Design, fabrication and experiment of photonic bandgap structures and devices

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Design, Fabrication and Experiment of Photonic Bandgap Structures and Devices

Selin Teo Hwee Gee

SCHOOL OF ELECTRICAL & ELECTRONIC ENGINEERING

A thesis submitted to the Nanyang Technological University
in fulfilment of the requirement for the degree of
Doctor of Philosophy

2007

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research and has not been submitted for a higher degree to any other university or institution.

Date

Selin Teo Hwee Gee

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Signature:

SUMMARY

This doctorate thesis focuses on the innovation of photonic integrated circuit (PIC) devices with a new class of material known as photonic bandgap (PBG) crystals for control of photons not achievable with legacy dielectric waveguide systems. Specifically, silicon is the material of choice being investigated for the PBG PIC devices designed to address the objectives of macro-to-micro optical system integration; ultra compact optical device footprint; high optical performance; realization of deep sub-micrometer length scale photonic crystal devices and also demonstration of PIC PBG functionalities.

Based on the physical and mathematical derivations for different PBG structures, the various aspects of PIC PBG were studied and modeled. Simulations were carried out based on derived transmission characteristics for one-dimensional PBG; the plane wave method (PWM); the finite difference time domain (FDTD) method and also the coupled mode in time analyses. Besides the dynamic frequency responses obtained through the transmission characteristic simulations, dispersion relations of band structures in PBGs that detailed the eigenmodes allowed or prohibited from existing within the PBG lattice were also obtained. Together with gap maps generated for parametric analyses, design optimizations were carried out to yield a novel large absolute bandgap lattice in a high symmetry square Brillouin zone PBG.

In device simulations, PIC applications to designs of single line embedded and orthogonally crossing optical intersection resonators were studied and then verified

experimentally. To enable such extensive experiments, the non trivial fabrication tour-de-force challenges required to realize PBG structures useful for the fiber optical-communication wavelengths centered at 1550 nm, must first be successfully addressed. The difficulties involved in PBG fabrication arises due to the scaling property of PBG which requires a length scale of less than half the wavelength of operation for sensitive photonic control. Hence, in the fabrication process, much works were carried out in the deep ultraviolet lithography and deep reactive ion etching (RIE) modules. Record high resolution and aspect ratio PBG structures were realized together with monolithic integration of disparate dimension and etch-depth test structures; achieved using a specially designed synthesized processing technique. The devices fabricated from silicon-on-insulator (SOI) substrates were then tested experimentally, with effective macro to micro level coupling between the optical fibers (of more than a hundred micrometers diameter) and the PBG PIC waveguides (of width less than a micrometer width). Through the use of background level isolating designs and adiabatically tapered waveguiding structures, experiments based on a set-up of pump and probe lasers (consisting of high and low photon energy beams respectively) were carried out on the realized PBG devices. Passive and dynamic optical experimental results were obtained for dispersion characterizations and optically induced switching in output levels. These novel experimental demonstrations of such PBG PIC devices not only verified theoretical design predictions, but also provided many insights useful for future designs of PIC device with active control applications.

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LIST OF ABBREVIATIONS

<i>1D</i>	One-Dimensional
<i>2D</i>	Two-Dimensional
<i>3D</i>	Three-Dimensional
<i>a</i>	Lattice Period
<i>Å</i>	Angstrom (A ten thousand-millionth of a meter)
<i>ArF</i>	Argon Fluoride
<i>BARC</i>	Bottom Anti Reflection Coating
<i>C₄F₈</i>	Octa-Fluoro-Cyclo-Butane
<i>CAIBE</i>	Chemical Assisted Ion Beam Etch
<i>CAR</i>	Chemically Amplified Resist
<i>CD</i>	Critical Dimension
<i>CF</i>	Correction Factor
<i>CMOS</i>	Complementary Metal Oxide Semiconductor
<i>CMP</i>	Chemical Mechanical Polished
<i>Cu</i>	Copper
<i>dB</i>	Decibel
<i>DBR</i>	Distributed Bragg Reflectors
<i>DF</i>	Dielectric Fill Factor
<i>DI</i>	Distilled
<i>DM</i>	Density of Modes
<i>DOF</i>	Depth of Focus
<i>DPN</i>	Dip-Pen Nanolithography
<i>DRIE</i>	Deep Reactive Ion Etching
<i>DUV</i>	Deep Ultra-Violet
<i>DWDM</i>	Dense Wavelength Division Multiplexing
<i>E</i>	Exposure Energy
<i>E-beam</i>	Electron Beam
<i>EBL</i>	Electron Beam Lithography
<i>ECP</i>	Electro Chemical Plating
<i>EF</i>	Experiment Factor
<i>EM</i>	Electromagnetic
<i>eV</i>	Electron Volt
<i>F</i>	Focus
<i>FDTD</i>	Finite Difference Time Domain
<i>FEM</i>	Focus Exposure Matrix
<i>FF</i>	Finesse Factor
<i>FIB</i>	Focused Ion Beam
<i>FIBL</i>	Focused Ion Beam Lithography
<i>FP</i>	Fabry-Perot
<i>FSR</i>	Free Spectral Range
<i>FWHM</i>	Full Width at Half Maximum

H_2O_2	Hydrogen Peroxide
H_2SO_4	Sulfuric Acid
<i>HAR</i>	High Aspect Ratio
<i>HIC</i>	High Index Contrast
<i>HL</i>	Holographic Lithography
<i>HMDS</i>	Hexa-Methyl-Di-Silazane
<i>ICP</i>	Inductive Coupled Plasma
<i>IPA</i>	Isopropyl Alcohol
<i>k</i>	Wavevector
<i>KrF</i>	Krypton Fluoride
<i>LE</i>	Lithographic Error
<i>LIL</i>	Laser Interferometric Lithography
<i>MFP</i>	Mean Free Path
<i>n</i>	Refractive index
<i>NA</i>	Numerical Aperture
<i>NIL</i>	Nano-Imprint Lithography
<i>nm</i>	Nanometer (A thousand-millionth of a meter)
<i>OAI</i>	Off Axis Illumination
<i>OL</i>	Optical Lithography
<i>OPC</i>	Optical Proximity Correction
<i>OPE</i>	Optical Proximity Error
<i>OSA</i>	Optical Spectrum Analyzer
<i>OTS</i>	Optical Testing Structures
<i>PBG</i>	Photonic Band Gap
<i>PECVD</i>	Plasma Enhanced Chemical Vapor Deposition
<i>PhC</i>	Photonic Crystal
<i>PIC</i>	Photonic Integrated Circuit
<i>PML</i>	Perfectly Matched Layers
<i>PSM</i>	Phase Shift Masking
<i>PVD</i>	Physical Vapor Deposition
<i>PWM</i>	Plane Wave Method
<i>Q</i>	Quality Factor
<i>QED</i>	Quantum Electro Dynamics
<i>R</i>	Resolution
<i>RIE</i>	Reactive Ion Etch
<i>sccm</i>	Standard Centimeter Cube per Minute
<i>SEM</i>	Scanning Electron Micrograph
<i>SF</i>	Shape Factor
SF_6	Sulphur Hexafluoride
<i>SLED</i>	Super-Luminescent Light Emitting Diode
<i>SMF</i>	Single Mode Fiber
<i>SOI</i>	Silicon-on-Insulator
<i>SPL</i>	Scanning-Probe Lithography

<i>Ta</i>	Tantalum
<i>TE</i>	Transverse Electric
<i>TIR</i>	Total Internal Reflection
<i>TLS</i>	Tunable Laser Source
<i>TM</i>	Transverse Magnetic
μm	Micrometer (A millionth of a meter)
<u><i>USG</i></u>	<u>Undoped Silicate Glass</u>
<i>V</i>	Mode Volume
<i>ZPAL</i>	Zone Plate Array Lithography

CHAPTER 1

INTRODUCTION

1.1 Motivation

This PhD research topic project arose in motivation from expectations, that the performance of photonic integrated circuits (PICs) can be greatly improved with the innovative use of a relatively new class of meta-material proposed only twenty years ago [1, 2]. Known as photonic bandgap (PBG) or photonic crystals (PhCs), this new class of material achieves unprecedented wavelength-scale control of light propagation [3, 4], through introduction of ‘defect’ states within a PBG - much like how defects in semiconductors are used to make useful devices. In solid state physical analysis of PhCs lattice reciprocal spaces, precise designs of such periodically arranged structures can be effected to yield perfectly opaque or strongly dispersive [5, 6] optical characteristics. Such extensive control in propagation properties, over a large bandwidth, with light speed processing photonics are consequently intensively researched for optical technological innovations, and also potential physical discoveries.

Albeit PBG makes direct reference to the word “photonic”, this technology has a principle that applies equally well to electromagnetic (EM) radiations of all wavelengths. At the same time, due to its scaling property, any PBG structure can be re-scaled in proportion to any arbitrary wavelength of interest without requirement of re-design. Further, PhCs can also be considered and understood in analogy to

their electronic counterpart – the semiconductor crystals. In semiconductor crystals, the electronic bandgaps arise because electrons behave partly like a wave, and the electron's waves scatter off the lattice of semiconductor atoms. Part of the electron's wave is scattered back in the source direction. For particles with characteristic wavelengths of similar dimensions to the characteristic length scale of the atomic structure, all the backscattered particle's waves can add up coherently such that the wave is reflected back completely, as if having hit a mirror. Similarly, for an optical bandgap where light is scattered by periodic contrasts of refractive indices, an interaction directly analogous to the electrons of the semiconductor case occurs for periodic structures of varying refractive indices with sufficient contrast. Hence, photons in PhCs have analogies of band structures in electronic crystals, where a full optical bandgap is formed, when there is perfect reflection occurring over a range of wavelengths for any wavevectors.

Yet, as intuitive as this analogous description of the PhC effect, it was initially not easy for scientists to correctly predict which type of structure would give rise to an effective optical bandgap. In the beginning, there was no rigorous numerical method for the determination of band structures. Added to this was the erroneous approach to use scalar instead of vector calculations, which prevented derivations of the right solution for PBG structures. Although analytical formulations were often followed directly by experiments, PBG scientists worked with the belief that such a man-made material was possible for many years without being able to demonstrate any prototype until four years after the initial proposals. Since then, much effort has been invested into the fabrication of PBG and the field has been under intense international research. The major developments in PBG technology can be summarized as given in Table 1.1.

Table 1.1 The milestones of major developments in photonic bandgap technology.

Year	Description
1987	Inhibited spontaneous emission for lasers of higher efficiency proposed [1]
1987	Photon-atom bound states for localization of light proposed [2]
1990	Macroporous silicon etching method formulated, later adapted for PBG [84]
1991	First PBG structure demonstrated – the “Yablonovite” [3]
1992	PBG found for FCC structures and simple-square configurations [3]
1994	“Woodpile” PBG structures for microwave wavelengths fabricated [6]
1995	Advent of the self-assembly fabrication method [6]
1996	Method for anisotropic plasma etch; inductive coupled plasma etch [154]
1997	Method of calculation for two-dimensional PBG formulated [3]
1998	First application of self-assembly inverse opal structure for PBG [6]
1999	PBG fibers (PCFs) proposed and fabrication method demonstrated [5]
1999	PBG incorporation into semiconductor laser demonstrated [49]
1999	Tunable PBG proposed with liquid crystal infiltrated [6]
1999	Demonstrated line defect waveguide with bends in slab photonic crystal [9]
2001	Proposal for square spiral 3D PBG fabrication [7]
2001	Proposal and development for all optical transistor with PBG [22]
2002	Band edge tuning of two dimensional PBG via optical injection [104]
2004	Demonstration of ultra high quality factor photonic crystal microcavity [70]
2006	Structure for “invisibility” at radio frequency demonstrated [155]

While the applications found for PhCs were broad and innumerable, the more prominent examples would include the resonant microcavities for lasers where PBG built from photo-emissive materials, such as III-V semiconductors and glasses doped with rare-earth atoms, can be used to make narrow line-width lasers that could potentially be integrated with other components in an optical-communications system. A second application of PBG to active optical devices lies in the reflectors of LEDs, which are used extensively in optical-communication systems. PBG mirrors reflect a selected wavelength of light from any angle with high efficiency and hence can be integrated within the photo-emissive layer to create a LED that emits light at a specific wavelength and direction with high efficiency.

