashed line represents the cross section shown in (b). (b) Time intensity calculated by the plane wave expansion method in crosssection view.

guided mode for the W1 PhCW and W0.66 PhCW by the PWE method. In Fig. 6.4
6. A COMPACT ELECTRO-OPTIC MODULATOR BASED ON PHOTONIC CRYSTAL

The intensity distribution for the W0.66 PhCW has a much more compact lateral size than that for the W1 PhCW, while most power is localize inside the Si slab in vertical direction for both structures. Some recent experiments indicate that the dominant loss in PhCW is the coupling loss, following a power law dependence of the group index [35]. It is believed that the coupling loss is mainly induced by the mismatch between the slow guide mode and input mode of a silicon strip waveguide. As the optical distribution in strip waveguide is smaller than that in a W1 PhCW, a taper structure is usually required to improve the coupling efficiency [35]. With the assuming W0.66 PhCW, whose cross section is similar to the normal strip silicon waveguide (e.g. 223 nm × 460 nm in [35]), we believe that this setting will lead to a better mode matching and reduce the insertion loss of a PhCW device.

Figure 6.5: (a) Intensity distribution in longitudinal-section view an plotted on a normalized scale (integrated over one unit cell) for the W1 PhCW and W0.66 PhCW.

Fig. 6.5 shows the time averaged power density profile of the photonic crystal mode in longitudinal section view and plotted on a normalized scale (integrated over one unit cell) for the W1 PhCW and the W0.66 PhCW. It can be seen clearly that the power profile in the W1 PhCW, where the power is small when the absolute value of the lateral position is bigger than 1.5 μm, has a wider lateral distribution than that in the width-reduced one, where the power is small when the absolute value of the lateral position is bigger than 2.4 μm. The time averaged power density reaches the maximum in the center of both waveguides, however, when the distance from the center of the waveguide increases, the time averaged power density for the W1 PhCW decreases sharply at first, increases slowly after reaching the first air array beside the center region and decreases again after leaving the first air array, while that for a width-reduced line-defect PhCW decreases dramatically all the time. The compact optical field profile in the width-reduced PhCW would allow a narrower intrinsic layer zone. When the heavy doped zones are put closer to each other,
the path for the carriers will be shorter and the carriers will be under higher electrical field assuming that the same bias voltage is applied. Hence, the electrical response is expected to be improved, without the expense of the optical loss.

6.3 Conclusion

We investigate the optical characteristics of the width-reduced line-defect photonic crystal waveguides within lateral p-i-n structures. Compared with the classical line-defect photonic crystal waveguides, the width reduced photonic crystal waveguide has much stronger capacity in optical confinement in plane, which can allow a narrower intrinsic layer that leads to a fast electric response.
6. A COMPACT ELECTRO-OPTIC MODULATOR BASED ON PHOTONIC CRYSTAL
Chapter 7

Nanobeam photonic crystal devices for sensing

Optofluidics, referring to a class of optical systems that are synthesized with fluids, is an emerging technology for synthetic/analytical chemistry and nanobiotechnology. Here, light is used for controlling and efficiently analyzing fluids, colloidal solutions, solids in a fluid, etc, in microscale devices [126, 127]. Sensors are among the fundamental elements of optofluidics. Miniaturization of label-free optical sensors is of particular interest for realizing ultracompact lab-on-a-chip applications with dense arrays of functionalized spots for multiplexed sensing, that may lead to portable, low cost and low power devices. Many efforts exist to realize small devices and among them are photonic crystals (PhCs). So far, many kinds of PhC sensors relying on regular PhCs, PhC waveguides and PhC cavities have been demonstrated [21–25, 128–132].

Recently there has been much interest in cavities realized in free standing nanobeams patterned with a one-dimensional lattice of holes [133–138]. Single nanobeams are studied for their exceptional high quality (Q) factor and small modal volume [133, 134]. Coupled nanobeams with air slot are invented to tune the modes [135, 137] and achieve an optomechanical cavity [138]. These structures were made in passive materials as Si [133, 135, 137], SiO$_2$ [134] or SiN [138]. Very recently, single nanobeams made in III-V semiconductors are fabricated to achieve lasing [139, 140]. In all these structures, the cavities are made by changing the lattice constant, or by modifying the radius of the holes and the distance between the holes. In addition, because of the strong optical fields that exists in the slot region [130, 132, 141], these devices are proposed to have applications in sensing. However, no experiment about sensing based on these structures has been reported until now.

In this chapter, we investigate InGaAsP PhC slot nanobeam slow light waveguides with embedded InAs quantum dots (QDs) consisting of two parallel suspended beams
7. Nanobeam Photonic Crystal Devices for Sensing

Separated by a small gap, each patterned with a one-dimensional (1D) line of holes. Such a structure exhibits a resonance near its band edge frequency where the group velocity is near zero. No modification is made to form a local cavity. By measuring the resonant wavelength for different analytes, we report a high sensitivity $S = \Delta \lambda / \Delta n$ of $7 \cdot 10^2$ nm/RIU (refractive index unit) in section 7.1. For another structure with a cavity, a sensitivity of $9 \cdot 10^2$ nm/RIU is measured in section 7.2. A new design with both high sensitivity and high Q factor is proposed in section 7.3.

7.1 Nanobeam

![Figure 7.1: Schematic sketch of a PhC slot nanobeam slow light waveguide from (a) top view, (b) cross-sectional view. A unit cell is marked by two dashed lines. (c) Band structure of the waveguide. The gray region is the light cone of water. The inset shows the intensity distributions of four band-edge modes in the central plane from bottom to top accordingly. (d) The electrical field ($E_y$) profile of the slot mode of a finite waveguide with some extra mirrors infiltrated with distilled water in the central plane.](image)

Figure 7.1: Schematic sketch of a PhC slot nanobeam slow light waveguide from (a) top view, (b) cross-sectional view. A unit cell is marked by two dashed lines. (c) Band structure of the waveguide. The gray region is the light cone of water. The inset shows the intensity distributions of four band-edge modes in the central plane from bottom to top accordingly. (d) The electrical field ($E_y$) profile of the slot mode of a finite waveguide with some extra mirrors infiltrated with distilled water in the central plane.
A PhC slot nanobeam slow light waveguide was designed by using MIT photonic bands software package (MPB) \[60\] and three-dimensional finite-difference time-domain method \[61\]. The top view and cross sectional view of the unit cell of waveguide used in the bandstructure calculation is shown in Fig. 7.1(a) and (b), respectively. The waveguide is defined by the lattice constant (490 nm), width of single nanobeam (450 nm), width of the slot area (200 nm), distance between the symmetric holes (650 nm), diameter of the holes (310 nm) and the thickness of the membrane (220 nm). Since the nanobeam is intended as a liquid sensor, the bandstructure calculation from MPB is performed for an environment refractive index of 1.333, corresponding to water, and is displayed in Fig. 7.1(c). There are four bands under the light cone of water, whose cutoff wavelengths are at 1706.8 nm ($\omega a/2\pi c=0.2871$), 1631.5 nm ($\omega a/2\pi c=0.3003$), 1404.7 nm ($\omega a/2\pi c=0.3488$) and 1336.9 nm ($\omega a/2\pi c=0.3665$), respectively. The intensity distributions of four band-edge modes in the central plane of the unit cell are shown in the inset of Fig. 7.1(c). We calculate the cutoff wavelengths shift by changing the environment refractive index to 1.342. Then we get the approximate sensitivities of different band edge modes. The results are shown in Tab. 7.1. Mode 3 gives the highest sensitivity. For the mode 3, the light is strongly localized inside the slot region and holes. We will call it slot mode later. The slot mode profile of this waveguide is similar to the even mode profile around cavities in coupled nanobeams as described in Ref. \[135–137\] but is not the same, which will be discussed later.

<table>
<thead>
<tr>
<th>Mode</th>
<th>Sensitivity (nm/RIU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mode 1</td>
<td>441</td>
</tr>
<tr>
<td>Mode 2</td>
<td>315</td>
</tr>
<tr>
<td>Mode 3</td>
<td>736</td>
</tr>
<tr>
<td>Mode 4</td>
<td>655</td>
</tr>
</tbody>
</table>

Table 7.1: The sensitivities of different modes.

<table>
<thead>
<tr>
<th>Width (nm)</th>
<th>Sensitivity (nm/RIU)</th>
<th>Q factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>180</td>
<td>717</td>
<td>3500</td>
</tr>
<tr>
<td>200</td>
<td>724</td>
<td>3000</td>
</tr>
<tr>
<td>220</td>
<td>744</td>
<td>2000</td>
</tr>
</tbody>
</table>

Table 7.2: The relationship between the width of the slot area, sensitivity and Q factor.

For a real sample, the length of waveguides is always finite. Additionally there is a constraint on the length of these waveguides because they need to be able to support their
own weight and survive in the fabrication and processing. A PhC slot nanobeam slow light waveguide with 27 periods was designed. In our simulation, the slot modes of the waveguide infiltrated with distilled water (n=1.333) and sugar/water solution (n=1.342) are at 1416.5 nm and 1422.8 nm respectively, with Q factors of 2000. Because the structure is finite, losses occur near the two ends. To decrease these losses, additional PhC mirrors with lattice constant of 490 nm and hole diameter of 400 nm were added, which increased the calculated Q factors to 3000. The electrical field $(E_y)$ profile of the slot mode of the finite waveguide with the extra mirrors infiltrated with distilled water in the central plane is presented in Fig. 7.1(d). The light is strongly localized in the central part of PhC slot nanobeam slow light waveguide. The light localization of the band edge mode in the central part of our 1D finite length waveguide is analogous to the light localization of band edge modes in finite two dimensional photonic crystals in Ref. [142]. By relating the peak position change with the change of refractive index, we obtain an impressive sensitivity value of 724 nm/RIU. Comparing with the even mode in the coupled nanobeams cavity [cf. Fig. 2 in Ref. [136]] where the light is localized in the slot region but also in the semiconductor, our slot mode has more light confined in the low refractive index region, i.e., in the slot region but also in the holes. Here we would like to introduce a figure of merit, $Q \cdot S$, which will be discussed in detail in section 7.3. To study the effect of the width of the slot area, the relationship between the width of the slot area, sensitivity and Q factor is given in Tab. 7.2. As the width increases, the sensitivity increases while the Q factor decreases. However, the increase in the sensitivity is marginal while the decrease of the Q factor is big. Therefore, the sensor performance is expected to be better for smaller slot widths for slot widths in the region of 200 µm.

The sample was fabricated with the method in section 2.2. Because for high sensitivity the nanobeams have strong requirements on the hole size and beam widths, they tend to be very fragile. These specifications are met by carefully adjusting the dose factors for the Electron Beam Lithography. We used SiN first to obtain the dose factors for the nanobeam with the correct parameters. Fig. 7.2(a) shows the Scanning Electron Microscope (SEM) image of a failed sample, which is not underetched. Fig. 7.2(b) shows the SEM image of a suspended nanobeam, in which both the diameter of the holes are smaller than what we want. Fig. 7.2(c) shows the SEM image, in which the parameters of the structure are good. Then with the proper dose factors found for the SiN mask, the structures were transferred to InGaAsP. Fig. 7.2(d) shows the SEM image of part of an array of InGaAsP slot PhC nanobeam slow light waveguides with the designed parameters, where the waveguide length was varied.

To measure the sensitivity of our structure, the sample was infiltrated with distilled water and sugar/water solution separately with known refractive indices [143] on the
set-up in section 2.3. The refractive indices of distilled water and sugar/water solution are 1.333 and 1.342, respectively. Fig. 7.3 shows the PL spectra from nanobeams with different lengths and larger radius than designed with the infiltration of water. There are two peak for the nanobeams with 25 and 27 period length, while only one peak for the other two. We find the peak appearing around 1525 nm is blue shifted as the length of the nanobeam increases. There are two reasons. First, when the length is increased, more slot area and more holes are opened. Second, holes and slots are marginally larger because of longer total exposure time due to larger overall doses resulting from electron scattering (“proximity effect”). Thus the two missing peaks for the nanobeams with 17
7. NANOBEAM PHOTONIC CRYSTAL DEVICES FOR SENSING

Figure 7.3: PL spectrum of the waveguide with the infiltration of distilled water $n=1.333$ and with length (number of periods) of (a) 17, (b) 19, (c) 25 and (d) 27.

and 19 periods are at longer wavelength and cannot be measured by the detector, which has a cutoff near 1600 nm. The separation between the two peaks is around 70 nm, which is consistent with the separation between mode 1 and mode 2 (75.3 nm), and between mode 3 and mode 4 (67.8 nm) as obtained from the band structure calculation. However, because the nanobeams have large holes, all the modes have blue shifts with respect with design. Thus the peak at shorter wavelength is from mode 2 and the other is from mode 1. Fig. 7.4 shows PL spectra from the another unsuccessful nanobeam with the infiltration of water and water/sugar solution. Because of the larger width of the slot area and holes, the peaks are blue shifted compared to the band edge modes in the simulation. There
are three peaks in both of the spectra. The two outer modes are attributed to the mode 1 and mode 1 from the simulations. The broad mode near 1540 nm is attributed to a mode formed between the slot area and mirrors, where can be seen in the calculated mode profile in Fig. 7.5. The modes are redshifted by replacing the water with water/sugar solution. This gives a sensitivity of 490 nm/RIU for mode 2, 280 nm/RIU for the mode formed between the slot area and mirrors, and 380 nm/RIU for mode 1.