Conversely, passive components such as optical filters and channel- add or drop multiplexes fabricated from passive materials, such as silicon dioxide and silicon

material could also make use of PBG to create filters that transmit only very narrow ranges of wavelengths. Such filters could be used to select a wavelength channel in a dense wavelength division multiplexing (DWDM) communications system. Another important passive PhC application is the integrated waveguide structure of small-scale optical interconnects, previously inhibited in miniaturization by the limits of bend radii in legacy low index contrast, index-assisted guiding waveguide systems. Using PBG, it is possible to form a narrow-channel waveguide within a PhC by creating ‘defects’ in an otherwise regular pattern such that light is confined within the line of ‘defects’ for wavelengths that lie within the bandgap of the surrounding PhC structure.

Besides its use in active and passive optical devices, PBG effects can also be incorporated into optical fibers, which is the backbone technology enabling high speed broadband and long haul transmission of optical signals in the ‘world-wide-web’. Instead of having a core with slightly higher refractive index as with conventional fibers, PCFs may have the central solid glass core removed to form a long air cavity, where light is guided along the low refractive-index air core by the PBG confinement effect. Since light is not actually guided by any material but in air, very high-power laser signals could potentially be transmitted along the fiber without damaging it. Other applications of air-core PhC fibers may also make use of the absence of material in the guiding core to avoid material dispersion effects.

The more recent developments in PBG technology had been focused on the tunable PhC effects; which had been proposed mainly for functions of developing dynamic functionality, compensation of fabrication deviations or modulation of signals etc. One of the first proposals for implementation of tunable PhC performance was based on PBG fabricated from a suspension of polymer spheres in a hydrogel

film or in shape-tunable structures. In the former, a synthetic polymer that absorbs water such as the hydrogel can have shrinking or expanding qualities that adjust the wavelength of the bandgap. The issue with such proposal lies within the implementation. Take for instance, colloidal structures, though easy to make, is not easily incorporated within an active hetero-structure of an LED or in other devices. Alternative proposals for tunable two-dimensional (2D) PhC circuits to achieve modulation of device characteristics include the use of thermo-optic effects, liquid crystal tuning, mechanical manipulations, material non-linearity, and also electrical and optical injection mechanisms. Of which, the slower modulation methods, such as the thermo-optical and mechanical tuning mechanisms can be used for state-changing applications, whilst the faster modulation methods, such as the optically controlled mechanisms of absorption and non-linearity induced material index changes can be used for real-time switching in dynamic network applications etc.

To implement these types of devices, PhCs structures with varying ability to control and prohibit the propagation of light within the PBG frequencies may be designed. Although only PhCs with periodicity in all three-dimensions have complete bandgaps, 2D PhC structures also possess many similar properties at much reduced complexity. In 2D PhCs, ‘defects’ positioned within a periodic lattice introduce light states into the photonic bandgaps (at frequencies otherwise prohibited by the bulk lattice), allowing EM radiation at these frequencies to be guided in-plane [9] along such ‘defect waveguides’. Whilst experimental confirmation of such theoretical waveguides was first demonstrated in the millimeter-wavelengths using PhC structures in a square lattice array of long alumina rods, optical waveguiding experiments were subsequently almost always carried out in slabs - with index guiding in the out-of-plane direction - since without this additional mechanism, 2D

PhC rod structures of insufficient aspect ratios suffer from prohibitive leakage due to lack of confinement in the out-of-plane direction. Yet, the design of innovative PhC devices (such as water contact angles controllers [12], table-top accelerators [13] etc) using the square lattice rod-type PhC structure were not abated [14-16].

Although square lattice rod-type PhC slabs were successfully demonstrated only recently, successful demonstration of PBG waveguiding in air without slab-type index assisted confinement in the vertical direction - along the lengths of the rods - has not been repeated in the optical communication wavelengths since the pioneering microwave experiments with long alumina rods. This progress has been hindered due to many short wavelength challenges. First, patterning of optical length-scale PhC structures with required ‘defects’ cannot be easily achieved without advanced processing techniques [25-26]. Second, unlike at longer operating wavelengths [27], the deep etch of such super-dense high aspect ratio (HAR) PhC rods of only 115 nm radii is non-trivial [28-29]. Since PhC structures without sufficiently small features and HARs are insensitive to the shorter optical communication wavelengths and suffer prohibitively high losses respectively, the fabrication of PBG waveguiding devices working at the optical communication wavelengths had been a critical issue.

Early fabrication efforts for PBG structures focused on drilling arrays of tilted holes so that the remaining structure consisted of materials with periodic variation in permittivity that corresponded to the different bandgap inducing structures. Whilst such methods had been demonstrated to exhibit complete bandgaps, it was difficult to fabricate and not readily amenable to mass fabrication. Hence, other methods were sought after. Two methods emerged eventually with the first being that of natural assembly. In this technique, the natural process by which gemstone opals were formed using micro-spheres positioned periodically into a three-dimensional (3D)

lattice - was emulated to obtain a mold of micro spheres in which deposited materials between these micro-spheres form a periodic array. Upon completion and formation of the deposited structure, the micro-spheres were etched away to leave a periodic PBG lattice crystal structure. Although self-assembly provides a simple, fast and large-scale method, its major drawbacks are the limited number of crystal structures that can be formed, the purity with which they can be formed, and the difficulty of efficiently incorporating specifically designed defects.

On the other hand, with use of the traditional electronic integrated circuit foundry processes - the expensive, precise and painstaking step-by-step fabrication processes already widely used by the semiconductor industry - the calculated construction of PhC structures, 'defects' and 'defect networks' may be enabled. Till date, there has been extensive work done with such approaches, namely in the area of direct electron beam (e-beam) write, laser interferometric and holographic techniques for patterning; and macroporous silicon etch, inductive coupled plasma (ICP) etch, focus ion beam (FIB) etch, chemically assisted ion beam etching (CAIBE) etc, for etching. Despite the tremendous range of techniques in fabrication efforts, none has been well received enough for dominant adaptation mainly due to limiting technology, exclusive machineries and high cost factors, of which these key attributes are summarized and tabulated in Table 1.2.

Table 1.2 Mainstream sub-micron fabrication of photonic bandgap crystals

Method	Advantages	Limitations
Electron beam	Flexible & allows definition of arbitrary patterns	Inefficient for extended structures due to sequential writing characteristic
Laser interferometric & holographic	Suitable for extended three dimensional periodic structures with high efficiency	Only regular patterns possible with difficulty in 'defects' definitions
Macroporous Silicon etch	Highest aspect ratio achievable	Only large uniform arrays in homogeneous Si <100> orientation & exact n-type doping
Inductive coupled plasma	Process independent on wafer doping level. Good mask selectivity.	Etch only in direction of RF bias
Electron cyclotron resonance	Low temperature etch for reduced tradeoffs in etch rates, selectivity & side etch profiles	Resonant technique - no independent control of ion energy, poor uniformity over large areas
Focused ion beam	Etch in any direction without mask	Small spot size pose similar efficiency problem as e-beam described above
Chemical assisted ion beam	Better performance than physical FIB with pre-structured pores	Limited by resistance of mask and ion beam deflection on side walls

In summary, the advent of PhC technology has brought about unprecedented control of light with suitable design of device properties. Through nano-fabrication techniques, it is possible to make use of the ubiquitous material of choice for integrated circuits – silicon - in application to photonic integrated circuits.

1.2 Objectives

Motivations for this research arise in view of the potential improvements, which may be made possible in the important area of integrated photonic circuits, through the development of PhC technology, which inherent advantages are: (i) its ability to tailor the dispersion properties of light; and also (ii) its sub-wavelength scale lattice dimensions which allows for miniaturization of device sizes. Currently, many optical circuit elements make use of the 'total internal reflection (TIR)' mechanism for optical confinement and guidance. This method is excellent in optical fibers used

extensively in long haul optical communication applications. However, in photonic integrated circuits, such as silica waveguides, the devices which make use of such a system are typically limited in terms of miniaturization potential, due to the large critical bend-radii requirement - which prevents tight bends with sharp angles (required for small circuit layouts) since prohibitively high losses results. Such constraint however is circumvented when these waveguides are made from high index contrast (HIC) material systems instead, which typically make use of material with high refractive index such as silicon ($n_{\text{si}} \sim 3.4$) etc, in contrast against air ($n_{\text{air}} \sim 1$) – so that their effective refractive index contrast may be high (~ 2.4) ; a requirement that needs to be satisfied in PhC systems also (since photonic bandgaps do not open unless there is sufficient contrast in refractive index between the lattice building blocks). Hence, due to their large index contrast, the confinement of the optical waveguides can be tighter, resulting in smaller critical bend radii, and therefore allowing for smaller circuit sizes since connections may then be routed around sharper bends. In this way, when waveguides of higher index is used within a lattice of PhC array, both index guiding and bandgap guiding are employed for waveguiding and confinement.

Hence, the objectives of this study are to develop theoretically sound PhC device designs, applicable for nano-photonic integrated circuits; through appropriate polarization modes analysis, physical models and also effective frequency and time domain simulations. In the implementation front, PhCs using silicon processing technology for application in the optical communication regime (inclusive of both theoretical investigations and experimental implementations) are to be realized. The progression of subject matter encompasses the theory of designing large complete PBGs and also the design of miniature size effective photonic circuit elements of functionalities amenable to large scale integration. This is followed through with the

nano-fabrication aspects (of sub-wavelength lithography and super dense reactive ion etching techniques), which in turn enables high density integration and also demonstrations of innovative light-tuned-light PhC properties with especially designed macro-to-micro coupling schemes and pump-probe laser source and detection set-ups.

First, design of large complete optical bandgaps (in terms of designed overlaps in the orthogonal transverse-electric and transverse-magnetic polarizations' bandgap frequencies) necessary to facilitate understanding of the PBG effect as well as its improvement to integrated photonic PhC device properties (which pivots on the span of the bandgap frequencies) are investigated. In the simulation of PhC bandgap devices, effective boundary conditions and also suitable frequency and time domain simulation parameters need to be determined in order for meaningful PhC device analysis. The PhC structures (to be studied specifically) include microcavities; embedded line defects and also intersecting waveguides configurations with resonators embedded. The system in which such structures are to be advantageously implemented has been identified to be in the rod-type configuration of 2D PhCs, in single crystal silicon for PBG waveguiding demonstration - in both single line and crossing PhC waveguides.

While single-line 'defect' PhC waveguides are important for sub-micrometer length-scale optical waveguiding; crossing PhC waveguides are important for forming large angle crossings between the former. Similar to the PhC waveguides, the crossing configuration also allows for tailored dispersion properties. At the same time, these PhC optical intersections also have compact working areas (as small as $5 \times 5 \text{ } \mu\text{m}^2$) and can be applied in optical integrated circuits for interconnections, an important component of photonic integrated circuits as they allow for interaction of

many waveguides within a small footprint. However, the disadvantage of these small-size PhC devices is that, due to the sub-wavelength scale of such crossings, optical input waves undergo diffraction at the intersections, resulting in high crosstalk and reflection levels, lowering effective transmissions. Such obstacle to device performance may be removed for these PhC optical intersections by the inclusion of a center cavity rod, so that low crosstalk and reflection levels can be obtained with high transmission. In which case, although the width of PBG waveguides are less than the wavelengths of light used, diffraction at such microscopic optical intersections may be circumvented.

To realize such PhC optical intersections in experiments, PhC optical intersection devices need to be fabricated with high resolution and also aspect ratio in single crystal silicon wafers. Monolithic integration of large scale optical testing structures (OTSs) are also necessary in order to facilitate experiments carried out to characterize any of the fabricated PhC devices. In this way, first demonstrations of sub-micrometer scale PhC optical intersection devices sensitive to the canonical optical communication wavelengths centered at 1550 nm may be achieved with varying resonator quality (Q-) factors – with dynamically tunable properties based on light modulations.