Fig. 7.6(a) shows the PL spectrum of the InGaAsP slot PhC nanobeam slow light waveguide with the anticipated parameters and with the infiltration of distilled water. The peak at 1386.5 nm is the slot mode, with a Q factor of 500. Fig. 7.6(b) shows the PL spectrum of the same waveguide with the infiltration of sugar/water solution. The peak redshifts to 1392.4 nm. This gives a sensitivity of $7 \cdot 10^2$ nm /RIU, which has been confirmed several times later. A sensitivity close to the predicted value of 724 nm/RIU, implies that the calculated mode pattern agrees with experiment. Previously the high intensity in a different slot structure was measured by locally probing the EM field.
distribution by a scanning near-field optical microscopy experiment \[135\]. In the present work we probe it directly by a sensitivity experiment as previously demonstrated \[25\]. The structure is promising for application after improving the Q factor, while the Q factor can be improved by introducing a better mirror just on the ends of the slot region \[142\]. The slight discrepancy between simulation and experiment of the peak position, Q factor and sensitivity can be attributed to several effects, including the uncertainty of the membrane thickness after an O\(_2\) plasma and H\(_3\)PO\(_4\) etch, and the roughness in the slot region which weakens the localization of the light inside the slot region.

### 7.2 Nanobeam with a cavity

Because of the over etching of one device caused change in device geometry, we also have an InGaAsP PhC slot nanobeam slow light waveguide with stuck nanobeams, which is shown in Fig. 7.7(a). In this device, the parameters are the same as those we mention above, except for the hole diameter, which is increased to 330 nm. However, for this waveguide, the nanobeams bend inward which makes the slot region narrow in the central part and a cavity is formed. The bend may be due to the weak wall because of the larger hole diameter. We measure the sensitivity of this structure in the same way used before. Fig. 7.7(b) shows the PL spectrum of the cavity with the infiltration of distilled water. The peak at 1502.2 nm is the slot cavity mode, with a Q factor of 700. Fig. 7.7(c) shows the PL spectrum of the same structure with the infiltration of sugar/water solution. The
peak redshifts to 1510.3 nm. This gives a sensitivity of about $9 \cdot 10^2$ nm/RIU. Compared to the normal waveguide, the resonant wavelength shows a red shift of 100 nm, while this cavity has a higher sensitivity and a higher Q factor. The red shift of the resonant wavelength is due to the decrease of the separation between the two nanobeams [136, 137]. We have also modeled the bend case in our simulation, and found that the slot modes of the cavity infiltrated with distilled water (n=1.333) and sugar/water solution (n=1.3417) are at 1477.0 nm and 1482.6 nm respectively, which gives a sensitivity of 643 nm/RIU. The intensity distribution of the slot mode of the cavity type waveguide infiltrated with distilled water in the central plane is presented in Fig. 7.7(d). The light is still strongly localized in the slot region. The difference between the experiment and simulation results is caused by parameters uncertainty as inferred from SEM image. The higher sensitivity in the experiment may be also caused by the larger hole size in the bend structure.
7.3 Nanobeam with a designed cavity

The sensitivity alone is not sufficient for quantitatively characterizing the ability of the sensor to identify and to quantify the targeted material in the sample. Equally important is the ability to precisely measure the spectral shift that results from the sample. Sensor resolution ($\delta \lambda$) characterizes the smallest possible spectral shift that can be accurately measured. If infinitely high spectral resolution were available and absolutely zero system noise were present, the sensor performance could be characterized by the sensitivity alone. However, spectral resolution and system noise detract from the precision and accuracy with which the true center of the resonant mode can be located. The minimum error in determining the actual mode spectral position leads to finite sensor resolution, and subsequently to the need for the sensor detection limit. Detection limit (DL) is the smallest change in refractive index $\delta n$ that the refractometer can still accurately detect. It is determined by the ratio of the smallest spectral shift $\delta \lambda$ that can be accurately detected, i.e., the sensor resolution and the sensitivity. The spectral resolution can be approximated as

$$\delta \lambda = \frac{3 \cdot \Delta \lambda}{4.5 \cdot \left(SNR^{0.25}\right)}$$

(7.1)

with $\Delta \lambda$ the full width at half maximum of the mode resonance, which is related to $Q$ by $Q = \lambda/\Delta \lambda$, SNR the signal-to-noise ratio (in linear units no in dB). Eq. 7.1 expresses the fact that a peak position can be determined with an accuracy much better than the bandwidth, provided there is little noise. Therefore the DL can be written as

$$DL \equiv \delta n = \frac{\Delta \lambda}{S} = \frac{3 \cdot \lambda}{4.5 \cdot \left(SNR^{0.25}\right) \cdot Q \cdot S}$$

(7.2)

From Eq. 7.2 we can see both sensitivity $S$ and $Q$ factor are important. Although the sensitivity is high in our structure, the $Q$ factor is not high. In this section, we make new designs to have a high $Q$ factor. Because our InGaAsP wafer has the strongest emission around 1.55 $\mu$m, the lattice constant ($a$) is changed from 490 nm to 520 nm to shift the slot mode (at around 1.4 $\mu$m in the previous experiment) to a longer wavelength. In the previous section, we find that the $Q$ factor can be increased by decreasing the width of slot area, while the sensitivity will not be sacrificed. Except that, we also increase the width of single nanobeam and increase the distance between the symmetric holes. The new waveguide is defined by the lattice constant (520 nm, 490 nm), width of single nanobeam (490 nm, 450 nm), width of the slot area (160 nm, 200 nm), distance between the symmetric holes (670 nm, 690 nm), diameter of the holes (310 nm) and the thickness of the membrane (220 nm), where the previous parameters are also written in Italic for comparison. The band structure for the infiltration of water is shown in Fig. 7.8.
bands can be shifted upwards by increasing the width of the slot area, increasing the diameter of the hole size, decreasing the lattice constant, decreasing the distance between the symmetric holes. In fabrication, the width of the slot area and the diameter of the holes are very hard to be precisely changed either because of the fabrication error or because of the roughness at the side wall of the opened area. In our simulation, we only use the other two methods to obtain cavities. Firstly, a nanobeam waveguide with 36 periods and without any modification at the two ends was simulated as reference. The slot mode is at 1566.8 nm with a Q factor around 3000. Because we want to keep the slot mode, the central part of the waveguide is unchanged only the two ends are modified.

Then the lattice constant is decreased in four different ways to obtain cavities. The configuration of four different nanobeams with varying the lattice constant are shown in Fig. 7.9. These four different nanobeams are referred as design 1, 2, 3 and 4. The positions of the slot mode and Q factors from the reference waveguide and designs are listed in Tab. 7.3. The $E_y$ distribution of the slot modes from reference waveguide and design 1 to 4 are shown in Fig. 7.10. For the reference waveguide, the slot mode spreads around 20 periods at the central part and part of light leaks out from the two ends, which causes a Q factor about 3000. The Q factor increased by just decreasing the lattice constant around the ends, which decreases the leak from the two ends. The Q factor is even significantly increased by enlarging the central part of the waveguide. Design 2 gives the highest Q factor about 17000, which is improved a lot.

Then the distance between the symmetric holes away from the center is decreased to achieve a cavity. The configuration of four different nanobeams by changing the distance...
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Figure 7.9: The lattice constant versus hole number in (a) design 1, (b) design 2, (c) design 3 and (d) design 4.

between the symmetric holes are shown in Fig. 7.11. These four different nanobeams are referred as design 5, 6, 7 and 8. The positions of the slot mode and Q factors from design 5 to 8 are listed in Tab. 7.3. The $E_y$ distribution of the slot modes from design 5 to 8 are shown in Fig. 7.12. The Q factor can be significantly increased by just decreasing the distance between the symmetric holes, which decreases the leak from the two ends. The peak position of the slot mode hardly changes, while the Q factor can be optimized by tapering the two ends slowly. So far design 8 gives the highest Q factor about 30000. To test its sensitivity, another simulation was made by repeating the simulation with a refractive index corresponding to that of water/sugar solution as previously done. A sensitivity about 710 nm/RIU was found. From these simulations it was decided to decrease the distance between the symmetric holes to make a new nanobeam waveguide.
7.3 Nanobeam with a designed cavity

Figure 7.10: The $E_y$ distribution for the slot modes of the waveguide infiltrated with distilled water in the central plane from (a) reference waveguide, (b) design 1, (c) design 2, (d) design 3, and (e) design 4.

This method is not applied before and differs essentially from the double nanobeam cavity of Foubert et al [135]. Technologically, it can be made in practice. Consequently, a sort of mode gap in the heterostructure is achieved. The central part of the slot nanobeam has a slightly lower frequency than the surrounding waveguide. In this way, a high Q factor sensor is obtained without sacrificing the sensitivity. The modulation method is different
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<table>
<thead>
<tr>
<th>Types</th>
<th>Wavelength (nm)</th>
<th>Q factor</th>
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</thead>
<tbody>
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<td>Reference</td>
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<td>∼3000</td>
</tr>
<tr>
<td>Design 1</td>
<td>1562.1</td>
<td>∼4400</td>
</tr>
<tr>
<td>Design 2</td>
<td>1564.8</td>
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<td>Design 3</td>
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</tr>
<tr>
<td>Design 4</td>
<td>1563.8</td>
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<td>Design 5</td>
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</tr>
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<td>Design 6</td>
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</tr>
<tr>
<td>Design 7</td>
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</tr>
<tr>
<td>Design 8</td>
<td>1565.4</td>
<td>∼35000</td>
</tr>
</tbody>
</table>

Table 7.3: The position of the slot mode and Q factor from the reference and design 1 to 8.

from Kuramochi et al [145], where they modified the central part to design a ultrahigh Q cavity.

Based on design 8, the fabrication is made. SEM pictures are shown in Fig. 7.13(a). Because the length is long, the nanobeam is easily bent due to strong capillary forces (stiction) in the rinsing liquids during drying. The PL spectrum with air from the bent nanobeams is shown in Fig. 7.13(b). The measured Q factor of the peak around 1558 nm is about 2500 which is limited by the detector resolution. In the future fabrication, supporting bars from the side will be made, which hardly affect the device parameters but will keep the nanobeams away from each other.

### 7.4 Conclusion

We presented the sensitivity to the refractive index changes of the analyte of InGaAsP PhC slot nanobeam waveguides. We report a high sensitivity of $7 \cdot 10^2$ nm/RIU for a normal structure and a higher sensitivity of $9 \cdot 10^2$ nm/RIU for a cavity type structure. These record high values for $S$ correspond directly to the large overlap of the mode field with the analyte [25], particularly in the slot region. A new design with both high sensitivity and Q factor is proposed. Although experimental results for the sensitivity are needed, this kind of structure based on luminescent III-V semiconductors is attractive as it offers the full on-chip integration with sources, or the operation as lasers to increase the refractive index resolution [23]. In addition, it can be employed using remote readout, not requiring the delicate attachment of optical fibers or electrical wiring.
7.4 Conclusion

Figure 7.11: The distance between the symmetric holes versus hole number in (a) design 5, (b) design 6, (c) design 7 and (d) design 8.
Figure 7.12: The $E_y$ distribution for the slot modes of the waveguide infiltrated with distilled water in the central plane from (a) design 5, (b) design 6, (c) design 7, and (d) design 8.
Figure 7.13: (a) SEM image of newly designed InGaAsP PhC slot nanobeam waveguide; (b) PL spectrum of the waveguide in air. Note that only the central waveguide has a slot. The outer ones are stuck.
7. NANOBEAM PHOTONIC CRYSTAL DEVICES FOR SENSING
Chapter 8
Independent control of different photonic crystal nanocavity modes

High-quality factor (Q) photonic crystal (PhC) nanocavities that strongly confine light in volumes of wavelength dimension have attracted much attention in fundamental and applied research areas [13, 17]. Nowadays many efforts have been made on exploring the possibilities to use PhC nanocavities in quantum electrodynamics (QED). A number of experiments have already demonstrated the potential of QD-based solid-state cavity QED in applications such as single-photon sources [146, 147]. Many more applications of the nanocavities have been shown. In section 8.1, we demonstrate how different modes can be controlled with application of tuning the degeneracy status of modes. In section 8.2, we demonstrate the independent mode tuning can be used for realizing encoded cavities for a biosensor.

8.1 Controlling the mode degeneracy in a photonic crystal nanocavity with infiltrated liquid crystal

The degenerate modes, having the same frequency but different polarizations, could provide a new application to manipulate the polarization state of a photon in a PhC nanocavity [148, 149], while the non-degenerate modes are needed for specific polarization state cases. In these applications the active tunability of the cavity modes is required. So far, different tuning methods relying on the effective refractive index (n_{eff}) change of the cavities via temperature or near-field probe have been demonstrated [150-152]. Another way to tune the cavity modes is to infiltrate liquids into the PhC holes. Liquid crystal (LC) has attracted much attention in combination with PhC cavities since it enables to change the cavities’ n_{eff} by changing the temperature or electric field [153-157]. A birefringence-
induced mode-dependent tuning has also been reported recently [158]. In chapter 8.1, we demonstrate the control of the degeneracy of the quadrupole mode by LC infiltration into an InGaAsP membrane PhC nanocavity. The mode splitting exists only in the anisotropic nematic LC state, but not in the unfilled or isotropic LC state above the phase transition temperature. The theoretical explanation is given through three-dimensional (3D) finite difference time domain (FDTD) computations [61].

![Image](8.1SEM.png)

Figure 8.1: (a) SEM image of the InGaAsP PhC nanocavity. (b) Schematic diagram for the incomplete infiltration of LC into a PhC nanocavity.