1.3 Major Contribution of the Thesis

The major contributions of this PhD thesis are in the various aspects of the theory, design, fabrication and experimental demonstration of the optical PBG phenomenon. Specifically, PhCs optical intersections (which focus on the properties of ‘line-defect’ waveguides with embedded resonator cavities) were the focus of this work as detailed below:

- (i) A novel square lattice type 2D PBG structure was designed based on the transverse electric (TE) and transverse magnetic (TM) bandgap model, where each of these respective polarizations have specially designed large bandgaps spanning a maximum range of normalized frequency, which at the same time have coinciding center bandgap frequencies - to ensure largest complete overlapping bandgaps. (See Chapter 3).
- (ii) Improved configurations of embedded microcavities system were proposed and analyzed in 'single-line defect' PhC waveguides to incorporate high Q-factors and also multiple resonances. Tunability for device operation is designed with detailed simulations for functionalities and device performance so that light-tuned-light operations were realized. (See Chapter 3).
- (iii) Nano-fabrication of PBG was realized with deep ultra-violet (DUV) lithography, without expensive phase shift masking (PSM) to obtain highly-dense PhC rods array with sub-100 nm reduced radii PhC defect rods. An optical proximity error (OPE) correcting model was developed to yield optical proximity corrected structures, with corrected average measured deviations below three percent. Also, record HAR etching for 2D PhC rod-type structures at such sub-micrometer length-scale and high density was obtained using inductive-coupled-plasma (ICP) deep reactive ion etching (DRIE) method with integration to both large optical testing structures and the micrometer-scale PhC integrated optical intersection devices (See Chapter 4).
- (iv) The implementation of optical modulation via micrometer-scale PhC optical intersections was designed, with the physical and application aspects of ultra-fast free carriers' generation presented in detail - with respect to the PhC optical intersections made with varying Q-factors (See Chapter 5).

- (v) PBG characterization measurement results for rod-type 2D PhC without index guiding, (which have not been repeated at the optical wavelengths since the first pioneering PBG's microwave experiments) have been obtained. Based on this, bending and propagation loss characteristics of PhC rod-type devices were successfully measured at the optical communication wavelengths, to obtain new bench marks not currently available in literature (See Chapter 6).
- (vi) All-optical switching has been achieved using an experimental set-up designed specifically for this purpose. Through successful localization of free carriers' introduced via optical injection, the PhC devices were modulated so that dynamic control may be implemented in the native optical form. The control and signals may be further pulsed so that switching speeds are limited only at the picoseconds level due to the relaxation times of the carriers (See Chapter 6).

1.4 Organization of the Thesis

This thesis is structured into seven chapters. An introduction to the thesis, which covers the motivation, objective, and major contributions, is presented in this current Chapter. The motivation section explains why and how this research was carried out. The objective section states the main focus of this work whilst the contribution section lists the resulting findings and innovations.

In Chapter 2, the relevant literature for PhC devices, fabrication and also PhC optical experiments were reviewed. These important background works provides the direction and impetus for this research, and also lays the technological foundation on which the works of this thesis were built upon.

In Chapter 3, the theory and design of PhC bandgap devices, beginning from the most basic one-dimensional (1D) PBG, followed by the design of a large optimized 2D PhC is presented. Next, the analysis and design of embedded PhC micro-resonators in single-line; cascaded resonators; and also crossing waveguides optical intersection configurations are presented before the chapter is rounded up with the design of OTSs for monolithic implementation with the various PhC devices.

In Chapter 4, the fabrication tour-de-force required to realize PhC devices operational at the telecommunication wavelengths centered at 1550 nm is presented. The design of process flow necessary for realizing disparate exposure areas and etch depths of the macro-size fiber grooves with the micro-size PhC integrated circuit devices were explained in technicalities. The details of the lithographic and multiplexed reactive ion etch processes are then presented with their nuances.

Chapter 5 presents the principles of PhC optical modulations, especially the physical background of such phenomenon, including the electrons-holes model of such free carriers' plasma generation process, the saturation conditions, together with the mechanisms for scattering, diffusion and recombination of carriers etc. Following which, the design of the PhC devices to enable optical modulation by free carriers' generation was presented - with differentiation between the plasma carriers' and thermo-optics effect.

Chapter 6 presents the experimental techniques required for experimental measurements of the fabricated PhC devices, including the design of set-up and also methods of measurements. The characterizations of the miniature size PhC devices in both HAR and slab configurations were carried out in both static and dynamic experiment conditions, with discussions on the obtained results - based on necessary comparisons against simulated predictions.

Finally, Chapter 7 concludes the major findings of this doctorate research thesis, and provides recommendations for further works in future studies.

CHAPTER 2

LITERATURE SURVEY

This chapter presents a review of PhCs technologies, as foundation to this thesis. A general survey on various aspects of the quintessential photonic circuit element, the PhC microcavities is first presented, including the basis principles; research milestones; current problems and possible opportunities for different configurations of PhCs resonators with various types of ‘line defect’ waveguides. Moving on, the focus will then be placed on the review of PhCs fabrication tour-de-force techniques developed thus far; which have helped realized in recent years, demonstrations of PBG performances in many innovative designs, and also observations of much intriguing physical phenomenon for further investigations. Specifically, the fabrication process modules that concern the areas of deep sub-micrometer resolution patterning and etching of highly dense PhC arrays are delved into. For each of these modules, the pros and cons of the various processes available are discussed and compared. Progressing further, some of the recent developments and endeavors of the PBG research community in the area of PhC experimental demonstrations techniques are then reviewed. Here, the techniques for coupling of micro-scale PhC devices to macro-scale optical fibers, sources and detectors etc are first looked into. Following which, the 2D rod-type PhC photonic integrated circuits, classified broadly into the categories of HAR and slab type configurations are then differentiated and presented according to their experimental demonstrations. Such

ground works therefore lays the foundation for the contributions of this thesis in the categories of design, fabrication and experiment.

2.1 Microcavities Principles and Schemes

Microcavities refer to structures capable of confining light in small volumes by the action of resonant recirculation. Devices based on optical microcavities are indispensable for a wide range of applications, for example in semiconductor lasers; read/ write heads in optical disc players; and also direction specific quantum optical emission devices [30]. However, photonic microcavities have been identified as one of the most elusive for design and implementation [31] since design rules developed for its counterparts in the physical, sound or microwave domains are not applicable in the design of optical microcavities. A theoretically perfect optical microcavity should be capable of confining light indefinitely without loss and have resonant frequencies at precise values. The criteria for practical designs of such optical resonant microcavities is described by the microcavity volume; the quality (Q)-factor – proportional to the confinement time in units of the optical period – where the ideal condition is described by a cavity with infinite Q-factor and cavity finesse (which measures the quality of cavity confinement without inclusion of propagation effects within the cavity that the Q-factor includes).

Such optical microcavity structures are greatly diverse, including strong-coupling cavity quantum electrodynamics (QED) [32, 40]; enhancement and suppression of spontaneous emission [33]; novel sources [34]; dynamic filters in optical communication [35]; commercial semiconductor lasers [36]; soliton effects [37]; chaos [38] and effects in quantum-well microcavities [39]. To achieve ever

increasing strong-coupling effects has therefore been an impetus for research into ultrahigh Q-factor, small-volume resonant microcavities [41, 42]. Following this, microcavities enhancement and suppression of spontaneous emission through the Purcell effect [43] makes use of local enhancement in the continuum density of modes (DM) function and quasi-mode of the microcavity resonator to enhance atomic decay rates and directionality of emission. Hence, weak coupling that results from dissipation, overwhelming the fundamental Rabi dynamic is prevented via use of such microcavities. Especially, with PhC proposed for spontaneous emission suppression, PhC microcavities Purcell enhancement was therefore expectedly much researched [44]. At the same time, applications of microcavities for novel sources such as microcavities droplets [45]; silica [46], semiconductors disks [47]; vertical cavities [48]; and PhC cavity source [49] has been demonstrated for lasing. Here, small cavity volumes and high Q-factors have allowed the obtainment of sub-microwatt optical pump thresholds in microspheres [50] and microamp-scale current thresholds in semiconductor lasers [51]. Such developments have further taken on increased importance with the emerging prominence of multi-wavelength communication systems, whereby new filtering functionalities for future systems are anticipated. For such dynamic microcavity filters, the resonant transfer of optical power between two waveguides has been the structure most studied [52, 53]. The figures of merit for microcavities suitable for these applications are listed as in Table 2.1.

Table 2.1 Figures of merit for microcavity design applications.

Application	Figure of merit*
Spontaneous emission rate enhancement via Purcell effect	Maximum Q/V
Nonlinear optical effects	Maximum Q^2/V
Strong coupling of cavity QED	Maximum ratios of $Q/V^{0.5}$ and $1/V^{0.5}$

*Q: quality factor; V: mode volume.

2.1.1 Devices in Application of the Fabry-Perot Configuration

These wide ranges of microcavities applications may be sorted out in terms of confinement mechanisms. Here, the three main categories would be the Fabry-Perot (FP), whispering gallery and the PhC mechanisms. First, in the FP configuration, micropost (or micropillar) [54] cavities employ 1D Bragg mirrors [55] for cavity confinement and dielectric-air guiding for lateral (in-plane) confinement. Used in application of the Purcell enhancement effect [56] to trigger single-photon sources, the micropost FP configuration offers small cavity volume and relatively high Q-factors, with emission patterns that are well suited for coupling, and manipulation of emitted photons even with optical fibers and can incorporate quasi-atomic, quantum dots as emitters. In such FP configurations whereby the coupling energy exceeds the thermal energy of an ultra-cold atom, the atomic center of mass motion can be altered by the interaction with the vacuum cavity mode such that atomic motions can be entrained by QED coupling. In this way, very high Q-factor may be achieved by such FP bulk optical cavities [57].

2.1.2 Whispering Gallery Configurations of Microcavities

Second, in the whispering gallery category, two of the common configurations include the micro-disks [58] and the add/drop filters [59]. In the latter, a most common configuration of microcavities add/drop filters involve two buried waveguides vertically coupled to a disk whispering gallery resonator [47]. Such a structure can be fabricated by first creating optical waveguides through lithography and etching, then wafer bonding an initially mechanically separated second wafer containing layers that ultimately become the micro-resonator.

In such structures, critical gaps between the waveguides and the resonator disk control the field-coupling determined by thin-film crystal growth methods as opposed to lithography and etching as is the case in side-coupled structures. Typically, a drop frequency is designed to be resonant with a mode of the disk and is subsequently coupled through to the waveguide on the opposite side of the disk resonator while an add frequency is non-resonant. Such configurations of microcavities may be made dynamic by inclusion of electrically controllable loss or refractive layers within the resonator. To improve the Q-factors of such whispering gallery microcavities, excellent surface finish is critical [61]. This requirement can be satisfied by fabricating the microspheres and micro-toroid whispering galleries through a molten state so that only surface roughness of not more than a few nanometers exists [62].

2.1.3 Photonic Crystal Implementations

Third, the final confinement method in microcavities by PhC mechanisms is relatively new - compared to the previous two mechanisms of FP and whispering gallery. Yet, due to its potential for ultra small volume confinement [63] with high Q-

factors, PhC microcavity research has become very intense worldwide [64 - 66]. A typical PhC microcavity is formed by dry etching periodic arrays of holes in a membrane, with a single hole left intentionally un-etched (to create a ‘defect’ in the array and therefore a defect mode in the optical spectrum).

The defect mode in the PhC is confined to the interior of the array by Bragg reflection in the plane of periodicity and conventional waveguiding in the vertical direction out of plane due to the higher refractive index of the membrane material. Since initial reports of PhC microcavities [67-69] with Q-factor one order of magnitude smaller than the first very high Q-factor PhC microcavity of 600,000; the latest design of PhC microcavity with Gaussian and sinc-type cavity modes derived by inverse problem approach has derived ultra high Q-factor PhC microcavities with Q-factor of more than a million [70]. A summary of the typical properties for each of these microcavities confinement methods are presented in Table 2.2.

Table 2.2 Typical properties of the various microcavities confinement mechanisms.

Confinement properties*	Fabry-Perot	Whispering gallery	Photonic crystal
Conventional configurations	Micropost, micropillars $Q \sim 2 \times 10^3$ $V \sim 5(\lambda/n)^3$	Microdisk $Q \sim 1.2 \times 10^4$ $V \sim 6(\lambda/n)^3$ Add/ drop filters $Q \sim 7 \times 10^3 - 1.3 \times 10^5$	Simple hole/ line defect cavities $Q \sim 1.3 \times 10^4$ $V \sim 1.2(\lambda/n)^3$
Optimized configurations	Fabry-Perot Bulk optical cavity $F \sim 4.8 \times 10^5$ $V \sim 1.7 \times 10^3 \text{ um}^3$	Microsphere $Q \sim 8 \times 10^9$ $V \sim 3 \times 10^3 \text{ um}^3$ Microtoroid $Q \sim 1 \times 10^8$	Inversely derived line defect Gaussian/ sinc- type photonic crystal cavity $Q \sim 4 \times 10^6$ $V \sim 1.0(\lambda/n)^3$

*Q: quality factor; V: mode volume; F: finesse of cavity.