A hexagonal PhC with cavities was fabricated on a 220 nm thick InGaAsP membrane which contains a single layer of self-assembled InAs QDs (density $3 \times 10^{10}$ cm$^{-2}$) [159]. Fig. 8.1(a) shows the Scanning Electron Microscope (SEM) image of a fabricated H1 InGaAsP nanocavity having a lattice spacing (a) of 510 nm and radius-to-lattice spacing ratio ($r/a$) of 0.34. (Here r is the radius of the holes in the hexagonal photonic crystal.) The radius of the six modified holes on the edge of the cavity is reduced to 130 nm. The LC 4-pentyl-4’cyanobiphenyl (5CB, Merck), which has the nematic-isotropic phase transition temperature (or clearing temperature) $T_c$ of about 35 °C, is infiltrated under ambient pressure. This is carried out by putting a drop of LC on the sample, while the sample and the LC are heated above $T_c$. The excess liquid is blown off the sample by dry nitrogen. Fig. 8.1(b) shows the schematic figure of the infiltrated H1 cavity, which will be discussed later. To investigate the temperature tuning, the infiltrated sample is placed on a current controlled heating stage. Because of the incorporated QDs, a photoluminescence (PL) experiment can be conducted easily by using a continuous wave He-Ne laser ($\lambda=632$ nm).

Fig. 8.2(a) shows the temperature dependence of the ordinary refractive index ($n_o$) and the extraordinary refractive index ($n_e$) of the LC in the nematic state at the wavelength of 1.5 µm, calculated from the parameters given in Ref. [160]. As the temperature increases up to about 35 °C, $n_o$ increases while $n_e$ decreases in the nematic state. At the clearing...
8.1 Controlling the mode degeneracy in a photonic crystal nanocavity with infiltrated liquid crystal

Figure 8.2: (a) Temperature-dependent refractive index change of the LC. PL spectrum of the nanocavity (b) before the infiltration, (c) after the infiltration of the LC in the nematic state at 24 °C, and (d) in the isotropic state. (e) Resonant wavelength shift of the modes with the increase of the temperature from 24 °C to 43 °C. The dots are the experimental results, while the solid lines are the simulation results.

At high temperature, they exhibit a sudden change showing the phase transition from the nematic state to the isotropic state. Above the clearing temperature, the LC has an isotropic refractive index \( n_i = 1.572 \). The PL spectrum collected from the modified H1 nanocavity before the infiltration is presented in Fig. 8.2(b). The peaks at 1456 nm and 1450.2 nm are the hexapole mode and degenerate quadrupole mode, which are confirmed later by 3D FDTD simulation. These two modes are referred to as \( H \) and \( Q \). The resonances of the H1 cavity we used have modest Q factors at the orders of 10^3. With this resolution, a possible mode splitting due to some fabrication imperfection is not observable. Fig. 8.2(c) shows the PL spectrum collected from the same cavity after the infiltration of the LC in the nematic state at 24 °C. The quadrupole mode is split into two modes separated by more than 11 nm after the infiltration, and these two modes are referred to as \( Q_1 \) and \( Q_2 \).
8. INDEPENDENT CONTROL OF DIFFERENT PHOTONIC CRYSTAL NANOCAVITY MODES

and $Q_2$. Fig. 8.2(d) shows the PL signal from the infiltrated cavity above the clearing temperature. The $Q_1$ mode and the $Q_2$ mode are merged again, since there is no splitting within the peak width when the holes are filled with an isotropic refractive index material. Fig. 8.2(e) shows the temperature-dependent resonance wavelength of $Q_1$ mode, $Q_2$ mode and $H$ mode after the infiltration. Below $T_c$ as the temperature increases, $Q_1$ mode and $Q_2$ mode shift smoothly in the opposite direction. At $T_c$ these two modes show a sudden jump in the opposite direction. The opposite shifts can be qualitatively explained if the shift of $Q_1$ mode is determined mainly by the change of $n_o$ instead of $n_e$, while the reverse is true for the shift of $Q_2$ mode. However, a comprehensive 3D FDTD computation is needed to analyze the splitting of the degenerate quadrupole mode in the nematic LC state.

First, it is necessary to find the filling degree of the PhC nanocavity. For this, the peak positions of the $Q$ mode and the $H$ mode in the isotropic state before and after infiltration are used. We first adjusted the radius of the holes within a reasonable range to match the calculated resonance positions to the measured ones in the unfilled case. A close match between the experiment ($\lambda_{Q} = 1450.2$ nm, $\lambda_{H} = 1456$ nm) and the simulation ($\lambda_{Q} = 1449$ nm, $\lambda_{H} = 1456.7$ nm) was obtained when $r/a$ is 0.34 and the radius of the six modified edge holes is 130 nm. Then we kept the refractive index of the LC in the isotropic state at 1.572 and varied the filling degree to match the experiment with the simulation. A good agreement (experiment: $\lambda_{Q} = 1529.4$ nm, $\lambda_{H} = 1561.3$ nm; simulation: $\lambda_{Q} = 1529.5$ nm, $\lambda_{H} = 1559$ nm) could be obtained assuming that the holes are approximately half filled and the upper side of the membrane is completely filled (see Fig. 8.1(b)).

Next we investigate the effect of the LC molecular orientations (MOs) on the degenerate quadrupole mode. The electric field directions of the degenerate mode in the center plane and in the cross section are shown in Fig. 8.3. It is assumed here that the H1 cavity is filled with the LC as found above. The degenerate quadrupole mode in a hexagonal PhC nanocavity, consists of two states that are mutually orthogonal [161]. The degenerate mode tends to split into these two modes under perturbation [149]. The electric field directions of these two modes are plotted in Fig. 8.3. Comparing Fig. 8.3(a) and (b), one sees that these two modes have nearly uniform polarizations inside the modified, most relevant holes at the edge of the cavity, but their orientations are perpendicular to each other. In Fig. 8.3(c) and (d), we notice that the fraction of the mode that extends in the surface layer is still predominantly TE-polarized (the electric field is in-plane).

Three kinds of LC MOs inside voids of small diameter are theoretically proposed: uniform axial (MOs are perpendicular to the plane of the PhC membrane surface), planar polar (MOs are in-plane), and escaped radial (MOs have both perpendicular and in-plane component) [162]. Because most of the electric field is in-plane, the LC orientation
8.1 Controlling the mode degeneracy in a photonic crystal nanocavity with infiltrated liquid crystal

Figure 8.3: Calculated electric field distributions of two orthogonal bases of the degenerate quadrupole mode (a), (b) in the central plane of the membrane; (c), (d) in the cross section. The dashed lines shown in (a) and (b) represent the positions of the cross sections. Fields in indicated holes are magnified in insets for clarity.

can be divided into three components, fraction $\alpha$ which is perpendicular to the plane of the PhC membrane surface (parallel to the hole axis), fraction $\beta$ which is in-plane and perpendicular to the $E$ field, and fraction $\gamma$ which is in-plane and parallel to the $E$ field. Then we can assume that for one of the modes, e.g., the $Q_1$ mode, $n_{\text{eff}}$ can be written as $n_{\text{eff}}Q_1 = \alpha n_o + \beta n_o + \gamma n_e$, because fraction $\alpha$ and fraction $\beta$ have the contribution of $n_o$ to $n_{\text{eff}}$ of the LC, while fraction $\gamma$ has the contribution of $n_e$ to $n_{\text{eff}}$ of the LC. Since $Q_1$ and $Q_2$ modes are perpendicularly polarized inside the holes, we have the same expression for $n_{\text{eff}}Q_1$, but with $\beta$ and $\gamma$ exchanged. The positions of both Q-peaks at 24 °C can be matched with the experimentally measured values if we set $\alpha$, $\beta$ and $\gamma$ as 48%, 41% and 11%, respectively. Thus in the nematic state, for $Q_1$ mode the contribution of $n_o$ is 89% and that of $n_e$ is 11%, while for $Q_2$ mode the contribution of $n_o$ is 59% and that of $n_e$ is 41%. Keeping $\alpha$, $\beta$ and $\gamma$ fixed, the temperature dependence of $n_{\text{eff}}$ of the LC in the nematic state can be obtained from the temperature dependence of $n_o$ and $n_e$ (Fig. 8.2(a)).
The peak positions of $Q_1$ mode and $Q_2$ mode in the nematic state obtained by using the temperature dependence of $n_{eff}$ of the LC are shown as solid lines in Fig. 8.2(e), which quantitatively agree well with the experimental results.

So far, we have assumed that only the MOs in the holes are relevant. Then we need the escaped radial configuration to explain the experiments. However, in practice, under our filling configuration, both the hole and the surface layer are equally important. Our averaging over $n_o$ and $n_e$ includes the configuration of orientation of the LC in the surface layer, because the electric field orientations outside the membrane are similar to those in the center plane of the membrane and the amplitude of the electric field decreases from the center of the plane [see Fig. 8.3(c) and (d)]. The phenomena reported here are typically observed for the LC infiltrated cavities. However, the magnitude of the splitting in the isotropic case (i.e. the degeneracy) depends on the accidental fabrication imperfection, whereas the magnitude of the LC-introduced splitting varies somewhat between infiltrations [158].

8.2 Spectrally encoded photonic crystal nanocavities by independent lithographic mode tuning

The ability to quantify multiple proteins, cytokines, or nucleic acid sequences in parallel using a single sample allows researchers and clinicians to obtain high-density information with minimal assay time, sample volume, and cost. To realize such multiplexed analysis with an as large as possible number of probe molecules, the individual reaction sites must be minimized and either positioned in micro-arrays as in Lab-on-a-Chip systems [163] or suspended as free particles in a single small sample of target analyte [164]. For suspension assays, particles with different probes must be distinguished and thus a particle encoding technique is essential. Spectrometric encoding by color coding the particles with luminescent dyes or nanocrystals is mostly used so far [164–166]. The maximum number of codes would be greatly enhanced by particles that can be made to display a number of very sharp peaks of independently adjustable wavelengths. Then the number of codes is $N^M$, where $M$ is the number of peaks and $N$ is the number of distinguishable wavelengths (inversely proportional to the linewidth). PhCs could satisfy this requirement and are already widely pursued as individual (bio)sensing elements [167], and for integration in planar arrays [23, 168]. PhC cavities coupled to bus waveguides [168] must also be recognized as an optical code. One-dimensional (1D) PhC particles with multiple peaks ($M > 1$) [169, 171] and three-dimensional (3D) PhC particles with a single peak ($M = 1$) [172] in their reflectivity spectrum have been used for encoding. The 1D multilayer structure consists of a layer stack to modulate the refractive index and therefore
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is necessarily several wavelengths thick (~10µm). It is made in the passive material Si, so it can only be read out by reflection. In addition, because the incident and reflected beams must be perpendicular to the surface of the 1D layer stack, the particles need a large area and also must be aligned. The 3D PhC used in Ref. [172] has a low quality factor and a single reflection peak, so the encoding capacity is modest. The technology to make other 3D PhCs is currently very limited and certainly very difficult.

Two-dimensional (2D) air-hole PhC cavities would be very attractive because of their ease of fabrication, small size, and the existence of multiple very sharp peaks (thus a potentially huge number of codes based on 2D PhC cavities could be achieved). They can be easily incorporated with either internal [173] or external [174] light emitters for a simple orientation-insensitive read-out by photoluminescence (PL) experiment. Using techniques analogous to those of the 1D PhC particles [169–171], they could be made as independent free particles. Such 2D PhC cavities were recently exploited for spectrally tagging different reaction sites even when all targets were fluorescently labeled with the same marker [175]. The peaks were sharp enough that 150 codes were claimed with only a single peak \( N = 150, M = 1 \). Moreover it was shown that the strength of the fluorescence from the conventional labels at resonance was enhanced by several orders of magnitude. To approach the potentially much larger number of codes of \( N^M \), with \( M > 1 \), it is necessary that different resonance peaks can be individually controlled. In this section, we theoretically and experimentally demonstrate the feasibility and strategy of independent lithographic mode tuning for the smallest possible, so-called H0 (or M0) PhC nanocavities [176]. Different modes are selectively tuned by modifying a particular subset of holes that comprise the defect. Methods other than lithography are necessarily post-fabrication processes. To address each cavity individually with a post-fabrication process will be very elaborate. As an example, using infiltration requires high resolution local micro-infiltration, which should not change over time due to fluid flow or evaporation. Similar arguments hold for other post-fabrication processes, such as local wet or dry etching, or local deposition. To show the general validity of the approach, we demonstrate the design guidelines also for a H1 cavity, consisting of one missing central hole with modified neighboring holes. The independent tuning of two H1 cavity modes was recently shown for a different cavity type made in a thick layer of a low index material that does not have a photonic band gap [177].