From Table 2.2, it is clear that PhC presents outstanding advantage in terms of the ultra small microcavity volume achievable. In terms of achieving ultra-high Q-

factor however, simplicity in PhC structures does not suffice. Although theoretical ideal confinement should arise based on 3D PhC with perfect bandgaps, 2D PhC of finite depth, employing distributed Bragg reflection (DBR) are much more compatible with existing PICs implementations and have also been proven to be suitable for attainment of ultra-high Q-factor [31]. Here, the main challenge is the minimization of out-of-plane loss by imperfect TIR, which becomes progressively severe for shrinking microcavity volume designs. Further, as with all other confinement mechanisms, the attainment of high Q-factor and small mode volume requires much in terms of fabrication technological developments, which will be presented in the following section.

2.2 Fabrication Tour de Force for Optical Photonic Crystal

PhC fabrication had been fraught with many challenges since its nascent beginnings [71]. These arise mainly due to the small size of PhC needed in order to work at the optical wavelengths. First, patterning of optical length-scale PhC structures with required ‘defects’ cannot be achieved easily without advance processing techniques. Second, unlike at longer operating wavelengths, the deep etch of such super-dense HAR PhC rods without slab type confinement is non trivial. Since rod-type PhC structures without sufficiently small features and HARs are insensitive to the shorter optical wavelengths and suffer prohibitively high losses respectively, the fabrication of PBG waveguiding devices working at the optical communication wavelengths had been a critical issue. To fabricate PhC devices operating at optical communication wavelengths centered about 1550 nm, the corresponding critical dimensions (CDs) required are in the hundred nanometers range. This requires not only the reduction of the optical lithographic wavelength

from 365 nm I-line to 248 nm DUV, but also the ability of such DUV lithographic scanner systems to work at the sub-lithographic wavelength order. At the same time, because the ultra-small CDs also shrink the process windows of all the other processing modules - especially in dimension sensitive reactions such as etching - advance fabrication techniques for each of these fabrication modules need to be developed. Further, the challenges of integrating structures of disparate dimensions also requires much work, as with the other requirements of minimized etch surface roughness; lithographic resolution limits etc.

2.2.1 Deep Sub-Micrometer Patterning

In the area of patterning, the definition of large periodic PhC arrays of rods/holes with CDs a mere few hundred of nanometers is not possible without the use of advance patterning tools such as electron beam lithography (EBL) [72]; zone-plate-array lithography (ZPAL) [73]; focused ion beam lithography (FIBL) [74]; laser interferometric lithography (LIL) [75]; holographic lithography (HL) [76] or deep-submicron wavelength optical lithography (OL) [77], nano-imprint lithography (NIL) [150], micro-contact printing [151], scanning-probe lithography (SPL) [152] and dip-pen nanolithography (DPN) [153] etc. While EBL, FIBL, DPN, and SPL are flexible, allowing definition of arbitrary patterns, they are sequential processes that can be inefficient for definition of large area arrays of PhCs. In particular, EBL also pose additional stitching error implications. On the other hand, while LIL and HL are suitable for patterning with high efficiency, extended 3D periodic structures, they are suitable mainly for regular patterns such that there are difficulties in patterning arbitrary “defect structures” where necessary. Here, while ZPAL, NIL and micro-contact printing are not constrained in this way, such systems are still not easily

available and are also typically not compatible with the standard complementary metal oxide semiconductor (CMOS) standard (adopted by most fabrication plants and hence not portable to these clean-rooms with operations limited to CMOS compatible processes).

Hence, OL is a promising technique for 2D PhC definition due to its batch processing nature and also its ability to incorporate flexibility in the patterning of arbitrary defects. Further, as the workhorse of silicon circuits, it is the most amenable to large scale manufacturing, important for the cost-control factor. However, the feature size required of PhC applicable to the communication wavelengths has CD of less than the DUV wavelength of Krypton Fluoride (KrF) lithographic laser systems. Such sub-lithographic wavelength OL is diffraction limited and special efforts are needed to enable successful patterning. As such, PhC lithography requires not only the reduction of OL wavelength from 365 nm I-line to 248 nm (DUV wavelength) but also the use of resolution enhancement techniques (RETs) since the reduction of lithography proportional constants for improvement of resolutions leads to problems of OPEs etc - affecting the performance of size sensitive PhC device structures adversely. This is especially so since the DUV OL system in use has numerical aperture (NA) of less than 0.7 and partial coherence of not less than 0.30.

Previously, OL at the DUV wavelength was investigated to realize hole-type PhC [25] with accompanying photonic wires. To make such hole-type PhC, silicon-on-insulator (SOI) wafers with silicon device thickness of 220 nm and buried oxide layer thickness of 1 μm was used. Since different CD structures such as the photonic wire and PhC holes array would likely have dissimilar exposure dosage, they are preferably printed with optimized lithographic energies. Yet, accurate alignment would be best achieved by printing such structures in a single step. To enable single

exposure lithography for different CD structures, mask bias was applied to the isolated photonic wires. An example of the optimal dose for a triangular lattice of PhC holes with 300 nm diameter, spaced 500 nm apart in lattice pitch is 25.6 mJ/cm^2 . At this energy, a photonic wire drawn to be 500 nm would be printed as 450 nm wide. Hence, a 50 nm bias was applied at the design stage. Based on such works, DUV lithography was used to demonstrate functional photonic wire components like racetrack resonators, and also hole-type PhC waveguides. However, as such reference works deal with interconnected PhC holes structures, as opposed to the disconnected rod-type structures, fundamental differences in lithographic characteristic have to be taken into consideration since the OL characteristics for line and space type patterns are considerably dissimilar. Such differences similarly extend to other process modules, especially apparent in the etching processes.

2.2.2 Etching of Super Dense Arrays of Photonic Crystal

Similar to the situation of lithography, deep etching of small PhC CD openings involves many challenges. First, due to the reason that it is not a typical process (unlike that of hole-type PhCs, which are like vias of integrated electronic circuits), there are relatively fewer studies that can be drawn on for references. Second, the choice of etching method is limited for PhC devices due to the reason that precisely designed defect structures over a potentially large area, are necessary for fulfillment of unique device operation properties [83] - take for instance the removal of a path of rods/holes for waveguiding and the strategic placement of a tunneling defect for reduction of crosstalk at an intersection. Although macroporous silicon etching [84] has been demonstrated to be capable of achieving HAR etch with high selectivity, it makes demand on the doping levels of the silicon wafer and also faces

challenge in achieving precise control of etched areas due to mask effects [85]. FIB etch can be employed to perform etching in any direction without mask [86], but poses a similar efficiency problem as discussed before for EBL. CAIBE with pre-structured pores, though performs better than physical FIB, is limited by resistance of etch mask and ion beam deflection on sidewalls [87]. Therefore, electron cyclotron resonance (ECR) [88] and ICP [89] etch may be used for etching in the direction perpendicular to wafer surface - with lower requirement in resistance of etch mask and wafer doping levels. However, due to the reason that ECR is a resonant technique, control parameters cannot be fully independent. At the same time, all time-multiplexed etch processes suffer from the formation of wave-like surface undulations – scallops – that translate to surface roughness detrimental to optical performances.

In addition, existences of sidewall angles that are typically negligible for larger dimension structures, are typically sufficient to cause total etch failures in the deep submicron length scale regime. Take for instance (see Fig. 2.1 for illustration), with a microelectromechanical (MEMS) cantilever of 2 μm thickness, 10 μm depth and arbitrarily long length, an etching angle of 0.5 degree would result in an undercut of 87 nm on each facet. Therefore, the resulting width at the bottom of the beam would be 1.825 μm . However, for the case of a 200 nm diameter PhC rod; the undercut all-round would leave for a similar etching depth of 10 μm , a bottom diameter of only 23 nm. Such a weak base tends to topple the rod, causing catastrophic etching failure.

Further, line edge roughness [90], etch-lag [91], and notching effects [92], (which have typical length scales ranging from hundreds of nanometers to a few micrometers) become critical to the successful fabrication of the hundred nanometers-

scale PhC CD structures. At the same time, the other processes of electrode metallization [93], post processing buried oxide release [94] (for air bridge PhC structures etc) also constitute challenges arising not only from the requirement of material compatibility [95], and contamination control [96], but also from etch aspect ratio specifications [97] and movable structures release stiction issues [98, 99]. These issues will be addressed in detail, in Section 3 of Chapter 4.

Fig. 2.1 Illustration of non-vertical etch phenomenon for a 0.5-degree etch angle, at a similar etch depth of 10 μm, for a (a) 2 μm-wide MEMS cantilever, and (b) a 200 nm diameter photonic crystal rod.

Hence, the nano-fabrication of PhC at the sub-micrometer length scale requires development in many of the process modules and is critical to the demonstration of optical wavelengths sensitive PhC integrated circuit devices.

2.3 Experiments with Two-Dimensional Photonic Crystal Circuits

Of the two main types of 2D PhCs, the hole-type structure had been demonstrated much more extensively than the rod-type PhC [6]. While the hole-type PhC was found to have the largest bandgaps in a triangular/ hexagonal lattice structure (for the mode where electric field propagation is polarized in-plane), the latter rod-type PhC typically uses a square lattice structure for its largest bandgap (for the mode where electric field propagation is polarized out-of-plane). Further, the hole-type PhC typically requires a thinner slab for a larger bandgap than the rod-type PhC [115].

Thus, the square lattice rod-type PhC which requires a higher aspect ratio fabrication process is relatively more difficult to realize at the deep sub-micrometer length-scale. Despite so, the square lattice rod-type PhC structure remains a very attractive design due to its: (i) potential for PBG guiding; (ii) unique disconnected topology; and (iii) its four-fold symmetry (also known as C_{4v} symmetry). These properties allow for design of applications [18] with high symmetry defects of nano-cavities [19], linear waveguides [20] etc with imposed cavity modes symmetry conditions that facilitate intuitive design [21] and high performances [22]. Hence, many rod-type innovative PhC devices have been proposed and demonstrated [12-14].

For such 2D PhC devices, the key for experimental demonstrations often lie in the successful coupling between the sub-micrometer scale PhC integrated circuit structures and the macro-scale discrete optical components such as the laser sources, optical fibers, photo-detectors etc with dimensions of more than a hundred micrometers. To do so, many different methods have been proposed for the coupling

of PhC structures for optical measurements, focused mainly in the area of various waveguide coupling schemes.

2.3.1 Photonic Crystal Device with Waveguide Coupling

To study the coupling techniques for PhCs, it is useful to first identify that integrated single-mode waveguides (which are able to convert the spot size of a propagating optical field and consequently provide low-loss large alignment tolerance coupling between semiconductor waveguide devices and flat end fibers) are becoming essential for future PhC integrated circuits [123]. This can be attributed to the fact that while PhC devices generally make use of tightly confined waveguides with mode field diameters of at most a few micrometers, standard single-mode fibers (SMFs) have a relatively larger circular mode field diameter of about 10 μm . Hence, the simple and efficient butt coupling between integrated PhC devices and SMF ribbon arrays will particularly require an efficient mode conversion medium. This is useful for PhC devices (even though PBG light guiding has no parallel in traditional dielectric waveguides, which typically relies on TIR to confine light) since the mode size conversions are carried out adiabatically.

Unlike TIR in low index contrast waveguides, which is effective only for specific directions of propagation, and needs a physical structure size much larger than the optical wavelength to operate effectively; PhC devices with HIC are slated to improve traditional low index contrast TIR waveguiding drastically due to many of its unique abilities: such as potential for free space confinement; large dispersions and also control over a wide range group velocities that can be designed for. Line defect waveguides with air cladding in PhC devices can guide optical signals supported by PhC defect modes falling below the light line, defined as

$$\omega = \frac{ck}{n}, \quad (2.1)$$

where ω is frequency, k is wavevector, c is the speed of light, and n is refractive index. Since modes above the light line are leaky due to overlapping with radiation modes in the cladding, PBG modes below the light line are truly guided and have no theoretical propagation loss. At the same, since photons fundamentally do not interact efficiently with materials or with other photons (making it generally very difficult to control or confine the paths of photons), and light-matter interaction in materials is strongly influenced by the group velocity of light; PhC can be used as opposed to traditional waveguide devices to enhance optically nonlinear phenomenon. Hence, these characteristics not only make PhC very attractive for various applications relating to optical interconnections, they also make PhC devices an obvious candidate for applications employing the effects of optical nonlinearities.

Coupling of light between sections of waveguides based on index guiding and Bragg reflection guiding mechanisms is far from trivial. This is due to the fundamental differences between traditional index guiding and PBG guiding. While the former possess continuous spatial translational symmetry along the mode propagation direction, the later possess only discrete translational symmetry. To couple such systems together, there have been many coupling structures and techniques proposed till date: (i) the grating-coupler based structures [124, 125] make use of configurations between dielectric guides and grating couplers offering possibilities of perpendicular to guide and out-of-plane coupling [126]. (ii) A coupler structure resembling a letter ‘J’ (also known as a J-structure) [127] makes use of a reflective structure to focus light from a feed waveguide into a PhC channel. (iii) Tapered waveguides [128, 129] make use of continuous slow varying spatial translational symmetry along mode propagation direction to achieve condition of

mode transformation. (iv) Also, the concept of waveguide taper was also applied to PhC coupling in the form of inserted tapered waveguides [130, 131] and also (v) the tapering of PhC waveguides [132, 133]. Besides the high transmission performance (up to 98 % [134]) within such 2D simulations, (vi) coupling schemes with ridge waveguide access guide and the straight PBG guide have also been realized [135] allowing power transmissions of up to 95 %. Experimentally, adiabatic mode connector designed [136] to be monolithically integrated in a PhC slab chip using SOI wafer was realized and demonstrated for a connection loss of 0.8 dB per port [123]. However, such adiabatic mode connectors does not work as well with PhC slabs with air cladding since no straight forward waveguide size matching can be carried out for the different material systems, which requires further design and investigation. The distinctions between these cases are as presented below.

2.3.2 Rod-Type Photonic Crystal Waveguides Demonstrations

Experimental implementations of PhC type of devices are complicated due to the wide range of PhCs structures possible. Even though complete bandgaps in 3D are required for complete control of light wave propagation [7], 2D PhC also possess many similar properties as their 3D counterparts, at much reduced complexity [8]. The first experimental confirmation of such theoretical waveguides was demonstrated in the millimeter-wavelengths using PhC structures in a square lattice array of long alumina rods [10]. In the work, a 2D PhC was constructed from a square array of circular alumina rods having a dielectric constant of 8.9 and radius 0.2 times the lattice constant, which was chosen to be 1.27 mm. For such a 2D PhC, a large PBG exist for light polarized parallel to the rods, extending from a normalized frequency of 0.32 to 0.44, that is, from 76 GHz to 105 GHz. By removing a row of alumina rods, a

line defect was created inside the crystal. This line defect introduces an optical mode inside the crystal. By having the ends of two such line waveguides meet orthogonally, a 90 degrees sharp corner was formed.

The equipment used to verify the PBG effect was a HP8510C mm wave source unit with range from 75 to 110 GHz. The electric field of the emitted waves was polarized parallel to the rods and coupled into the PBG waveguide using two metallic waveguides. By measuring and comparing transmission amplitudes of such PBG waveguides with different lengths, the propagation loss is estimated to be 0.3 dB/cm. Testing of the sharp bending corners was also carried out in a similar experiment set-up, where it was shown that these PBG bends exhibits near perfect transmission at the resonant frequencies supported by the designed structure. Based on this work, overall transmission efficiency larger than 80 % was obtained, a significant improvement from the 30 % efficiency typically obtained by similar high-index dielectric waveguides.

At the optical wavelengths however, repetition of this pioneering experiment was prevented for many years due to the difficulty of fabricating such PhC structures in HAR, since such wavelengths would require PhC with super dense lattices of period less than half a micrometer. Another reason for this was also due to the lack of wave confinement in the vertical direction. Hence, optical wave guiding experiments were subsequently almost always carried out in slabs - with index guiding in the out-of-plane direction [11] - since without this additional mechanism, 2D PhC rod structures of insufficient aspect ratio suffer from prohibitive leakage due to lack of confinement in the out-of-plane direction.

2.3.3 Slab Type Photonic Crystal Experiments

Square lattice rod-type PhC slabs were successfully demonstrated recently by two independent groups of researchers [23-24], (with the former achieving low propagation loss of 4.8 dB/mm). In both these cases, out-of-plane optical confinement for the PhC slabs were provided by the introduction of reduced diameter rods in place of completely removed rods as the PhC line waveguide. By replacing missing rods of the previous alumina rod type PhC demonstration (in the mm wavelength range [10]) with that of smaller rods with similar height as the PhC slab; such slab type PhC makes use of index-confinement within the reduced diameter defect rods along the PhC waveguide to confine light in the vertical direction.

In the first reference work [23], a rod type PhC slab was fabricated on SOI wafer substrate, with silicon device layer of 1.3 μm and buried oxide layer of 4 μm . For a lattice constant of 0.43 μm , the bulk PhC rod diameters were 0.23 μm and the reduced radii waveguide rods had diameters of 0.15 μm . Such PhC pattern was created using EBL and subsequently transferred by ICP etching. A polymer coating was then deposited over the fabricated PhC device up to a thickness of 5 μm . Since the polymer has an index of 1.45, similar to that of the bottom cladding, there is mirror symmetry in the vertical direction. In the experiments, light was input into a cleaved end of the PhC waveguide using a hemispherical-end optical fiber while output light was detected from the opposite end with another fiber, using an optical power-meter. A 1.8 mm long straight waveguide was used in measurement. Since the theoretical minimum of the coupling losses were calculated to be 4.9 dB per end. By subtracting the coupling losses from the insertion loss of 18.5 dB, a propagation loss 4.8 dB/mm was estimated.

In the second demonstration [24], PhC rod-type slab was fabricated in a different material system of GaAs/ Al_xO_y . This 2D array had high-index dielectric

rods with period $0.5\ \mu\text{m}$, diameter of $0.29\ \mu\text{m}$ and reduced radii rods diameter of $0.24\ \mu\text{m}$. Fabrication of the device was also carried out using EBL and ICP etch process. The fabricated devices were then cleaved to create the input and output facets for optical testing. In the experiment, light was coupled directly from a fiber to the PhC waveguide by encapsulating the structure with a low index polymer [24]. Transmission measurement made of such device having two and four rows of rods were made and an increase in transmission observed within the measured bandgap is deduced to indicate demonstration of lateral guiding due to PBG effect rather than TIR.

2.4 Summary

This chapter provides a brief overview of the works relevant to the research in this thesis, as they were found in literature. In the three main sections, the principles and achievements of previous works carried out for: (i) optical PhC and rod-type 2D waveguides with microcavities; (ii) the difficulties of fabricating deep sub-micrometer scale PhC optical waveguides with monolithic integration of optical testing structures were presented together with (iii) the challenges involved with experimental measurements, such as the implementation of coupling structures etc are presented. Based on the theoretical studies of the PhC waveguides and resonator cavities designed and implemented thus far, innovation in device operations may be realized. With the development of deep reactive ion etching process development, optical quality PhC structures which have high quality sidewalls may be fabricated in the much reduced process window, while the integration of optical waveguides and also coupler interfaces enables macro (more than a $100\ \mu\text{m}$) – to – micro (less than a micrometer) optical signal coupling and measurements of the PhC structures.

Collectively, the review of these three areas not only provide the technological base required as foundation for the subsequent chapters, but also affirms the high potential of PhC design, fabrication and measurement as a way forward for integrated photonic circuit implementations.

CHAPTER 3

THEORY & DESIGN OF PHOTONIC CRYSTAL DEVICES

The objective of this chapter is to develop the theory and principles behind the design of 1D and 2D PhC waveguides and microcavities structures suitable for application in optical integrated circuits. PhCs can be used in a menagerie of devices where miniature photonic volumes are to be tailored through structural designs, useful in fulfilling many unique applications. It is of interest to design a large complete PBG for 2D photonic integrated circuit applications with large operating frequency ranges. Further, there is also intense research interest in the areas of PhC waveguiding effects, especially with incorporation of PhC nano-cavities where very small mode volumes are to be created. Here, it is the goal of this research to develop high performance, novel tunable optical PhC intersection devices through the maximal leverage of the following core inherent advantages of optical PhC: (I) Unprecedented control of optical dispersion properties, not attainable with legacy optical waveguiding material based on TIR principles. (II) Ultra-compact sub-micrometer size PhC integrated circuits functional at the canonical optical communication wavelengths scale, centered at 1550 nm (with large resonator Q-factor of strong cavity confinement properties even within a minute volume).

To do so, this chapter begins with the work based on the most fundamental form of PhC (in a 1D periodic PBG), where analytical solutions of such high optical contrast, layered structures were used to design applications in the FP resonant filter

configurations. This is followed by the derivation of 2D PBG band structures design, via theoretical Bloch formulations that gave rise to the derivation of a record size full bandgap in a highly symmetric square PhC lattice structure. Finally, based on the above works, further designs of 2D PhC devices in single line and intersecting waveguides configurations were studied and designed to enable practical demonstrations of such PBG effects; aided in demonstration with the appropriate integration of OTSs.

3.1 One-Dimensionally Periodic Bandgap Structures

For the fundamental 1D periodic PhC structure, having alternating material stack of high and low dielectric index constants [60] (as shown in Fig. 3.1), the transmission and reflection coefficients can be calculated in the following way:

Fig. 3.1 A one-dimensionally periodic photonic crystal with alternating layers of high and low index dielectric material.

$$Z_j = \sqrt{\frac{\mu_j}{\epsilon_j}}, \quad (3.1)$$

$$E_{jy} = A_j e^{jk_j(L-L_{j-1})} + B_j e^{-jk_j(L-L_{j-1})}, \quad (3.2)$$

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$$H_{jx} = \frac{1}{Z_j} \left[A_j e^{jk_j(L-L_{j-1})} - B_j e^{-jk_j(L-L_{j-1})} \right], \quad (3.3)$$

where the wave impedance is governed by Eq. 3.1 and the electromagnetic field in each layer subscript j is as shown in Eqs. 3.2 and 3.3 respectively. Here, μ and ε denotes the magnetic permeability and electric permittivity respectively whilst k_j , d_j and ϕ_j represent the propagation constant, thickness and phase shift ($k_j d_j$) in layer j respectively. L_j yields the coordinate between layer j and layer $j+1$. For a “ n ” number of layers structure, there would be $2n$ linear equations. However, since the amplitude of incident wave (A_{n+1}) is known and Z_j and d_j can be obtained, these unknowns can be solved using the property that tangential components of electric fields are continuous across boundaries. By the same token, since it is not the magnitude at each boundary which is of interest but the reflection ratio (B_{n+1}/A_{n+1}) and transmission ratio (A_1/A_{n+1}), some manipulations are then carried out as follows to derive these ratios for the implementation of computation codes.