A hexagonal PhC with cavities was fabricated in a 220 nm thick InGaAsP membrane which contains a single layer of self-assembled InAs QDs (density \( 3 \times 10^{10} \) cm\(^{-2} \)) [159]. The H0 cavities are formed by reducing the diameter or/and shift the positions of some neighboring holes in the pattern without leaving any holes out [23, 176, 178, 25, 179]. In this work, the nearest four neighbor holes are reduced and shifted outwards in all the
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Figure 8.4: (a) SEM image of an H0_Y2 InGaAsP PhC nanocavity. Schematic diagrams for the PhC nanocavities of (b) H0_Y2, (c) H0_Y6, (d) H0_X2, (e) H0_X8, and (f) H0_X6. \( D_x \) and \( D_y \) are the modified hole diameters. \( S_x \) and \( S_y \) are the shifts of the modified holes.
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cavities to obtain a high Q factor [179]. All the H0 cavities have a lattice spacing (a) of 500 nm and radius-to-lattice spacing ratio (r/a) of 0.33. (Here r = 165 nm is the radius of the holes in the hexagonal photonic crystal.) The positions of all holes are kept fixed for all cavities, but the radii of suitable subsets of holes may vary to modify the resonance positions. The shifts in x direction (S_x) and y direction (S_y) are 70 nm (0.14a) and 20 nm (0.04a), respectively. Fig. 8.4(a) shows the Scanning Electron Microscope (SEM) image of a fabricated H0_Y2 InGaAsP nanocavity, with the diameters of the nearest four neighbor holes of 210 nm. Four other kinds of cavities, H0_Y6, H0_X2, H0_X8 and H0_X6, were also made. The schematic figures of these cavities are shown in Fig. 8.4(b)-(f). The dark shaded holes represent the subset of the holes whose diameters are adjusted, while the light shaded holes are the holes whose diameters are fixed to 210 nm.

A 3D finite-difference time-domain simulation [61] is used to verify our experimental results in the following paragraphs. We used the experimental parameters in our simulation. However, there is a discrepancy of several tens of nanometer (4%) between the peak position of the simulation and that of the experiment, which may be attributed to an uncertainty of the parameters of the real samples. The simulated dependence of the peak wavelengths of different modes on the modified hole diameters is shifted along the frequency axis to coincide with the experimental value at one specific case.

8.2.1 H0 cavities

For H0 cavities, the two lowest order modes are monopole mode and dipole mode. The calculated modal profiles (H_z) of the modes are shown in the insets of Fig. 8.5(b) (Here only the magnetic field is plotted, however the analysis and conclusion are the same when the electric field is considered). From the mode patterns of these two modes, we expect that by modifying the nearest two neighbor holes in y direction (i.e., H0_Y2 cavities) the resonance position of the monopole mode will not change too much while that of the dipole mode will have a large shift. The opposite is expected when modifying the nearest two neighbor holes in x direction. The PL spectra collected from a series of H0_Y2 cavities are shown in Fig. 8.5(a). The two sharp peaks are monopole mode and dipole mode with Q factors of about 2000. As the hole diameters decrease, both the monopole mode and the dipole mode show redshift, as expected since the average refractive index increases. Fig. 8.5(b) shows the relation between D_y (defined in Fig. 8.4(b)) and the peak wavelengths of the modes. When the modified holes are large, the wavelength of the monopole mode is longer than that of the dipole mode. However, the monopole mode is not as sensitive to D_y as the dipole mode. When the hole diameters decrease, the dipole mode has a much larger redshift than the monopole mode and the wavelengths of the
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Figure 8.5: (a) PL spectrums collected from a series of H0_Y2 cavities and the relation between the diameters of the varied holes and the mode positions of (b) H0_Y2, (c) H0_Y6, (d) H0_X2, (e) H0_X8, and (f) H0_X6 cavities. The inserts in (b) are the calculated modal profiles ($H_z$) of the monopole and the dipole modes. The solid curves are the experimental results, while the dashed curves are the simulation results. Error bars represent average error introduced by the fabrication error, estimated from variations in resonance positions of different, but nominally identical, cavities.
two modes cross. To enhance this effect, H0\textsubscript{Y6} cavities are fabricated. Fig. 8.5(c) shows the relation between $D_y$ and the mode wavelengths of H0\textsubscript{Y6} cavities. Since the mode overlap with the six modified holes is larger than that with the two holes [cf. the insets of Fig. 8.5(b)], the dipole mode has a larger redshift with decreasing $D_y$ (average slope of 1100 nm/\(\mu\)m) than that of H0\textsubscript{Y2} cavities (average slope of 750 nm/\(\mu\)m). The dipole mode is particularly affected by the additional holes with decreased radius, and thus it now already has a larger wavelength than the monopole even at $D_y=0.21$ \(\mu\)m so that the two modes can no longer cross. With the six modified holes, however, the redshift of the monopole becomes appreciable, particularly at smaller $D_y$. A better independent tuning of the dipole mode could be obtained by allowing unequal changes for the six modified holes.

The next goal is to keep the dipole mode wavelength almost unchanged and vary the monopole mode wavelength. From the mode profile, one may expect that this might be realized by changing the nearest two nearest neighbor hole diameters in $x$ direction. Fig. 8.5(d) shows the relation between $D_x$ and the position of the modes of H0\textsubscript{X2} cavities. Different from the expectation, both the monopole mode and the dipole mode show almost the same redshift when the hole diameters decrease. The reason is that the nearest two neighboring holes in $x$ direction are also close to the amplitude maxima of the dipole mode [cf. the insets of Fig. 8.5(b)]. When the hole diameter decreases, both the modes are affected. To achieve an independent tuning of the monopole mode, H0\textsubscript{X8} cavities are fabricated by modifying the nearest eight neighbor holes in $x$ direction [cf. Fig. 8.4(e)]. Fig. 8.5(e) shows the relation between $D_x$ and the modes of H0\textsubscript{X8} cavities. Indeed, the monopole mode now has a larger redshift than the dipole mode, but the shift of the latter is still appreciable. To minimize the effect on the dipole mode, H0\textsubscript{X6} cavities are made by modifying the six nearest neighboring holes in $x$ direction, while the two nearest neighbors in the $y$ direction are unaffected [cf. Fig. 8.4(f)]. Fig. 8.5(f) shows the relation between $D_x$ and the mode wavelengths of the H0\textsubscript{X6} cavities. The dipole mode is now only weakly affected and shows a much smaller redshift than the monopole mode. For H0\textsubscript{X8} cavities and H0\textsubscript{X6} cavities, the dipole modes are crossed by the quadrupole modes [cf. the insets of Fig. 8.5(e), (f)]. This is because the monopole mode and the dipole mode move to the short wavelength when the modified hole diameters increase and the quadrupole mode is more sensitive to the holes around the defect area. Comparing these experimental results (marked by the solid lines) with the simulation results (marked by the dash lines), we find good agreement for the slope of the curves. This shows that the simulations reliably predict the resonant frequencies of the cavities.

So far, we have shown the modes tuning by changing the hole diameters around the defect area of the PhC cavities both experimentally and numerically. For H0\textsubscript{Y2} cavities,
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a tuning of the dipole mode nearly independent of the monopole mode was realized [cf. Fig. 8.4(b) and 8.5(b)]. The opposite is true for H0_X6 cavities [cf. Fig. 8.4(f) and 8.5(f)]. To obtain a more independent tuning of the monopole mode and the dipole mode, we designed H0_X6+Y6 cavities and H0_X8+Y2 cavities. The schematic figures of these two kinds of cavities are shown in Fig. 8.6(a), (b), respectively. The dark shaded holes represent the subset of the holes whose diameters are decreased, while the grid shaded holes represent the subset of the holes whose diameters are simultaneously increased.

By decreasing $D_y$ and increasing $D_x$ simultaneously or decreasing $D_x$ and increasing $D_y$ simultaneously, the dipole mode or the monopole mode can be tuned very independently [cf. Fig. 8.6(c) and (d)]. The quadrupole mode may occur in the same wavelength range of the monopole mode and the dipole mode. Even if it is not used as an independent coding mode, it will serve as an extra check for the two-mode coding. Because the linewidth is of

Figure 8.6: Schematic diagrams for the PhC nanocavities of (a) H0_X6+Y6 and (b) H0_X8+Y2. Relation between the diameters of the varied holes and the mode positions of (c) H0_X6+Y6 cavities and (d) H0_X8+Y2 cavities.
the order of 1.5 \( \mu \text{m} \) (\( Q \sim 10^3 \)) and the dipole mode is nearly independently tunable over a \( \sim 80 \) nm range [cf. Fig. 8.5(b)], the dipole mode may have 80/1.5\( \approx 50 \) positions when the monopole mode is always at a specific position. This gives 50 codes. The positions of both monopole mode and dipole mode can be tuned easily by modifying the nearest two neighbor hole diameters in \( x \) direction over a \( \sim 60 \) nm range. Then the monopole mode may have 60/1.5=40 positions. Thus the combination of H0_X2 and H0_Y2 cavities, i.e., H0_X2+Y2 will offer a two-digit bar code with \( \sim 50 \times 40 \) or \( \sim 10^3 \) number of codes. With the higher \( Q \) factors that can be achieved with the H0 cavities [179], and/or using more peaks, a huge number of (\( > 10^5 \)) codes are in principle achievable. Of course, in a sensing application, a certain bandwidth can be reserved for the identification. Any peak appears within this bandwidth will have the same code. Within this bandwidth, the peak position will deviate from the relationship in Fig. 8.5. The deviation, however, is expected for sensing. This is possible when the \( Q \) factor is high enough so that the linewidth is much smaller than the bandwidth reserved for sensing. Thus the sensing can also be achieved while not reduce the present encoding capacity.

### 8.2.2 H1 cavities

Fig. 8.7(a) and (b) show the approach for encoding with H1 cavities. All the H1 cavities have a lattice spacing (\( a \)) of 480 nm and radius-to-lattice spacing ratio (\( r/a \)) of 0.31. (Here \( r=150 \) nm is the radius of the holes in the hexagonal photonic crystal.) The radius of the six modified holes on the edge of the cavity is reduced to 90 nm to obtain a high \( Q \) factor. Two kinds of the cavities, H1_X4 and H1_X2, are fabricated. The schematic figures of these cavities are shown in Fig. 8.7(a) and (b), respectively. The dark shaded holes represent the subset of the holes whose parameters are adjusted. For H1_X4, the diameters of the light shaded holes are fixed and the diameters of the dark holes are varied. For H1_X2, the light shaded holes are fixed, as are the radii of the dark holes, while the positions of the dark holes are modified. The calculated modal profiles (\( H_z \)) of the dipole modes are shown in the insets of Fig. 8.7(c). For the simple H1 cavity, which retains the hexagonal symmetry, these dipole modes are degenerate. The dipole modes are referred to as DX and DY, respectively. From the mode patterns of these two modes, we expect that by modifying the four neighbor holes in \( x \) direction around the defect holes (i.e., H1_X4 cavities) the resonance position of DY mode will not change too much while that of DX mode will have a large shift. Fig. 8.7(c) shows the relation between \( D_x \) and the position of the modes of H1_X4 cavities. As expected, the DX mode now has a larger redshift than the DY mode, but the shift of the latter is still appreciable and the shifts of both modes are not large. The relatively small shifts arise because both of the modes...
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Figure 8.7: Schematic diagrams for the PhC nanocavities of (a) H1_X4 and (b) H1_X2. (c) Relation between the diameters of the varied holes and the mode positions of the H1_X4 cavities. (d) Relation between the shifts of the varied holes and the mode positions of the H1_X2 cavities. The inserts in (c) are the calculated modal profiles ($H_z$) of the DX mode and the DY mode. The solid curves are the experimental results, while the dashed curves are the simulation results. Error bars represent average error introduced by the fabrication error, estimated from variations in resonance positions of different, but nominally identical, cavities.

...have relatively small overlap with the modified holes, being larger for DX mode than for the DY mode. Fig. 8.7(d) shows the relation between $S_x$ and the position of the modes of H1_X2 cavities. When the two holes near the defect area are shifted outwards along the $x$ direction, the DX mode has a large red shift while DY mode almost doesn’t move. An independent tuning of DX mode is achieved here, which is also confirmed by Ref. [177] in which the confinement of the mode was based on mode mismatch with the environment rather than band gap.
8.3 Conclusion

In summary, we have demonstrated the influence of the liquid crystal infiltration on the mode-degeneracy of the quadrupole modes of a PhC nanocavity. The mode splitting exists only in the anisotropic nematic LC state and not in the unfilled or isotropic LC state, which is attributed to the different interactions of the two orthogonal bases of the degenerate mode with the two components of the refractive index of the LC. Apart from temperature, the manipulation of the LC orientation with electric or optical fields will provide a new control for applications, such as a switch between a polarization-entangled quantum state and a specific polarization state of the generated photon from the PhC cavities containing semiconductor quantum dots.

We have also demonstrated that the resonances can be independently controlled by changing the hole around the defect area. Only the combination of the monopole mode and the dipole mode from the H0 cavities will already offer a two-digit bar code with a large number of ($\sim 10^3$) different codes. These encoded PhC nanocavities could be highly useful for biosensing in the future.
8. INDEPENDENT CONTROL OF DIFFERENT PHOTONIC CRYSTAL NANOCAVITY MODES
Chapter 9

Photonic crystal nanocavities as free micro-particles

The technology of combining different semiconductor materials on a single substrate has been a subject of research for many years now. Epitaxial lift-off (ELO) was first reported by Konagai et al in 1978 [180], and it showed the possibility of grafting GaAs solar cells onto an Al plate. Interest in thin film grafting techniques has increased rapidly recently, mainly due to the difficulties in heteroepitaxial growth. Lee et al demonstrate multiple growths of flexible, thin-film indium tin oxide-InP Schottky-barrier solar cells on a single InP wafer via ELO [181]. In 2010, a new printing method was reported by Ko et al [182]. The authors pattern the InAs films into narrow, nanoscale-thick strips that they release from the underlying substrate by selectively removing the AlGaSb with a chemical etchant. In a final step, they use a silicone rubber stamp to lift arrays of the nanoribbons from the substrate, and then deliver them to the silicon dioxide (SiO$_2$) insulator surface of a silicon wafer. Because the procedure can be used with different types of material, the authors refer to the resulting structure as 'X' on insulator, or XOI, where X represents a semiconductor, by analogy to the widely used acronym SOI for silicon on SiO$_2$/Si substrates. In section 8.2 chapter 8, we proposed that finely designed two-dimensional photonic crystal (PhC) cavities can be used as the encoded particles. However, in practice, as encoded particles for suspension arrays the PhC cavities must be liberated from the chip. In this chapter, we examine way to release PhC cavities from the original substrates for use as free cavities or to be attached to another carrier. In section 9.1, three releasing methods are discussed. To release the particles in a controlled way and keep track of individual particles, the printing technique analogous to the previous works was employed first. Scotch tape (9.1.1) and blue tape (9.1.2) were used respectively to take the cavities from the chip where “the tape” acts as a stamp for the printing method. The results by using a nano-manipulation setup are also presented (9.1.3). The optical
properties of the cavities on different substrates were investigated. In section 9.2, two applications of liberated nanocavities are introduced.

9.1 Releasing methods

Figure 9.1: (a) SEM image of the InGaAsP PhC nanocavity array. (b) The schematic figure of a 5 by 5 super array. This array in (a) is copied 25 times in a 5 by 5 super array in (b).

To enable the nanocavities to be taken easily from the chip, every nanocavity was weakly suspended by using two nano-bars. Fig. 9.1(a) shows the SEM picture of the overview of a PhC array. This array consists of a 5 by 5 nanocavity matrix. Every line consists of five different H0 cavities (see section 8.2). All the H0 cavities have a lattice spacing \( a \) of 500 nm and radius-to-lattice spacing ratio \( r/a \) of 0.32. \( D_x \) is 230 nm. \( D_y \) are 230 nm, 210 nm, 180 nm, 130 nm and 0, respectively, from column 1 to column 5. The width of the bar is decreased from top to bottom. They are 3.1 \( \mu \)m, 2.3 \( \mu \)m, 1.6 \( \mu \)m, 0.8 \( \mu \)m and 0.3 \( \mu \)m. Because the widths of the bars from the last row are so narrow, the bars are fragile and easily broken and some nanocavities fall into the holes (in the case of Fig. 9.1(a), all the nanocavities from the last row fell into the holes). For the application and the experimental tests, we need to have a large number of identical cavities. Therefore, the array of Fig. 9.1(a) was copied 25 times in a super array of 5 by 5 in Fig. 9.1(b). The cavity is labeled with \( i,j,u,v \), which means the cavity is from the \( j \)th row and \( v \)th column in the 5 by 5 matrix, \( i \)th row and \( j \)th column from the super array. Fig. 9.2(a) shows the PL spectra of the cavities from a single array out of the super array.

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On the horizontal axis are the different diameters from different columns. The scatter between nominal identical cavities from different rows is represented by the error bars. A 3D finite-difference time domain simulation is used to verify our experimental results here. We used the experimental parameters in our simulation. However, there is a discrepancy of several tens of nanometers ($\sim 4\%$) between the peak position of the simulation and that of the experiment, which may be attributed to an uncertainty of the parameters of the real samples. The simulated dependence of the peak wavelengths of different modes on the modified hole diameters is shifted along the frequency axis to approximately coincide with the experimental value. The comparison of the experimental results and the simulation result is shown in Fig. 9.2(b). There are at most six modes within the detector range, i.e., the monopole, the dipole, the quadrupole, the quasi-hexapole, the second order monopole and the second order quadrupole modes, which are referred as $M$, $D$, $Q$, $QH$, $SM$, and $SQ$. The calculated modal profiles of $M$ and $D$ modes are shown in the insets of Fig. 8.5(b), so the rest are shown in Fig. 9.1. The calculated dependence is given by the dashed lines in Fig. 9.2(b). The considerable deviations from the experimental data is attributed to deviation of fabricated hole diameters from the design. Note that these deviations are systematic while the random variations (indicated by the error bars) are much smaller.

9.1.1 Scotch tape printing

Fig. 9.3 shows the process-scheme of the transferring method by using Scotch tape. First, the Scotch tape was put on the surface of the chip. Then the Scotch tape was pressed a little bit. After that, it was taken from the chip. Fig. 9.4(a) and 9.4(b) shows the images of the chip and the scotch tape after the process. We can see that some nanocavities on the last several rows were transferred onto the scotch tape because the supporting bars are weak. The patterns on the chip and on the scotch tape match with each other very well. The next step was to transfer the nanocavities from the Scotch tape to other substrates, such as glass in this case. We glued the Scotch tape to the glass and pressed it. After we peeled it, there was no nanocavity transferred to glass which is because the glue on the Scotch tape was too sticky. To make the glue less sticky, we immersed the Scotch tape into aceton for 10 mins. Then we took the scotch tape out of aceton, put it on glass and dragged it with tweezers. Some nanocavities with glue on the Scotch tape were transferred to glass see Fig. 9.4(c). From the results above, we can see that the Scotch tape can be used to take the nanocavities from the chip, but it is hard to liberate the nanocavities from the glue and the nanocavities were not totally free.
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Figure 9.2: (a) PL spectra collected from a series of H0,Y2 cavities. Spectra from bottom to top are from column 1 to column 5. (b) the relation between the diameters $D_y$ of the varied holes and the mode positions. Error bars represent average error introduced by the fabrication error, estimated from variations in resonance positions of different, but nominally identical cavities. The standard deviation ($\sigma$) in one array are from 2 nm to 2.6 nm, from 1.3 nm to 5.1 nm, from 1.1 nm to 6.7 nm, from 0.8 nm to 8.5 nm, from 1.3 nm to 6.6 nm, 1.8 nm and 3 nm for the monopole, dipole, quadrupole, quasi-hexapole, second order monopole and second order of quadrupole modes, respectively. The dashed line are the simulation results. The calculated modal profiles ($H_z$) of (c) the quadrupole, (d) the quasi-hexapole, (e) the second order of monopole and (f) the second order of quadrupole modes.

9.1.2 Blue tape printing

In this subsection, we used a less sticky tape which is called blue tape. In order to know the effects of the environment on the cavities, the PL spectra were taken after every step. Because we don’t know which cavities will be transferred, the PL spectra of every cavity from the first array and the cavities at the last two rows from the rest 24 arrays were
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Figure 9.3: Process-scheme of the transferring method by using scotch tape. (a) put the tape on the surface of chip, (b) take the tape from the chip, (c) put the tape on a glass plate and (d) drag the scotch tape when it immersed into isopropanol. (Not in scale)

Figure 9.4: The surface of (a) the chip, (b) the scotch tape and (c) the glass plate after the processing with the scotch tape.
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Figure 9.5: The pictures taken (a) with an array in between the blue tape and the glass from the glass side, (b) with an array on glass; (c) the SEM image of the group containing six cavities; (d) the PL spectra of the cavity 5,3,4,3; The cavity is marked with a red circle in (a) and (b).

measured before the processing. The processing was similar to the one in Fig. 9.3, but no solvent was used in the last step. A sandwich configuration, i.e., glass/nanocavities/blue tape, was first achieved and measured. Fig. 9.5(a) shows the nanocavities in between the glass plate and blue tape, where the image was taken from the glass side. Overall, this image can be divided into two areas, the colored bright area and the dark area. The colored bright area is caused by the interference of the light reflected from the bottom surface of the glass plate and the top surface of the blue tape because there is air gap between the glass plate and blue tape. In all, there were two kinds of configurations of
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the nanocavity position, one is blue tape/cavity/glass plate see Fig. 9.6(a), the other is blue tape/cavity/air/glass plate see Fig. 9.6(b). After checking the PL spectra, the blue tape was peeled from the glass plate. Some cavities stayed on the blue tape, while the others were on the glass plate. To study the effects of different environment on the cavity modes, the PL spectra were taken. Note that the spectra of cavities on the chip were taken first, then when they are in between glass and tape (Fig. 9.6), and finally when they are on the glass plate or blue tape.

Figure 9.6: The schematic figure of the configuration of (a) blue tape/cavity/glass, (b) blue tape/cavity/air/glass. (Not in scale)

The cavity 5.3.4.3 was first transferred in between the blue tape and glass without air gap [see Fig. 9.5(a)] and then was transferred onto glass [see Fig. 9.5(b) and Fig. 9.5(c)]. Fig. 9.5(d) shows the PL spectra of that cavity. There were five peaks when the cavity was on the chip, i.e., $SM$ (at 1385.4 nm), $QH$ (at 1434.7 nm), $Q$ (at 1493.9 nm), $M$ (at 1556.4 nm) and $D$ (at 1560.1 nm). Here we focus on $QH$ mode to analyze the effects of different substrates. The $QH$ mode was red shifted by 100.8 nm when the cavity was in between. According to calculation, such a large red shift occurs because not only both of the sides are replaced by substrates with refractive index larger than 1 but also some holes of the cavity are infiltrated with the glue from the blue tape. The $QH$ had a blue shift of 73.3 nm back when the cavity was transferred on the glass and the tape was removed. Comparing with calculations, it is concluded that the blue tape and glue were removed from the cavity. The red shift for the glass plate case with respect to the suspended case is 27.5 nm and close to the simulation result (24.1 nm). Comparing the Q factors in different cases, we find the case on the chip gives the highest value, the case in between gives the second highest value because the contrast of the refractive index in the vertical direction becomes lower, and the case on the glass gives the lowest value because the symmetry in the vertical direction is the worst [123]. The behavior of other modes are similar to the $QH$ mode but the specific shifts are different, in agreement with the mode patterns of each mode.
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Figure 9.7: The pictures taken (a) with an array in between the blue tape and the glass from the glass side, (b) with an array on blue tape; (c) the PL spectra of the cavity 5_1.5.3. The cavity is marked with a red circle in (a) and (b).

The cavity 5.1.5.3 nominally same as 5.3.4.3, was first transferred in between the blue tape and glass without air gap and but was still attached to the blue tape after it was peeled off. Fig. 9.7(c) shows the PL spectra of that cavity. The QH mode is again used to analyze the effects of different substrates. The QH mode was red shifted by 101.3 nm when the cavity was in between, which is almost the same as the case for cavity 5.2.4.3 (Fig. 9.8(c)). The QH shifted back by 32.3 nm when the cavity was left on the blue tape. The large 100 nm first shift implies that the holes are filled by glue. The small back shift of 32 nm means that only the glass is removed, but glue remains in the holes. The Q
factor for the case in between is lower than that for the case on the blue tape. This may be because some dusts existed when the cavity was in between and was taken off when the cavity was on the blue tape.

Figure 9.8: The pictures taken (a) with an array in between the blue tape and the glass from the glass side, (b) with an array on glass; (c) the PL spectra of the cavity 5.2.4.3. The cavity is marked with a red circle in (a) and (b).

The cavity 5.2.4.3 also nominally the same as the one 5.3.4.3 and 5.1.4.3 but from another array, was first transferred in between the blue tape [see Fig. 9.8(a)] and glass with air gap and then was left onto the blue tape [see Fig. 9.8(b)]. Fig. 9.8(c) shows the PL spectra of that cavity. There are four peaks when the cavity was on the chip, i.e., $SM$ (at 1386.4 nm), $QH$ mode (at 1436.9 nm), $Q$ mode (at 1496.3 nm), and the sum of $D$...
and $M$ (at 1559.2 nm) modes. Comparing the PL spectra of cavity 5.3.4.3 and 5.2.4.3 on chip, the peak positions for the same modes were very close, within the typically fabrication fluctuations. We still focus on the $QH$ mode to analyze the effects of different substrates to have comparison with cavity 5.2.4.3. The $QH$ mode had a red shift of 53.9 nm when the cavity was in between. This is to be compared with the ~ 100 nm shift when the cavity was firmly pressed to the glass. It hardly shifted (only 5.2 nm) and the $Q$ factor hardly changed when the cavity was left on the blue tape after it was peeled off.

![In between](image1)  
![Tape released](image2)

Figure 9.9: The schematic configuration of three different cases. (Not in scale)

We find that if the configuration of the nanocavity position in between of the blue tape and glass is blue tape/cavity/glass, some nanocavities will be transferred to the blue tape (such as cavity 5.3.4.3) and some others will be left on the glass (such as cavity 5.1.5.3) plate which depends on the force between the nanocavities and blue tape caused by glue and the van der Waals force between the nanocavities and the glass. If the configuration of the nanocavity position in between of the blue tape and glass is blue.
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tape/cavity/air/glass, the nanocavities are transferred to the blue tape (such as cavity 5,2,4,3) because of glue. The schematic configuration is shown in Fig. 9.9. In view of the small size, it is impossible to see these nanostructural composition clearly, either from the optical or electron microscope.

After the nanocavities have been transferred to the glass, the bonding between glass and the nanocavities caused by the van der Waals is very strong. The nanocavities are still on the glass after we blew them with nitrogen gun, immersed them in water and blew them again. Because the thickness of the cavity is just 220 nm, the cavities are flexible. Even the surface of the substrate is not very flat, the cavities can follow the surface profile after pressing it which gives the strong bonding. From the results above, we can see that the cavities can be taken from the chip and transferred to another substrate (glass in our case) by using blue tape. The method could be suitable for mass production.

9.1.3 Nano-manipulation

As we see from the blue tape experiment, the binding between the nanocavities and the glass is very strong. The van der Waals force could even be used to liberate the nanocavities from the chip. In this subsection, we describe how we use a glass micro-tip to liberate nanocavities.