For layer number $n+1$,

$$E_{n+1,y} = A_{n+1} e^{jk_{n+1}(L-L_n)} + B_{n+1} e^{-jk_{n+1}(L-L_n)}, \quad (3.4)$$

$$H_{n+1,x} = \frac{1}{Z_{n+1}} \left[A_{n+1} e^{jk_{n+1}(L-L_n)} - B_{n+1} e^{-jk_{n+1}(L-L_n)} \right], \quad (3.5)$$

For layer number 1,

$$E_{1y} = A_1 e^{jk_1 L}, \quad (3.6)$$

$$H_{1x} = \frac{A_1}{Z_1} e^{jk_1 L}, \quad (3.7)$$

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For layer number 2 on interface $L = 0$, by definition of $Z_1 = \frac{E_{2y}}{H_{2x}}$

$$\left. \frac{E_{2y}}{H_{2x}} \right|_{L=0} = \frac{A_2 + B_2}{\frac{1}{Z_2}(A_2 - B_2)} = Z_1 = \frac{E_{1y}}{H_{1x}}, \quad (3.8)$$

Therefore, the reflection ratio is given by

$$R_E^{(1)} = \frac{B_2}{A_2} = \frac{Z_1 - Z_2}{Z_1 + Z_2}, \quad (3.9)$$

Defining the input impedance on the interface $L = d_2$ to be $Z_{in}^{(2)}$

$$Z_{in}^{(2)} = \left. \frac{E_{2y}}{H_{2x}} \right|_{L=d_2} = \frac{A_2 e^{jk_2 d_2} + B_2 e^{-jk_2 d_2}}{\frac{1}{Z_2}(A_2 e^{jk_2 d_2} - B_2 e^{-jk_2 d_2})}, \quad (3.10)$$

Letting $\phi_2 = k_2 d_2$,

$$Z_{in}^{(2)} = Z_2 \frac{Z_1 + jZ_2 \tan \phi_2}{Z_2 + jZ_1 \tan \phi_2}, \quad (3.11)$$

Expressing $Z_{in}^{(1)} = Z_1$,

$$Z_{in}^{(2)} = Z_2 \frac{Z_{in}^{(1)} + jZ_2 \tan \phi_2}{Z_2 + jZ_{in}^{(1)} \tan \phi_2}, \quad (3.12)$$

Similarly for layer 3, the reflection ratio is then

$$R_E^{(2)} = \frac{Z_{in}^{(2)} - Z_3}{Z_{in}^{(2)} + Z_3}, \quad (3.13)$$

Similarly let Z at d_3 be $Z_{in}^{(3)}$,

$$Z_{in}^{(3)} = Z_3 \frac{Z_{in}^{(2)} - jZ_3 \tan \phi_3}{Z_3 + jZ_{in}^{(2)} \tan \phi_3}, \quad (3.14)$$

Hence, the reflection coefficient of layer $n+1$ is derived as

$$R_E^{(n+1)} = \frac{Z_{in}^{(n)} - Z_{n+1}}{Z_{in}^{(n)} + Z_{n+1}}. \quad (3.15)$$

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Input impedance on the interface $L = d_n$ as $Z_{in}^{(n)}$ is

$$Z_{in}^{(n)} = Z_n \frac{Z_{in}^{(n-1)} + jZ_n \tan \phi_n}{Z_n + jZ_{in}^{(n-1)} \tan \phi_n}, \quad (3.16)$$

For the transmission coefficient, using the continuity condition between layer j and layer $j+1$ ($Z = Z_j$),

$$E_y : A_j e^{j\phi_j} + B_j e^{-j\phi_j} = A_{j+1} + B_{j+1}, \quad (3.17)$$

$$H_x : A_j e^{j\phi_j} - B_j e^{-j\phi_j} = \frac{Z_j}{Z_{j+1}} (A_{j+1} - B_{j+1}), \quad (3.18)$$

The input impedance at the interface is

$$Z_{in}^{(j)} = \frac{E_{y,j+1}}{H_{x,j+1}} \Big|_{L_j} = \frac{A_{j+1} + B_{j+1}}{A_{j+1} - B_{j+1}} \cdot Z_{j+1}, \quad (3.19)$$

so that,

$$\frac{A_j}{A_{j+1}} = \frac{Z_j + Z_{in}^{(j)}}{Z_{j+1} + Z_{in}^{(j)}} e^{-j\phi_j}, \quad (3.20)$$

Therefore, the transmission coefficient is given by:

$$\frac{A_1}{A_{n+1}} = \prod_{j=1}^n \frac{Z_{in}^{(j)} + Z_j}{Z_{in}^{(j)} + Z_{j+1}} e^{-j\phi_j}, \quad (3.21)$$

Using this method, the reflection and transmission characteristics for a 1D PBG structure (made up of alternating layer of silicon $\varepsilon = 11.9$ and air $\varepsilon = 1$) is simulated using Matlab by substituting the respective values of the different material stack parameters into Eqs. 3.1 through 3.21 as and where necessary. For different number of layers ranging between a single Si-Air pair to five stacked pairs, the reflection characteristic for the 1D PBG is as expected of higher value for larger number of repeating stacks as shown in the calculated simulation result of Fig. 3.2 which plots the reflectance for 2, 3 and 4 layers of alternating dielectric stack.

Fig. 3.2 Simulation results of reflection characteristics derivation of a one-dimensionally periodic photonic bandgap crystal structure.

3.1.1 Fabry-Perot One-Dimensional Photonic Bandgap Structures

The 1D PhC structure may be applied to one of the most important applications used extensively in the area of optical filters, which are key components in the implementation of optical spectroscopy devices and DWDM networks. Capable of isolating one optical channel from all the rest, the filter design based on the FP resonator theory using the 1D PBG structure holds many similar figures of merit as described for the resonant cavities discussed extensively in Section 2.1. The basic FP resonator comprises two parallel reflective surfaces used to form a cavity with transmission (I_t) and reflection (I_r) intensities for a given input (I_i) in a medium of refractive index n and cavity length d as depicted in Fig. 3.3

Fig. 3.3 Schematic of a Fabry-Perot resonant filter.

The filtering function is accomplished by interfering the initially transmitted and reflected signal with many delayed versions of the input signal. The interference of a great number of transmission beams results in a set of transmission frequencies giving in effect a band-pass filter. In the same vein, a great number of reflection beams also resulted in a set of reflection bands, which can be used as a band-stop filter. Considering the input light striking the first interface at an incident angle of θ (with respect to the surface normal) such that the total optical path difference (Δ) inducing phase shifts during successive reflections between the two surfaces, it is expressed as a function:

$$\Delta = m\lambda = 2nd \cos \theta, \quad (3.22)$$

where m is an integer. For the specific case of a normal incidence in air, Eq. 3.22 can be simplified to:

$$\Delta = m\lambda = 2d. \quad (3.23)$$

Such a FP cavity formed by two reflective parallel plane surfaces with a small gap is able to transmit a comb of frequencies separated by the free spectral range (FSR), which is one of the two critical performance measures that define such filters. The FSR and the finesse factor (FF) are defined as:

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$$FSR = \Delta\lambda = \frac{\lambda_0^2}{2d}, \quad (3.24)$$

and

$$FF = \frac{\pi\sqrt{r_1 r_2}}{1 - r_1 r_2}. \quad (3.25)$$

While FSR is the wavelength spacing between peaks that determines the non-ambiguous tuning range, FF determines the channel spacing achievable with the filter. For the reflected and transmitted intensities of a FP etalon with different reflectance, the sum of the resultant amplitude of all reflected waves is given by:

$$\frac{A_r}{A_{in}} = r_1 + t_1' r_2' e^{-i\delta} \left[1 + r_1' r_2' e^{-i\delta} + r_1'^2 r_2'^2 e^{-i2\delta} + \dots \right], \quad (3.26)$$

where r_1 , t_1 , r_1' and t_1' represent the reflection and transmission coefficients as exemplified for an interface shown in Fig. 3.4. δ is the phase difference proportional to the optical path length difference, that is defined as

$$\delta = kP_L = \left(\frac{2\pi}{\lambda} \right) 2dn = \frac{4\pi dn}{\lambda}, \quad (3.27)$$

where λ and c represent their conventional qualities of the wavelength and vacuum speed of EM waves respectively.

Fig. 3.4 Definition of reflection and transmission coefficients at an interface between two materials.

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Together with the condition that energy is conserved; the ratio of reflectance and transmittance for the case of normal incidence is obtained as:

$$R = \frac{I_r}{I_i} = \frac{(r_1 - r_2)^2 + 4r_1r_2 \sin^2(2\pi nd / \lambda)}{(1 - r_1r_2)^2 + 4r_1r_2 \sin^2(2\pi nd / \lambda)}, \quad (3.28)$$

$$T = \frac{I_t}{I_i} = \frac{(1 - r_1^2)(1 + r_2^2)}{(1 - r_1r_2)^2 + 4r_1r_2 \sin^2(2\pi nd / \lambda)}. \quad (3.29)$$

3.1.2 Advantages and Optimization in Implementation

Using the qualitative relationships between the various filter design parameters, as laid out in the previous section, it can be observed that the use of PBG for designing a FP filter has several advantages over other types of traditional reflectors, such as the multilayer quarter-wave reflecting plates. First, due to the extensive, large reflection bandwidth of a typical 1D PhC as compared to other types of traditional reflectors (such as metal coated beams, which in addition suffers absorption losses), very high FF filters can be obtained, enabling improved channel spacing specifications. Next, the low frequency dependence of the 1D PBG reflectivities to wavelength changes also makes it an ideal reflector for FP filters used in the tuning of optical channels in broad bandwidths applications. An example of how a 1D PhC may be implemented in such configuration is shown in Fig. 3.5, where three layers of 1D PhC acts as partially reflecting mirrors on each side of the center resonant layer. Figure 3.6 shows the ideal high Q-factor filter response of a lossless FP filter while Fig. 3.7 shows filter responses with lower Q-factors. Here, it is noted that in non-ideal systems such as in Fig. 3.5, losses in the input/ output taper structures [156] will not only result in lower Q-factors, but also result in less than unity transmission levels.

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Fig. 3.5 Illustration of one dimensional photonic crystal Fabry-Perot resonator filter.

Fig. 3.6 Simulation result of one dimensional photonic crystal Fabry-Perot resonator filter.

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Fig. 3.7 Lower quality factor Fabry-Perot resonator filter response resulting in lower quality factor, broader bandwidths and lower contrast.

To optimize the PBG filter, it is first noted that compliant with the resonator theory described in Chapter 2, larger number of reflecting layers forming the 1D PBG on each side of the resonator give rise to higher reflectivity – which in turn results in the increment of Q-factor. Further, based on the qualitative derivations, the relationship between the parametric variables can be used to design a higher performance FP filter based on tailoring the properties of the PhC band structures. That is, through the design of a high reflectivity PBG structure, with bandgap frequencies spanning a sufficiently large range. This will enable a large FF for the filter being implemented with such PBG and would therefore directly increase the Q-factor of the filter, which consequently would also determine other filter parameters such as contrast and resolution. To do so, work as laid out in the following section will be used to obtain a record size complete 2D PBG.

3.2 Two-dimensional Photonic Band Structure Design

The performance of 2D PIC devices hinges on the existence of PBGs spanning a sufficient frequency range. Hence, there has been much interest in the search for large complete bandgaps since its early beginnings. Initiations into this field of study had been both theoretical [3] as well as heuristic [108]. Subsequent developments have led to the realization of PBGs with large complete 2D bandgaps, which have been designed using methods such as anisotropic material inclusions [109], crystal symmetry reduction [110], conjugate gradient optimization [111] and procedural derivations [112] etc. In all these methods, brute force calculations [114] are always required to determine the existence of complete 2D bandgaps in PhCs, since no simple analytical equations can be used to derive exact bandgaps without numerical calculations. However, brute force calculations should be minimized both for reduction of computational efforts and for derivation of larger bandgaps [144-147]. Therefore, in this work, a large complete 2D PBG was designed with a qualitative approach [113].

Here, the derivation of a simple 2D PhC structure spanning a very wide complete bandgap is presented. Through systematic physical insights, the required brute force computation efforts are reduced. For benchmarking purposes, the widely used material properties of silicon (with low absorption loss, high isotropic index of refraction 3.4 at the optical communication wavelengths) are employed. For plane wave method (PWM) calculations in 2D, the electromagnetic fields are decoupled into TM and TE polarizations. Here, TE modes have magnetic field along the plane of propagation and TM modes have electric field along the plane of propagation. By calculating the eigenvalue frequencies of the PhC system in which both polarization states are not present, a ‘complete’ bandgap can be identified. Calibration of the

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calculated results using 128 plane waves against that obtained using 1024 plane waves yield differences of less than 0.5 % for the overlapping photonic bands of both TM and TE polarization modes. Hence, the results presented can be estimated to be within 1 % of their true values.

3.2.1 PhC Eigenvalue Matrix and Modes

Due to the periodic nature of PhC lattices, the repeated unit cells of the PhC can be simplified from the Maxwell's equations into an eigenvalue equation [4] - such that the eigenmodes, which are solutions of the Maxwell's equations in a periodic macroscopic PhC system, can be solved using PWM. The eigenvalues of a plane wave expanded matrix are given by [8]

$$\sum M(K, \lambda; K', \lambda') H_{K', \lambda'} = (\omega / c)^2 H_{K, \lambda}, \quad (3.30)$$

where H , c , ω , K , and λ represents the magnetic field, the speed of light in vacuum, its frequency, the wave vector and the perpendicular axes respectively. The matrix M is defined as

$$\sum M(K, \lambda; K', \lambda') = |K| |K'| \begin{bmatrix} e_2 \cdot e_2' & -e_2 \cdot e_1' \\ -e_1 \cdot e_2' & e_1 \cdot e_1' \end{bmatrix}, \quad (3.31)$$

where the magnetic field has transverse components of e_1 and e_2 , forming an orthogonal triad with the wave vector in the Brillouin zone of the reciprocal lattice. Here, M as a physical operator for a real and even PhC dielectric function possessing inversion symmetry, will have its Fourier transform real symmetric and Hermitian [8].

After expansion of a numerically transformed PhC unit cell, by using the required number of plane waves for sufficient accuracy [5], the eigenvalues of M cannot be obtained analytically and have to be solved through iterative algorithms. However, by analytic as opposed to numerical Fourier transform for unit cell

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structures of standard shapes such as squares and circles, some trends can be observed for the factors affecting M . For example, the Fourier transform of a circular PhC unit cell is defined as

$$F(k) = \frac{1}{\alpha} \iint_{\alpha} f(r) e^{-i\vec{k} \cdot \vec{r}} ds, \quad (3.32)$$

where $i = \sqrt{-1}$, $f(r)$ is the dielectric function of the unit cell in real space and α is the area of the unit cell. The analytical Fourier transform of Eq. 3.30 yields for the whole lattice

$$F(G) = \varepsilon_b \delta(G) + 2(\varepsilon_b - \varepsilon_a) f \frac{J_1(GR)}{GR}, \quad (3.33)$$

where ε_a and ε_b are the dielectric constant of the material within and outside a cylindrical unit cell respectively, R is the radius, G is the reciprocal lattice, f is the ratio of the cylinder area to the unit cell, and J_1 is the Bessel function of the first kind. Based on such formulations, the general properties of the eigenstates may be expressed in their various lattice parameters. To develop from such analytical expressions (for parametric optimization), it is then necessary to proceed further through calculations of the various PhC structure variables.

For discussion applicable to both high and low index circular unit cells, a dielectric-filling fraction (DF) can be defined for a simple two material PhC systems, as the ratio of the area occupied by the dielectric material per unit cell (without regard of lattice geometry or unit cell shapes etc). Consequently, as the main diagonal elements of M , are proportional to the inverse of $F(G)$, increases in DF therefore correspond to decreases in the coefficients of eigen-values obtained in the expanded characteristic equation. Here, as the shape of the unit cell has not been included in the derivation of the Fourier transform, variations of symmetric lattice structures therefore does not affect the validity of Eq. 3.33. Beyond this consideration however,

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the solution to the characteristic equation of M cannot be expressed algebraically (except for certain special classes, as discovered around 1829 by the French mathematician Évariste Galois).

Hence, beyond the above analysis, it is also necessary to be able to express the above described process with physics for a better understanding. A physical description of the above mathematical formulations for PhCs can be considered and understood in analogy to their electronic counterpart – the semiconductor crystals. In semiconductor crystals, the electronic band-gaps arise because electrons behave partly like a wave, and the electron's waves scatter off the lattice of semiconductor atoms. Part of the electron's wave is scattered back in the source direction. For waves with wavelengths of similar dimensions to the characteristic length-scale of the atomic structure, all the backscattered electron's waves can add up coherently such that the wave is reflected back completely, as if having hit a mirror. Similarly, for an optical band-gap where light is scattered by changes of refractive index, an interaction directly analogous to the electrons of the semiconductor case occurs for periodic PhC structures of varying refractive index with sufficient contrast. Hence, photons in PhCs have analogies of band structures in electronic crystals where a full band-gap is formed when there is perfect reflection occurring over a range of wavelengths for any wave-vectors. Therefore, with all the above derived analytical formulations and also physical nature of the PhC band structures described, actual optimization for the largest complete photonic bandgap structures may be carried out, as described step-by-step in the following sections to finally yield a square lattice PBG of normalized wavelength range, spanning 0.20, which is then discussed and compared against other benchmark PhC structures

3.2.2 Band Structures and Dielectric Fill Fraction

For solution of the M matrix, the lowest band of mode solutions is known as the dielectric band while the next is known as the air band [115]. Bandgaps of PhC can be identified for normalized frequencies without any available eigenstates within the non-repeated wave numbers. By plotting the PhC bandgap size and center frequencies against their DF 's, a trend in PBG size can be observed such that generally, the occurrence of bandgaps along the DF axis peaks between extremes of minimum and maximum DF 's. This is illustrated for square lattices of air and dielectric cylindrical columns with dielectric constant 12, as shown in Fig. 3.8 (a), (b) and (c), (d) respectively. Here, for increasing rod radii or decreasing hole radii for the rod- and hole- type PhCs respectively (both scenarios corresponding to increasing DF s), the eigenmodes of the PhC system with frequencies within 0.8 ($\omega a/2\pi c$) are plotted for TE and TM mode polarizations as filled and unfilled symbols respectively.

(a)

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(b)

(c)

Fig. 3.8 Simulation results of photonic crystal band structure of varying bandgap sizes and center frequencies (plotted against increasing dielectric-fill fraction) for square lattices of air columns in (a), (b); and for dielectric columns (c), (d) respectively.

From the Fig. 3.8, it can be observed that besides having more pronounced TE and TM modes respectively for the isolated (rod type) and interconnected (hole type) structures, the formation of bandgaps can be seen to occur more readily at the lower range of DF values, from 0 to 0.6. At the same time, PBG center frequencies for TM eigenmodes are much lower in the interconnected lattice than in the isolated ones and vice versa for the TE polarization eigenmodes. Therefore, the TE and TM polarization bandgaps in both these structures do not exhibit complete PBGs, as their eigenmodes center frequencies do not coincide.

Qualitatively, this can be explained. First, as the frequency of radiation for a given wavelength is lower in dielectric material than in air, eigenmodes that have

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more character in the dielectric would have lower frequencies as compared to the less confined modes [108]. Therefore, another consequence of increasing dielectric character of eigenmodes with higher DF in the unit cells includes the “pulling down” of mode frequencies [8]. Effectively, gaps are progressively “squashed” by the pulled down states as DF increases till they disappears.

Second, PhC structures with larger DF values permit mode wave functions to spread over a larger area of the dielectric material, allowing greater confinement for the out-of-plane displacement fields. To illustrate these, the square lattice PhC band structures with the dielectric and air columns are altered by introduction of a hollow core and replacement with a square shape respectively. In the former, the dimension of the inner hollow cylinder is set to be half that of the outer dielectric column such that for the same outer dimension of column DF is reduced together with an increase in spatial dielectric contrast. For the latter, interconnected grids with circular arcs at intersecting branches are replaced by sharp cross shape unit cells.

3.2.3 Modes Fields and Dielectric Contrast

Figure 3.9a shows the out-of-plane displacement field amplitudes for a dielectric ring PhC unit cell, where the introduction of an air hollow within the dielectric column effectively reduces the amount of field character in the higher index dielectric material (as compared to that of the solid dielectric columns, as shown in Fig. 3.9b). This is corroborated with calculation of the mode effective index, $n_{eff} = |\vec{k}|/\omega$, which gives the ratio of the wave-vector modulus as a ratio of eigenmode frequency. As expected, n_{eff} of the TE dielectric band was indeed reduced from by 0.05 with the introduction of an air hollow within a solid core dielectric

column. At the same time, due to the increased spatial dielectric index contrast for the in-plane displacement fields of the TM modes, greater differentiation between the dielectric and air bands led to increase TM bandgap size as shown in Fig. 3.10.

Fig. 3.9 Simulation results of photonic crystal displacement field plots for dielectric band TE bandgap modes of (a) hollow and (b) solid dielectric column structures.

Fig. 3.10 Simulation results of photonic crystal bandgap sizes for hollow dielectric cylinders with increased spatial index contrast, as plotted against their dielectric fill factors.

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On the other hand, for the case of circular air columns replaced by square shape ones giving sharp dielectric crossing branches instead of rounded intersections, the displacement fields for the dielectric bands of the out-of-plane TE eigenmodes are as given in Fig. 3.11a and 3.11b respectively. Here, as expected, due to the reduced spread of spatial dielectric material, the modes in Fig. 3.11b tended to have less of their character in the dielectric than that of Fig. 3.11a. This, supported by the n_{eff} values calculated in Table 3.1 therefore attributes to higher bandgap frequencies. Here, the present unit cell structure, for its increased gap frequencies, may be coupled together with the isolated ring structure, for its enhanced TM gap sizes, for derivation through superposition, the square lattice unit cell structure of Fig. 3.12.

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Table 3.1 Mode effective indexes for dielectric bands of both TE and TM modes of circular and square shape holes in a square photonic crystal lattice.

	TE polarization		TM polarization	
	Dielectric band	Air band	Dielectric band	Air band
Circular Holes	2.922	2.629	2.596	2.414
Square Holes	2.742	2.437	2.394	1.834

Fig. 3.11 Simulation results of photonic crystal displacement field plots for dielectric band TE bandgap modes of (a) circular shape hole and (b) square shaped hole unit cell, in a square lattice photonic crystal structure.

Fig. 3.12 Enhanced isolated ring structures, with criteria of interconnectivity fulfilled by introduction of interconnecting grids, having defined parameters of pitch, R , R_2 and w .

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A coarse scan of this hybrid unit cell structure yields the band structure is shown in Fig. 3.13. For the same ring diameter as the isolated ring structure, the in-plane displacement field of the TM modes in the interconnect rings of Fig. 3.12 would be able to keep mainly within the dielectric material, hence allowing greater n_{eff} contrast against the air band, which correspondingly increases the size of the TM bandgaps. At the same time, the raised TM bandgap frequencies of the intersecting sharp crossing of Fig. 3.11b also enabled overlapping with the TE mode bandgap frequencies, which therefore yielded large complete bandgaps. To optimize this unit cell structure of interconnected rings, the parameters of outer-radii, inner-radii and interconnecting branch width (R , R_2 and w) are then scanned systematically for widest complete PBG. Here, without discrimination, there would be a great number of unit cell geometries for calculation. However, computation efforts can be greatly reduced by selective calculations for unit cells satisfying condition of DF ranging from 0.1 to 0.5.

(a)

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(b)

Fig. 3.13 Simulation results of photonic crystal bandgap (a) sizes, and (b) center frequencies of interconnected rings photonic crystal square lattices for increasing dielectric fill fractions.

Therefore, largest complete bandgap is found for an ideal overlap of TE and TM polarization bandgaps with similar gap size and center frequencies (Fig. 3.14). Here, the photonic bandgap as plotted along the high symmetry points of the irreducible Brillouin zone as indicated in Fig. 3.22 is given, with the positive slope hatchings correspond to TE polarization bandgaps while the negative slope hatchings correspond to TM polarization bandgaps. Cross-hatch regions therefore indicates the complete bandgap, centered at frequency of $0.515 (a/\lambda)$, where a is the pitch of the PhC and λ is the wavelength of operation. For dimensions of R , R_2 and w being $0.260a$, $0.456a$ and $0.0335a$, this complete bandgap spans normalized frequency range $0.103 (\omega a/2\pi)$, i.e. spanning 20 % the center frequency. Compared to the

case of the standard triangular lattice of air holes, this structure has a photonic bandgap spanning normalized frequency range 20 % larger. However, the minimum index contrast for which a complete gap opens occurs at 1.7 for the case of the triangular lattice of air holes while an index contrast of 1.8 is required in the case of this new structure. Hence, whilst this structure shows greater potential for the creation of larger complete bandgaps, it also imposes greater demand on the refractive index contrast of the constituting lattice elements.

In terms of robustness, for isolated variations in the unit cell dimensions, complete bandgaps were found to persist for R , R_2 and w being $[-20\%, +64\%]$, $[-70, +131\%]$, and $[-100\%, +73\%]$ of their designed values respectively.

Fig. 3.14 Band structure of optimized photonic crystal unit cell, yielding complete bandgap spanning normalized frequency of 0.103, centered 0.515.

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Hence, through frequency splitting effect between the orthogonal eigenmodes of PhC lattices, adjacent bands sufficiently differentiated in spatial dielectric localizations and eigenfrequencies are used to derive large bandgaps. For large DF value unit cells where characteristic frequencies of the orthogonal eigenmodes cannot be forced apart, large bandgaps do not occur and therefore may not be calculated for reduction of computation efforts required. For the large complete PhC bandgap structure derived, simple material system of dielectric columns in air may be realized with standard semiconductors such as silicon. The wide range of bandgap frequencies in this bandgap structure may be used for design of optical devices requiring extra wide bandwidths. As the derivation of this design has been presented in their sequential order, similar principles can be applied in general to other lattice structures including 3D ones.