![Figure 9.10: (a) The microscope image from of a tapered fiber tip. The diameter of the tip is about 1.5 \( \mu \)m. The tip was tilted and the focus was at the tip when this photo was taken. (b) The manipulation set-up. The SEM image of the tip is shown in the inset of (b).]

The tool used in the experiments is a tapered fiber tip. The tip is made from a step-
index silica fiber by heating it at the central part while pulling the two ends. The heating is done by using a flame produced by a hydrogen micro-torch. The fiber extents due to the force exerted on it. At a certain condition it cannot extend anymore and splits into two parts with each end having conic shape. Fig. 9.10(a) and the inset of Fig. 9.10(b) show the optical microscope image and the SEM image of a tip. The fiber is immobilized on a nano-manipulation stage so that the tip can be moved along the $x$, $y$, $z$ directions and the angle can also be changed. The sample is put on another nano-manipulation stage that can also be moved along the $x$, $y$ and $z$ directions. Fig. 9.10(b) shows the nano-manipulation set-up we used.

9.1.3.1 Cavities forced to a surface

We use the tip to exert force on the nanocavities. The bars are first broken and then the nanocavities are released from the chip. The released cavities are attached to the tip. Different sizes of bars were tested to determine which size of the bars gives successful results. We also tried to take the cavities that fall into the holes since it is hoped that the interaction between the cavity and the glass is strong enough to take the cavity out of the hole. It is found from the preliminary experiments that the cavities (including the fallen cavities) from the fourth and fifth rows could be taken. The ones in the third rows can also be taken but some of them are broken during the releasing manipulation. The cavities in the first two rows cannot be taken. The following experiments focus on the treatment of the cavities from the fourth and fifth rows while sometimes the ones from the third row are also used.

It is also very interesting to see the effect of the tiny tip on the nanocavity. Fig. 9.11(a) and 9.11(b) show the two different attached positions, one attached with its edge and one attached with its central part. Fig. 9.11(c) and 9.11(d) show the corresponding PL spectra. For the case of the cavity attached with its edge, the peaks are almost not shifted. This is because the tip is far way from the defect area and its effect is negligible. The case is different when the cavity is attached with its central part. For that case, there is about 10 nm red shift for each mode compared the PL spectrum with that on chip. The red shift occurs because the mode localized around the defect experiences the refractive index change caused by the tip.

The relative intensities of the peaks are changed with the respect to the spectrum on chip and also with respect to the two configuration in Fig. 9.11(a) and Fig. 9.11(b). The reason of the relative intensity changes is that different modes have different radiation patterns in the far field, while the numerical aperture of objective is only 0.5. Thus the amount of light collected by the objective depends on the orientation of the cavity with respect to the objective axis. The observations prove that the manipulation does not
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change the optical properties of the cavities, which is required in a real application.

In this way, the single nanocavity can be transferred to another substrate (a glass plate in this case) easily. The nanocavity is first taken by using the tip and then put horizontally on the glass plate. It is found that the taken cavity can be easily transferred to the glass plate in horizontal position. The binding between the cavities and the glass in this case is generally not weak enough that the transferred cavity can be moved on the glass surface by using the tip. Pressing them gently with the tip is needed to make the cavities stick well to the glass surface. Once they stick well, they cannot be moved again with the tip.
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Figure 9.12: The microscope images from the same nanocavity (a) on tip, (b) on glass and (c) on glass after pressing. (d) PL spectra of the same cavity in different positions.

Figs. 9.12(a), 9.12(b) and 9.12(c) show the images of the same free nanocavity when it is on tip and on glass, respectively. Fig. 9.12(d) shows the corresponding PL spectra. First, the nanocavity was taken and transferred to the tip end. Comparing the PL spectra of the cavity on tip with that on chip, we found that the $M$, $D$ and $Q$ modes have about 3 nm blue shift. The relative intensity of peaks also changes a lot. For example, the peak from
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The $QH$ mode disappears and that from the $SM$ mode becomes stronger. The reason of the small blue shift is attributed to removed material after the cavity was rubbed by the tip for many times. When the nanocavity was transferred from the tip end to the glass plate, there is an air gap between the nanocavity and the glass plate. This can be verified both from the color fringes on the nanocavity when observed under the microscope and the PL spectrum at this position is hardly affected as compared with the PL spectrum of the cavity on tip. The fringes became weak when the tip pressed the nanocavity on the glass. All the PL peaks are red shifted because of the proximity of the glass. However, comparing the PL spectrum on the glass plate 2 with the PL spectrum on the chip, it is seen that the $QH$ peak has a 14.1 nm redshift which is less than the simulation result (24.1 nm). There are two possible reasons. One is the cavity is broken. The other is there is still some air underneath which can be seen from the blur fringe.

9.1.3.2 Self-orientation of cavities on surfaces

During the manipulation, some unexpected phenomena were observed. Accidentally, cavities jumped from their positions and landed on the surface some tens of $\mu$m’s from their original positions. Rather than landing in the expected orientation face parallel to the surface, there appeared a preference for having the large face perpendicular to the surface. To study this in more detail, a manipulation technique was developed for deliberately throwing the cavities. Fig. 13 shows some SEM images of nanocavities standing on the surface of the chip. Systematic experiments were done to investigate this behavior of the single cavities. To make one cavity jump, it must be taken first by breaking the bars and letting it stick to the tip. The end of the tip is moved to the edge of the hole and force is exerted on it so that the tip was bent. By suddenly relaxing the tip from the hole, the cavity is thrown out. In Fig. 9.14, the states of the cavity before being thrown are observed under the optical microscope. It is found that the cavities tend to land on the InGaAsP surface with vertical position. With 26 cavities being thrown, only 9 are found landing on the chip horizontally. The remaining cavities land with either vertical or tilted positions. Even some of them are found to stand with extreme position, such as with its bar (see Fig. 9.13(b),(d) and (e)).

We suggest electrostatics is responsible for the phenomenon. For this we need the cavities to be charged after release from the chip. There are two potential origins for the charge.

**Electrostatic charging by the manipulating glass tip** Glass is most likely to be charged positively. The charging could happen in two ways. First, the glass tip can be easily electrostatically charged by friction. Second, the charging likely happened when
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Figure 9.13: The SEM images of nanocavities stand (a) vertically with edge, (b) tilted with bar, (d) vertically with bar and (e) vertically with edge on another nanocavity. The SEM images of (c) zoomed in bars of (b), and (f) overview of chip surface.

The glass tip was made by pulling it in a hot flame. This is a very harsh treatment in a plasma and charging is very likely. When the tip approaches the cavity, it will repel the like charge and attract the opposite charge in the conducting InGaAsP. After the bars are broken, the cavity particle is charged. It is more intuitive to express the charge \( Q \) in terms of an electrostatic potential \( V \) through \( Q = CV \). It is easier to get an order of magnitude estimate for \( V \) than for \( Q \), since it is shown that electrostatic potentials easily
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Figure 9.14: In the circle is the cavity particle attached to the tip while the tip is made bent by exerting force using the nano-manipulator. The inset shows the sketch.

can be very high, and lead to discharges. So it is reasonable to estimate it in the volt range, if not substantially larger. As an order of magnitude for the particle’s capacitance $C$, we take $C = \varepsilon_0 h$, where $h$ is a typical lateral dimension of the particle. It is not clear what $h$ should be taken. If it is the lateral size of the particle (about 15 $\mu$m), then we find $Q$ is in the range $10^{-16}$ C.

Charge transfer at the InGaAsP-InP interface  This occurs at a bulk InGaAsP-InP heterojunction as a result of differences in band alignments and bandgaps [183]. Typical surface charge densities are in the range of $10^{15}$ to $10^{16}$ electrons/m$^2$, or $10^{-4}$ to $10^{-3}$ C/m$^2$. Although it is not likely that all this charge is left after under etching, it is instructive to estimate the maximum amount of charge on the particle by multiplying with the surface area of 125 $\mu$m$^2$. This would yield a charge of $10^{-14}$ to $10^{-13}$ C, even much larger than the previous estimate. Translating this into an electrostatic voltage as above via $Q = \varepsilon_0 h V$ would give a voltage in the order of $10^2$ V.

As a result, it is plausible that by one or other mechanism the particle is charged to an electrostatic potential in the range of Volts or much more. Since the particle is conducting, the charges will be spatially separated as much as possible, and preferentially be located at extremes such as boundaries, and particularly the bars.

When the charged particle approaches the surface, the charged extremes induce oppo-
site charges near the surface. These opposite charges attract the extremes of the particles. When this attractive force is much stronger than the gravity force, a torque is exerted to the particle that tends to align it perpendicular to the surface, see Fig. 9.15. Due to the small cross-sectional size of side or leg, the bond to the surface may be very strong and keeps it perpendicular. The nature of the bond with the surface is not decisive here. Whether electrostatic, van der Waals, or other (e.g. fuse after spark discharge), in all cases the bond with the surface is strong.

Firstly, we need to estimate the minimum voltage which offers the electrostatic torque to align the nanocavity perpendicular to the surface. Assume the total induced charge in the nanocavity is $Q$, and assume it all moves to the end near the surface. A charge $q$ at a distance $d$ from the surface is attracted by its image charge. Assume conducting surface for simplicity, then the image charge is also $q$ at a distance $-d$. Then we have for the attractive force $F_{\text{attr}}$:

$$F_{\text{attr}} = \frac{q^2}{4\pi\varepsilon_0 4d^2}. \quad (9.1)$$

The electrostatic torque can only be significant if one side is significantly closer to the surface than the other side. So the torque only starts to work when the particle is near a distance $h$ from the surface. The force may be estimated by ignoring the far part, taking
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$h$ for $d$, and $Q$ for $q$. Eq. 9.1 can be rewritten as

$$F_{\text{attr}} = \frac{\varepsilon_0}{4\pi} V^2.$$  (9.2)

Here, we estimate the rotation of the nanocavity when it falls over a distance of the order of $h$. Thus the rotation angle $\beta_{\text{rot}}$ in the time $t_{\text{fall}}$ becomes

$$\beta_{\text{rot}} \sim \frac{1}{2} \alpha t_{\text{fall}}^2 = \frac{6F_{\text{attr}}}{mg + F_{\text{attr}}},$$  (9.3)

which approaches a constant ($\gg \pi/2$) if $F_{\text{attr}} > mg$, where $\alpha$ is the angular acceleration. Note that once $F_{\text{attr}}$ is large enough, $\beta_{\text{rot}}$ should be independent of $F_{\text{attr}}$, because the larger $F_{\text{attr}}$, the faster it will fall to the surface, and the faster it must rotate to arrive perpendicular to the surface.

The density of InP is $\rho \approx 5 \times 10^3 \text{kg/m}^3$. The volume of the nanocavity can be estimated by $\text{Volume} \sim h^2t = 4.5 \times 10^{-17} \text{m}^3$. Thus the mass is $m = \rho \cdot \text{Volume} = 2 \times 10^{-13} \text{kg}$. The weight $G$ of the nanocavity is $G = mg \sim 2 \times 10^{-12} \text{N}$.

When the attractive electrostatic force and gravity are equal, we can get the voltage

$$\frac{\varepsilon_0}{4\pi} V^2 = 2 \times 10^{-12} \text{N} \Rightarrow V \sim 3V.$$  This is a modest electrostatic potential, a reasonable order of magnitude. The attractive force rapidly increases when the sample approaches the surface, while gravity remains constant.

In the analysis above, a perfect conductor was assumed. However, it is also valid for a dielectric, if the image charge is taken as $q_{\text{image}} = -\frac{1}{\varepsilon + 1} q$ ($\varepsilon$ is the (static) permittivity of the dielectric), which is of the same magnitude as $q$, not only for an InP-like dielectric ($\varepsilon \sim 12$), but even for glass ($\varepsilon \sim 4$).

Once the nanocavity has arrived at the surface, it is strongly bound. No other forces need to be invoked then to keep it to the surface in any orientation. An analogous situation occurs for nanowires that can be grown epitaxially vertically on a surface. They are bound to the surface with a strong chemical bond and then very high aspect ratio wires remain upright at the surface in any orientation, unaffected by gravity. Wires with tens of nm’s diameter, micrometer long, have similar aspect ratio as our cavities.

The sample can be flipped 180 degree. Thus the bond to the surface must at least be large enough to carry the particle against gravity, so the bond force per unit area $\sigma_{\text{contact}}$ must be at least $mg/wt = 5 \times 10^{-4} \text{bar}$, where $w$ is the width of the nanocavity which is the length of side ($\sim 5 \mu\text{m}$) when it lands on its side, or is the width of the bar (same order as $t$) when it lands on its bar. The sample was rotated 90 degree at SEM holder. The bond force must also provide the torque to compensate the gravity when the particle is horizontal, see Fig. 9.16. The torque due to the bond force with respect to the pivot
point $P$ can be expressed with

$$
\tau_{\text{contact}} = \int_0^t x \sigma_{\text{contact}} \, dx = \frac{1}{2} \sigma_{\text{contact}} wt^2.
$$

(9.4)

When $\tau_g = \frac{1}{2} mhg$ due to the gravity equals $\tau_{\text{contact}}$, we get $\sigma_{\text{contact}} = 4 \times 10^{-2}$ bar.

The intrinsic genuine chemical bonding force may be expressed as a materials tensile strength. It is typically many orders of magnitude larger, e.g. $7 \times 10^4$ bar for crystalline Si. This confirms e.g. that long nanowires do not bend or break under their own weight.

InP has been bonded to crystalline Si by polishing and sputter cleaning both surfaces, after which they are immediately pressed together at room temperature, contacting over an area of $3 \times 3$ mm$^2$ under a pressure of 40 kgf, which corresponds to a pressure of 400 bar [184]. The adhesion was tested by a tensile stress experiment, and the bond already disrupted at a Si-In interface, apparently due to an initially P-depleted InP surface. Other work was cited that showed 3 bar rupture strength. The significance of this number is that even this very low bond strength between dissimilar material, realized by only cold pressing, is more than enough to resist gravity.

There are some options for the origin of the bond to the surface,

**Electrostatic bond** An electrostatic bond between the cavity’s charge and its image charge at the surface. For this case, an insulating layer of thickness ($t$) must be assumed. This could be present in the form of native oxides or depletion layers. In all cases, they should be very thin, in the order 1 to 10 nm. Assuming the same charges as above, the
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force per unit area of contact $\sigma_{\text{contact}}$ can be estimated. The force per unit area of contact is

$$\sigma_{\text{contact}} = \frac{Q}{wt} E.$$  \hfill (9.5)

The electric field follows

$$E = \frac{Q}{wt \varepsilon \varepsilon_0},$$  \hfill (9.6)

where $Q/wt$ is the surface charge and $\varepsilon$ is the permittivity of the assumed oxide. Then we can get

$$\sigma_{\text{contact}} = \frac{Q}{wt} \frac{Q}{wt \varepsilon \varepsilon_0} = \frac{Q^2}{w^2 t^2 \varepsilon \varepsilon_0}.$$  \hfill (9.7)

Assuming again $Q = \varepsilon_0 h V$, we get

$$\sigma_{\text{contact}} = \frac{\varepsilon_0 h^2}{w^2 t^2 \varepsilon} V^2.$$  \hfill (9.8)

Take for standing on a bar $w \sim t \sim 0.2 \, \mu m$, $h \sim 10 \, \mu m$, $\varepsilon \sim 3$, then we get

$$\sigma_{\text{contact}} = \frac{10^{-11} \times 10^{-10}}{2 \times 10^{-7} \times 3} V^2 \sim 1.25 \times 10^4 V^2,$$  \hfill (9.9)

which is $\sim 0.125$ bar for $V=1$ V. This is an order of magnitude larger than required to provide the torque, and larger than the bond pressure found in Ref. \[184\]. As mentioned above, it is likely that the charging voltage is much larger than the fraction of a volt estimated here. However, this larger voltage cannot exist across a thin layer as breakdown voltages of even good insulators are typically in the range of $\sim 1$ V/\mu m or lower. Thus the nanocavity will discharge to the substrate.

**Melting** If the discharge mentioned in last paragraph would occur by a violent breakthrough, local material modification, melting, or spot welding might occur. Mechanically however, this would lead to an even stronger bond at the surface. This is not likely to occur, as particles are easily taken, repositioned or moved across the surface.

**Van der Waals forces** If electrostatic bonding effects are eliminated, and the discharge has occurred by gentle recombination, then the last force present would be the Van der Waals force between surfaces. The classical Van der Waals force per unit area between two flat plates at a distance $d$ is $\sigma_{\text{vdW}} = \frac{A}{6sd^3}$ with $A$ the Hamaker constant \[185\], which is typically in the range $10^{-19}$ to $10^{-20}$ J. Disregarding any microscopic details, it can be seen that even at a distance of 1 nm, this force is already in the range of tens of bars, i.e. far larger than needed to resist gravity against falling.
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9.2 Application 1: 3D photonic crystal

Full confinement of photons and control of their interaction with materials can only be achieved with the use of three-dimensional photonic crystals (PhCs) with complete photonic bandgaps. We propose to use the microscope manipulation method as a means for building 3D PhCs. So far, there are several ways to fabricate 3D PhCs.

Layer by layer: First, a basic 2D structure is formed on one layer by electron beam lithography and dry etching techniques. Then the next layer will be built with a different patterning. Finally, the 3D PhCs can be made by continuing the layer by layer process. Fig. 9.17(a) and 9.17(b) show the SEM image of PhCs having band gap around telecommunications wavelength \[186, 187\]. Recently, some 3D PhCs were assembled by stacking planar components using a sophisticated micromanipulation technique \[188–192\] [see Fig. 9.17(c)]. The alignment is quite difficult. These experiments were done in electron microscope.

Self-assembly: First, latex spheres are made by a sol-gel method. Then the nanoparticles spontaneous organize into ordered structures by non-covalent interactions. Normally the face centered cubic (fcc) structures can be made because of thermodynamics. Fig. 9.17(d), 9.17(e) and 9.17(f) shows fabricated highly ordered 3D arrays of spheroidal voids \[193\], silicon inverse opal \[194\] and fcc PhCs \[195\], respectively.

Top-down: The top-down approach is a method based on the multi-directional (or multi-angled) etching of single-crystalline semiconductors or dielectric materials for the direct creation of high-quality 3D photonic crystals. Fig. 9.17(g) shows the schematic figure of two step etching \[196\].

Holographic lithography: Periodic microstructures are generated by interference of four non-coplanar laser beams. The intensity distribution in the interference pattern has 3D translational symmetry; its primitive reciprocal lattice vectors are equal to the differences between the wavevectors of the beams. Highly exposed photoresist is rendered insoluble; unexposed areas are dissolved away to reveal a three dimensionally periodic structure. Fig. 9.17(h) shows 3D PhCs by crosslinked polymer with air-filled voids \[197\].

Multi-photon polymerization: In this method, a liquid or block of gel containing various monomers and a 2-photon active photoinitiator is irradiated with a focused laser,
Figure 9.17: SEM images of PhCs generated by (a), (b) and (c) layer by layer, (d), (e), (f) self-assembly, (h) holographic lithography, (i) Multi-photon polymerization and (j) Glancing angle deposition methods. The schematic figure of (g) top-down and (j) glancing angle deposition methods.
which traces the 3D profile of the object to be created. The laser light initiates polymerization, but only at the focal point as a result of the nonlinear nature of the polymerization. The laser passes unperturbed through both polymerized and unpolymerized regions of the material. After this tracing is finished, the three-dimensionally structured object may be recovered by washing away the unpolymerized gel with common organic solvents. Fig. 9.17(i) shows a 3D PhC [198] made by Cumpston et al.

**Glancing angle deposition:** Toader proposed an alternative PhC architecture consisting of square spiral posts in a tetragonal lattice [199] [see Fig. 9.17(j)]. This structure has a large and robust 3D PBG occurring between the fourth and fifth electromagnetic bands and is amenable to large-scale micro-fabrication using glancing angle deposition (GLAD) technique. The SEM image is shown in Fig. 9.17(k).

As we see from the micro-manipulation [188–192], the manipulation with a slab is the key to build a 3D PhCs. In this section, we describe how we can align the nanocavities with different patterns or orientation in three dimensions. The manipulation includes taking the cavities from the chip by breaking the bar, changing the places and the orientation of them on the same substrate or on another substrate. It shows the potential of the nanomanipulation method for building 3D PhCs or other 3D structures.

**Controlled positioning of cavities**

Figure 9.18: The SEM image of the result of the experiments of stacking two cavities (a) vertically and (b) horizontally.
The experiments on controlling the orientation of the cavities in a horizontal position are done by first controlling the orientation when they are in vertical position, followed by pushing them face down to the surface. These experiments are followed by an attempt to perfectly stack two cavities. It is done by first putting a cavity vertically on top of another suspended cavity. The orientation of the cavity is controlled when it is in that position. After getting the correct orientation, the cavity is gently pushed down. The SEM image of the horizontally stacked cavities is shown in Fig. 9.18(a).

The stacking two cavities vertically on the substrate is also investigated. One of them is taken by the tip and brought to the other after being assured that they have the same orientation. After they touch each other, the tip is removed from the cavity. It is found under the optical microscope that it is possible to make the cavities touch each other while being aligned. The result can be seen in Fig. 9.18(b). Note that the SEM images are made after the alignment procedures are finished. From both Fig. 9.18(a) and Fig. 9.18(b), we can see that the alignment is not perfect which is because of the resolution of the optical microscope.

Figure 9.19: The SEM images of several cavities (a) standing in a line on InGaAsP substrate and (b) standing in a certain arrangement on a glass plate. The dark background behind the cavities in (b) is the scotch tape which is used to mark the areas of the cavities on the glass plate.

It is also found possible to touch the cavities with the tip and then to drag them to different positions. It is even possible to lift the standing cavities from the substrate and then land them on the substrate again. Changing the orientation of a standing cavity is also successfully done by making the tip touch one of its sides and using the tip to exert force on it. With all these findings, a fully controlled manipulation has been successfully
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done on several cavities to make them standing vertically in a line on chip as shown in Fig. 9.19(a) and in a pattern on glass plate as shown in Fig. 9.19(b). The controlled manipulation of nanocavities offers great potential for new 3D optical devices as 3D PhDs or all dielectric metamaterial. An application already pursued recently is to use similar cavities to control light extraction of arbitrary emitters on arbitrary surfaces [200]. Also a novel type of scanning cavity microscopy was proposed by the authors [200].

9.3 Application 2: Sensing

Optical fiber sensors are studied for a long time. By detecting intensity, phase, frequency, polarization of light in a fiber, different kinds of sensors can be made. Very recently, there is much interest to functionalize a fiber facet [201–204]. This is a very nontrivial problem since standard lithographic methods like spinning of photo- or ebeam resists cannot be applied to the small facet of an optical fiber easily. Lin et al transfer gold nanorod arrays to optical fiber tips for localized surface plasmon resonance biochemical sensing [201]. Andrade et al use multilayer silver nanoparticles-modified optical fiber tip for high performance SERS remote sensing [202]. King et al put a porous PhC to the facet of a fiber and used it for sensing organic vapor [203]. According to our experience above, the PhC cavity can be bound to the glass very well. In this section, we will give the description of making an innovative fiber sensor by attaching one PhC cavity to the facet of a single mode fiber.

In order to excite the PhC nanocavity modes efficiently, the laser should be focused on the defect area of the cavity. With a single mode fiber, this is already achieved to a considerable extent. A standard fiber (SMF-28-10 from Thorlabs) was used. The core diameter and the cladding diameter are 8.2 $\mu$m and 125±0.7 $\mu$m, respectively. The NA is 0.14. The cavity from column one is chosen for the experiments for two reasons. The holes in the defect area of cavities from column one have the biggest diameter which means the highest sensitivity. The modes wavelength of cavities from column one is shorter than the ones from the other four columns, so the modes have the highest possibility to reappear within the detector range after the infiltration.

Our cavities were not designed for the fiber coupling and generally radiate under angles well outside the small NA of the fiber. It is therefore relevant to have an estimate of the (poor) coupling efficiency. Some calculations based on Ref. [205] are performed to estimate the coupling efficiency of the cavity to the fiber.

The fiber mode profile in the radial direction is determined by two constants $k_T$ and $\gamma$, which are related to the fiber propagation wavevector $\beta$ in the axis direction by

$$k_T^2 = n_{\text{core}}^2 k_0^2 - \beta^2$$  \hfill (9.10)
\[ \gamma^2 = \beta^2 - n_{\text{clad}}^2 k_0^2 \]  

where \( k_0 \) is the wavevector in vacuum.

If we let \( X = k_T a \), \( Y = \gamma a \), the fiber’s dispersion relation \( \beta(\omega) \) is to be found from the characteristic equation,

\[ X \frac{J_{l+1}(X)}{J_l(X)} = \pm Y \frac{K_{l+1}(Y)}{K_l(Y)} \]  

where \( J_l(X) \) is the Bessel function of the first kind and order \( l \), \( K_l(X) \) is the modified Bessel function of the second kind and order \( l \). Eq. 9.12 was solved numerically for \( \beta \) at the cavities resonant frequencies, \( k_T \) and \( \gamma \) are known. With this, the mode profile is given by

\[ u(x) \propto \begin{cases} J_l(k_T r), & r < a \ (\text{core}) \\ K_l(\gamma r), & r > a \ (\text{cladding}) \end{cases} \]  

Both the fiber transverse mode profile and the cavity modes are Fourier transformed to find the necessary overlap of transverse k-vectors.

Fig. 9.20 (a) and (b) shows the momentum space intensity distribution obtain by Fourier transforming the in-plane field \( (|FT(E_x)|^2 + |FT(E_y)|^2) \) of the \( M \) and \( D \) modes at the input of the fiber. Fig. 9.20 (c) and (d) shows the momentum space intensity distribution obtain by Fourier transforming the fiber modes at the \( M \) and \( D \) modes frequencies. While clearly the overlap is poor, it is sufficient to expect a measurable signal.

The end of the fiber was cleaved and cleaned with isopropanol. The facet was made as flat as possible to attract the cavity very tight at the facet. The manipulation of transferring a cavity from the chip to the fiber facet was done by the modified setup which is shown in Fig. 9.21(a). The fiber is fixed vertically, i.e., the fiber facet is horizontal.

The bars were broken first and then the nanocavities were released from the chip. The released cavities were attached to the tip. The microscope image of a cavity on the tip is shown in Fig. 9.21(b). The cavity is in horizontal position when it was taken by the tip. The next step was to align the cavity to the core of the fiber. To make the nanocavity effectively excited, the nanocavity should be put at the center of the core area. To know the exact area of core, a red laser was sent through this fiber [see Fig. 9.21(c)]. The last step was to align the cavity with the core and make them overlapped. In the end, the cavity was transferred from the tip to the core area. Fig. 9.21(d) shows the microscope image of a cavity attached on fiber facet with laser on. We can see the defect area of the cavity coincidences with the center of the laser spot. Note that the cavity is largely transparent to visible light. This is due to the holes (30% of area occupied by the holes) and the penetration length at visible wavelengths which is comparable to the membrane.
Figure 9.20: Momentum space intensity distribution obtained by Fourier transforming the in-plane near field ($|FT(E_x)|^2 + |FT(E_y)|^2$) of (a) the monopole mode and (b) the dipole mode from the PhC cavity. Momentum space intensity distribution obtained by Fourier transforming the fiber modes at (c) the monopole mode frequency of PhC cavity and (d) the dipole mode frequency of PhC cavity. Note that the modes lack of the hexagonal symmetry because the defect is not hexagonally symmetric and (b) have been rotated with 90 degree for comparison. The dashed lines are used for alignment.

Because the fiber with a cavity for PL measurement is too long to be put on the SEM holder, Fig. 9.22(a) shows the SEM image of another cavity attached to the fiber facet where the fiber had been cut. Fig. 9.22(b) shows the zoom in image of the cavity in...
Figure 9.21: (a) The schematic figure of the manipulation set-up. The microscope images of (b) tip with a cavity, (c) fiber with laser on and (d) a cavity attached on the fiber facet with laser on.

Fig. 9.22(a).

The schematic figure of the measuring setup is shown in Fig. 9.23. A $2 \times 2$ fiber coupler (10202A-50-FC from Thorlabs) is used to connect the laser, the detector and the fiber with a cavity on its facet. First, the laser was sent through the fiber coupler to excite
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Figure 9.22: The SEM images of (a) a cavity attached to the fiber facet and (b) zoom in of the cavity in (a).

Figure 9.23: The schematic figure of the measuring setup.

the cavity mode of the PhC cavity. Then some part of the emission from the cavity was collected by the fiber connected to it and arrived at the detector through the fiber coupler.

Fig. 24 shows the PL spectra excited with laser power 0.2 mW with the fiber connected to the nanocavity and without the fiber. The intensity is quite high at the short wavelength and decays as the increase of the wavelength. This background can be from the spontaneous emission from the laser. However, the emission from the quantum dots is still dominant in the important range near 1500 nm for the sensing application.

Fig. 9.25 shows the PL spectra excited with different laser powers of 0.05 mW, 0.1 mW, 0.2 mW, 0.5 mW, 0.7 mW and 1 mW. The average intensity is comparable to the intensity of the modes from the nanocavity which are the $M$ (at 1588.5 nm) and $D$ mode (at 1567.4 nm) at low power. The period modulation at short wavelength is attributed to Fabry-Perot oscillations. The free spectral range (FSR) from Fabry-Perot mode can be
9.3 Application 2: Sensing

Figure 9.24: PL spectra excited with laser power 0.2 mW on laser display (a) with the fiber connected to the nanocavity and (b) without the fiber.

Figure 9.25: The PL spectra excited with different laser power, which are 0.05 mW, 0.1 mW, 0.2 mW, 0.5 mW, 0.7 mW and 1 mW on laser display.

calculated by

\[ FSR \approx \frac{\bar{\lambda}_0^2}{2nL} \]  \hfill (9.14)

\( \bar{\lambda}_0 \) is the central wavelength of the two adjacent peaks, \( L \) is the length of the Fabry-Perot cavity and \( n \) the refractive index of the mediumn between the mirrors. Set \( \bar{\lambda}_0 \) to 1506 nm, \( FSR \) to 6.5 nm and \( n \) to 1, we get \( L \) is 0.17 mm. In view of the length, the Fabry-Perot mode is likely formed between the two facets of the fibers inside the FC/PC connector which are manually adjusted.
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The peak positions of the two cavity modes shift about 3.7 nm when the laser power is changed from 0.05 mW to 1 mW ($D$ mode at 1571.1 nm, $M$ mode at 1592.8 nm). That is attributed to heating of the cavity and results from the refractive index increase of the InGaAsP as the temperature is increased. The red shift is $\sim$3.9 nm/mW which is in the reasonable range \[206\]. It means that cooling of the cavity to the glass is poor. We note that the $Q$ and $QH$ modes can not be recognized because they are immersed in the background.

![Figure 9.26: PL spectrum excited with laser power 1 mW on laser display with the fiber connected to the nanocavity infiltrated with distilled water (green curve) and without distilled water (red curve).](image)

To find out the sensitivity of the fiber with cavity, the vessel was filled with distilled water. To have a good signal to noise ratio, excitation with 1 mW power was used. Fig. 9.26 shows the PL spectrum with the fiber connected to the nanocavity immersed in distilled water. The $D$ and $M$ modes were red shifted to 1591.9 nm and 1616.5 nm. Compared with the mode positions without water, they were red shifted with 20.8 nm and 23.7 nm, which give sensitivities of 66 nm/RIU and 75 nm/RIU, respectively. In our simulation, if the surface and the holes are infiltrated with water, the $D$ mode and $M$ mode should have 37.2 nm and 33.3 nm red shift, if only the surface is covered with water, the two modes should have 12.7 nm and 12.4 nm red shift. Thus in our case, the surface is covered and part of the holes are infiltrated. The sensitivity is underestimated because in water the cavity is better cooled and is not expected to be heated with the laser power. The mode at 1550 nm is the $Q$ mode, which can now be recognized after shifting out of the strong background area.
9.4 Conclusion

In summary, we demonstrate three releasing methods to transfer the nanocavity on chip to other substrate. The effect of the surrounding materials were analyzed with the PL spectrum. We demonstrate that printing of cavities on other substrates is possible. The nano-manipulation method is successfully used to take the single nanocavity from the chip. Controlled positioning by manipulation like aligning several nanocavities vertically or horizontally on chip or glass plate has also been demonstrated. There is a large prospect in three dimensional PhC fabrication with this method. A fiber sensor with nanocavity on its facet was achieved. The sensitivity and the signal to noise ratio could be increased by optimizing the PhC nanocavity.
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Summary

Light control by nanostructured metal surfaces and photonic crystals in nanobeams and freestanding membranes

Photonic crystals (PhCs) are periodic nanostructures, which affect the motion of photons in a similar way as the periodicity of a semiconductor crystal affects the motion of electrons. Because of the spatial periodicity of the refractive index of the material, there exist band gaps. The light with energy within the band gaps is forbidden to propagate. Apart from the bandgap effect, another property which receives lots of attention is the abnormal refraction of light in a PhC when the frequency is near the PhC band edges.

A surface plasmon polariton (SPP) is a collective oscillation of the electrons at the interface between a metal and a dielectric. One of the major driving forces in the field of plasmonics is the ability of spatially confining electromagnetic energy at visible frequencies over a distance significantly shorter than the wavelength. At terahertz frequencies, a metal resembles in many aspects a perfect electric conductor. The metal leads to highly delocalized SPPs.

In this thesis we study theoretically and experimentally nanophotonic structures of dielectric PhCs and SPPs for application in integrated optics, imaging and sensing. The plane wave expansion and Finite Difference Time Domain (FDTD) methods are used to calculate the band structures of PhCs and to obtain the field distribution of a finite PhC, respectively. The PhC membranes are made in the clean room with the state of the art technology. The PhCs are characterized by the photoluminescence (PL) emitted by quantum dots incorporated in the semiconductor during epitaxial growth.

In the introduction, the theory and properties of PhCs are introduced. The reason why surface plasmon polaritons at THz frequencies don’t exist at a planar metal surface is given.

In chapter 2, the basic ideas of these two simulation methods, fabrication process and measurement set-up are given.

In chapter 3, we have studied the characteristics of the terahertz SPP propagation on a periodically structured Ag surface with the FDTD method. The dispersion relations
and the propagation losses of the SPP mode have been calculated. The influence of the groove width, the period, the sharpness of the groove corners, and the groove height, has been analyzed. We have found that the total area of the side-walls of the grooves per unit length has a major effect on the propagation loss. To slow down the speed of light at THz, we have introduced a metal waveguide consisting of two parallel thin metal slabs with subwavelength periodic corrugations on their inner boundaries. Compared with another metal waveguide based on engineered surface plasmons, our structure has obviously smaller absolute value of the group velocity dispersion parameter and lower propagation loss. As the waveguide is made of metal, the light can be confined tightly in a subwavelength region, which cannot be realized with a two dimensional (2D) PhC-based waveguide. The physical mechanism of the slow light for the proposed structure is that a portion of the field re-circulates back and forth through a number of directly coupled optical cavities.

In chapter 4, we have introduced a simple superlens formed by a one dimensional (1D) dielectric PhC. Off-axis subwavelength focusing has been achieved and explained with some equi-frequency contours analysis. Unlike in subwavelength focusing by a slab of some high-dimensional PhC of negative refraction, both positive refraction and negative refraction occur in the present subwavelength focusing. The present 1D PhC lens is easy to fabricate, and the spot size can be much smaller than that for a 2D or three dimensional (3D) PhC slab. The superlens properties, including the influence of the orientation of the surface termination to the image quality, have been studied with the FDTD simulation. The present superlensing structure can be much thinner than existing 2D or 3D PhC slabs for subwavelength focusing. The properties of on-axis image achieved by the combination of two such slabs of 1D PhC have also been studied. Although the present 1D PhC does not have any isotropic effective refractive index, the combination of two such slabs of 1D PhC can give some properties which usually exist only for some 2D or 3D PhC with an isotropic effective refractive index.

In chapter 5, the effects of disorder in a PhC on the extraction efficiency of the light emitting diode (LED) have been investigated by using a full-vectorial FDTD method. The extraction efficiency of the ordered PhC LED (EEOPL) and extraction efficiency of the disordered PhC LED (EEDPL) at several normalized emission frequencies are calculated to compare the extraction efficiency with different extraction mechanisms. The EEOPL and EEDPL are comparable when the frequency is in the leaky modes region. Other kinds of disorder have also been simulated (such as other kinds of random distribution, air grooves of half circle shape and triangles), but are not shown here. These simulations show that a similar conclusion can be expected for other kinds of disordered PhC LEDs in which the effect of the PhC band structure still exists. Thus when the emission frequency
is in a leaky modes region, the functionality of the PhC LED can be sustained even if disorder exists in the fabrication process and the Purcell enhancement of the ordered PhC LED and the disordered PhC LED are more or less the same.

In chapter 6, we investigate the optical characteristics of the width-reduced line-defect PhC waveguides within lateral p-i-n structures. Compared with the classical line-defect PhC waveguides, the width reduced photonic crystal waveguide has much stronger capacity in optical confinement in plane, which can allow a narrower intrinsic layer that leads to a fast electric response.

In chapter 7, we presented the sensitivity to the refractive index changes of the analyte of InGaAsP PhC slot nanobeam waveguides. We report a high sensitivity of 700 nm per refractive index unit (RIU) for a normal structure and a higher sensitivity of 900 nm/RIU for a cavity type structure. These record high values for sensitivity correspond directly to the large overlap of the mode field with the analyte, particularly in the slot region. A new design with both high sensitivity and Q factor is proposed. In the new design structure, both the high sensitivity and high Q factor can be achieved. Future work about the sensitivity test should be done.

In chapter 8, we studied the properties of PhC nanocavities. First, we have demonstrated the influence of the liquid crystal infiltration on the mode-degeneracy of the quadrupole modes of a PhC nanocavity. The mode splitting exists only in the anisotropic nematic LC state and not in the unfilled or isotropic LC state, which is attributed to the different interactions of the two orthogonal bases of the degenerate mode with the two components of the refractive index of the LC. Second, we have also demonstrated that the resonances of PhC nanocavities can be independently controlled by changing the holes around the defect area. Only the combination of the monopole mode and the dipole mode from the cavities will already offer a two-digit bar code with a large number of ($\sim 10^3$) different codes. These findings can be applied to realize encoded particles with large coding capability ($> 10^5$) for biosensing.

In chapter 9, printing and nano-manipulation techniques are employed to transfer the membrane cavities to another substrate (glass) and to manipulate them as chiplets. The remarkable phenomenon that the chiplets preferentially orient themselves with their plane perpendicular to the surfaces is observed and studied. A fully deterministic positioning of them is demonstrated. Their PL spectra are measured at each experimental step to study the effect of the environments and the nature of the bonding between the chiplets and the surfaces. A single chiplet is attached to the facet of an SMF-28 optical fiber as the first application. Its PL spectra when coupled to the fiber are measured with the excitation and luminescence guided through the same fiber while the facet is exposed to air and immersed in water. The observed spectral shift demonstrates the working principle of a
novel optical fiber-based sensor. More applications in sensing and 3D manufacturing are anticipated.
List of publications

Part of the thesis

Journals


Conferences


Part out of the thesis

Journals

Conferences

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Curriculum vitae

Bowen Wang was born on July 3, 1984 in Nanjing, China. He received his B.Eng. degree in Nanjing University of Science and Technology, Nanjing, China, in 2006. He started PhD studying in Centre for Optical and Electromagnetic Research, Zhejiang University, Hangzhou, China, in 2006. His research included theoretical study of the metamaterial and to investigate its applications (National Basic Research Program (973) of China (under Project No. 2004CB719800)), and the dependence of the light extraction efficiency of a light emitting diode on the lattice irregularities of the photonic crystals (Brainbridge project).

In November 2009, under the framework of the BrainBridge project with Philips Research, TU/e and Zhejiang University, he continued his research in the Photonics and Semiconductor Nanophysics group, Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands, in the area of photonic crystal optical sensors.