3.3 Photonic Crystal Cavities in Single Line Resonators

As discussed in Section 2.1, microcavity resonators refer to structures capable of confining light in small volumes by the action of resonant recirculation. Photonic microcavities have been identified as one of the most elusive for design and implementations since design rules developed for its counterparts in the physical, sound or microwave domains are not applicable in the design of optical microcavities. To investigate this, PhC cavities will be studied in progressively higher Q-factor single line resonators, spatially shifted resonators, and cascaded configurations.

3.3.1 Single Line Photonic Crystal Resonator Cavities

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In the single line PhC resonator configuration, the line defect waveguide is created by removing a line of rods (or reducing the diameter of a line of rods within a periodic lattice), and coupled together with a resonator of a reduced/enlarged rod embedded within some PhC rods of the bulk PhC structure. The waveguiding mode of a reduced diameter PhC line defect waveguide is exhibited in the 2D simulation result of Fig. 3.15, where there is an additional PhC guiding mode within the bandgap frequencies. For slab type PhC with finite dimensions in the vertical plane, this mode diagram is further divided by a diagonal “light line” arising from the material cladding - in this case, air. PhC modes which are guided within the bandgap frequencies become resonant above the light line, such that they extend deeply into the surroundings, losing their lossless guiding properties.

Fig. 3.15 Diagram of photonic bandgap mode for a single line defect waveguide, with addition of the light line indicating the resonant states.

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For such configurations of single line resonators, a single rod on each side of the resonator gives a 3×3 structure, while two rods on each side of the resonator gives a 5×5 structure, and so on for the case of three rods on each side [115] (see Fig. 3.16). Hence, with increasing number of PhC rods on each side of the resonator, increasing reflectivity of the confining cavity is obtained (analogous to the mirrors of a confining FP cavity [4]).

Fig. 3.16 Schematic of single line photonic crystal waveguides with a single embedded resonator, (a) 1×1 , (b) 3×3 , (c) 5×5 , where the shaded areas indicate high refractive index material set against a low index background such as air.

Hence, it corresponds that for a higher number of rods placed on each side of the embedded resonator, a higher Q-factor for the cavity mode results. Figure 3.17 gives the frequency response of the 1×1 , 3×3 and 5×5 embedded PhC resonator with normalized transmission for lattice constant of $0.52 \mu\text{m}$. From the spectrums, it can be seen that for progressively increased orders of the single resonator structures, the transmittance increases in Q-factors. This is accompanied by a corresponding reduction in the bandwidth, which is the range of transmitted wavelengths about the

center resonance wavelength. Such increase in Q-factors for these increasing orders of single line resonators therefore results in correspondingly reduced full widths at half maximum (FWHM) for the 1×1 , 3×3 and 5×5 single line resonator structures, respectively.

Fig. 3.17 Transmission spectrums for progressively higher order single line resonators.

With such frequency response results, the effect of changes to the center resonator rod sizes and refractive index may be predicted for their sensitivity, which corresponds directly with the Q-factors of the resonator structures.

3.3.2 Spatially Shifted Resonators

If however, the center cavity rod is not altered in its properties while remaining in its original position, but spatially shifted, the properties of the shifted resonator structures may no longer be predicted directly based on the order of the

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resonator's structure which determines the resonator Q. This is depicted for a 3×3 embedded single line PhC resonator, shifted in the two orthogonal directions towards its nearest vertical and horizontal neighboring rods. Figure 3.19 shows how the spatial shifting of Fig. 3.18 affects the transmittance and reflectance of the embedded resonator.

Fig. 3.18 Schematic representation of the spatial shifting performed in simulations of a position shifted embedded resonator rod.

(a)

(b)

Fig. 3.19 Surface plot of (a) reflectance, and (b) transmittance levels, simulated by finite difference time domain method at steady state level for a 3×3 embedded single line resonator with center cavity rod shifted in the orthogonal directions

Based on these two results of Fig. 3.19, it is clear that shifts of $0.1 \mu\text{m}$ in either orthogonal direction reduce the transmittance levels of the resonator structure the most. This is accompanied by a corresponding increase in the reflectance levels.

3.3.3 Cascaded Configurations

If more than one resonator rod is embedded within the PhC line defect [157], such as that of a double resonator arranged in tandem - in a cascaded configuration such as that shown in Fig. 3.20 - more than a single resonance frequency may be obtained. Figure 3.21 gives the simulated spectrum response of such a structure,

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where the transmission is represented by a solid line and the reflection spectrum is represented by a dash line.

Fig. 3.20 Schematic layout of two resonator rods embedded in a cascaded configuration in a single line defect photonic crystal waveguide.

Fig. 3.21 Frequency response of a cascaded configuration, double resonator.

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In Fig. 3.21, the two resonant wavelengths of the cascaded resonator structure (with two resonators) are located at within the bandgap spanning 1.35 μm to 1.8 μm , at 1.547 μm and 1.576 μm to give a free spectral range of 0.029 μm . By increasing the number of cascaded, embedded resonators, for example, to three embedded resonators, the number of resonant frequencies within the bandgap frequencies can be correspondingly increased to three, therefore correspondingly squeezing and reducing the free spectral wavelength range. Hence, with an increased number of resonances, different wavelength channel applications can be effected.

Therefore, based on such studies of miniature PhC resonator structures with very small layout size of less than ten micrometers - in various configurations of single line, single resonator; shifted resonator; and cascaded multi resonators - identified as key components to next generation integrated photonic circuits' development, the properties and sensitivity of each configuration to effects of perturbations in the resonator properties was determined and may be used in application to ultra-fast modulations of light-tuned-light PhC integrated circuit devices.

To do so, the PhC optical intersection may be used. Comprising of single line defect PhC waveguides, PhC optical intersections are important for sub-micrometer length-scale optical waveguiding with capability of forming large angle crossings. Since the PhC waveguide crossings can be tailored to produce various required dispersion properties and at the same time maintain a small layout size, it may potentially be applied for optical integrated circuits as interconnections, which will allow for interaction of many waveguides within a small area. This work is therefore developed in detail, as described in the following section.

3.4 Photonic Crystal Optical Intersections

From the basic device structure of a square lattice rod-type periodic PhC, removal of a single line of PhC rods introduces defects that create the single line waveguide. By intersecting orthogonally two such waveguides, PhC optical intersections (Fig. 3.22a) with four-fold symmetries [17] as illustrated in Fig. 3.22b are formed.

(a)

Fig. 3.22 (a) Schematic representation of a photonic crystal optical intersection as an orthogonal crossing of two single line defect waveguides in a two-dimensional array of silicon rods with square lattice periodicity. (b) Illustration of high symmetry, four fold operations in the Brillouin zone of the square lattice photonic crystal reciprocal space representation.

These PhC optical intersections can have compact working areas (as small as $5 \times 5 \text{ um}^2$) and can be applied in optical integrated circuits for small form large angle crossings [117, 118]; an important component of photonic integrated circuits as they allow for interaction of many waveguides within a small footprint [115].

3.4.1 Principles of Four Ports Intersections

However, due to the sub-wavelength scale of such crossing waveguides, inputs undergo diffraction at the intersections [118], resulting in high crosstalk and reflection levels lowering effective transmissions (as illustrated graphically in Fig. 3.23a). This

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is collaborated by the steady state FDTD simulation results of Fig. 3.23b; where the electric field propagating along the z axis with alternating maximum positive and negative amplitudes along the waveguides are shown in the lowest order, 1×1 form without any center cavity rod. In the figure, the circles drawn in the schematic indicates the positions of the PhC silicon rods set against an air background. For optical intersections with the inclusion of an optimized center cavity rod, crosstalk may be eliminated to obtain high transmission as shown in Fig. 3.23c.

Fig. 3.23 (a) Schematic of diffracting radiation, through sub-wavelength intersecting waveguides. (b) Steady state FDTD simulation of photonic crystal intersection without, and (c) with center cavity resonator rod.

Here, such an optical intersection with a single cavity rod in the center can be referred to as a 1×1 intersection cavity, similar to that of the single line resonator convention. If increasing layers of bulk PhC rods are introduced to each branch of the intersecting waveguides near this center cavity rod, where rods were previously removed from lattice sites to form the line defect waveguide, progressively larger cavities of 1×1 , 3×3 , and 5×5 orders (as shown in Fig. 3.24) are formed. For these progressively higher order cavities, there is increasing confinement effect at the center cavity rod (since such additional layers of PhC rods around the center cavity rods act like “Bragg” mirror layers similar to that found in a typical FP resonator), leading to correspondingly increasing cavity Q-factors but smaller frequency bandwidths as given in the 2D simulation results of Fig. 3.25.

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Fig. 3.24 Photonic crystal optical intersection configurations with progressively higher order configuration for correspondingly higher factors.

Fig. 3.25 Frequency response of the different configurations of photonic crystal optical intersection resonators.

Here, Fig. 3.25 gives as expected progressively sharper frequency responses as expected for correspondingly higher Q resonators with higher orders of PhC confinement effect by 2D FDTD simulation. It is to be noted that such frequency

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spectral plots requires simulation with sufficient time duration so that smaller steps in the frequency result domain may be obtained and high quality resonator peaks may be observed. At the same time, the boundary conditions for such domain limited simulations are also particular to the terminations at the simulation boundaries. In such cases, perfectly matched layer (PML) boundary conditions, which typically works well for the FDTD method fails for such periodic media [158]. By circumventing such computation cell boundary reflection issues, normalization issues may be avoided. Hence, FDTD may be used effectively to calculate for these configurations of the PhC optical intersections, two degenerate modes in the frequency range of interest may be supported [121]. These degenerate modes have similar frequencies, which therefore allows for their superposition. Figures 3.26a and 3.26b depicts the electric field mode profiles of the in-phase and out-of-phase superposition of these degenerate modes for the 1×1 optical intersection. Similar to Fig. 3.23, the field representations of the mode profiles are given by the maximum positive and negative amplitudes of the propagating electric field in and out of plane along the z-axis as labeled. From these mode plots, it is therefore easy to visualize how the cancellation of opposite phases at the crosstalk branches by the two degenerate modes enables the elimination of crosstalk.

Fig. 3.26 Profile plots of electric field modes for the in-phase and out-of-phase superposition of the degenerate modes in the 1×1 photonic crystal optical intersection.

3.4.2 Analytical Formulations using Coupled Mode Theory

To analyze such four port PhC optical intersection, the coupled mode theory in time (CMT) [119] is used to qualitatively describe the optical properties of the 1×1 optical intersection. For an arbitrary PhC optical intersection with a center rod for coupling cavity such as that shown for example in the ‘black box’ diagram of Fig. 3.27, where there is a center coupling cavity joint to four orthogonal side branches; there may exist the two degenerate modes as described earlier in the previous section, with amplitudes denoted as a and b , and resonance frequency ω_0 in the frequency of operation.

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Fig. 3.27 Illustration of a four port photonic crystal intersection device consisting of four waveguides as ports connected to an arbitrary cavity.

Qualitatively, the behavior of this system described by CMT [119, 121] is formulated as follows: After intrinsic loss with decay rate $\frac{1}{\tau_0}$, and a waveguide branch transfer rate $\frac{1}{\tau_e}$ and input excitation s_{+1} , with coefficient κ describing the coupling between the intersection cavity and the excitation radiation, the effective mode amplitude is given by:

$$\frac{da}{dt} = j\omega_0 a - \frac{1}{\tau_0} a - \frac{1}{\tau_e} a + \kappa s_{+1} \quad (3.34)$$

For source at frequency ω , with $e^{j\omega t}$ as time dependence, at steady state:

$$a = \frac{\kappa s_{+1}}{\frac{1}{\tau_0} + \frac{1}{\tau_e} - j(\omega - \omega_0)} \quad (3.35)$$

To express κ in terms of τ_e , assuming no internal loss with no source and only one waveguide branch, the mode decay

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$$\frac{d|a|^2}{dt} = -\frac{2}{\tau_e}|a|^2 = -|s_-|^2, \quad (3.36)$$

where s_- is the wave traveling away from the coupling cavity. For the time-reversed solution, it is converted into an incident wave, s_+ , such that energy in the coupling cavity builds up rather than decays, with time dependence $e^{\frac{2t}{\tau_e}}$. For ‘positive frequency’ amplitudes of time reversed solution $\hat{a}$,

$$\frac{d|\hat{a}|^2}{dt} = \frac{2}{\tau_e}|\hat{a}|^2 \quad (3.37)$$

the time reversed solution is “driven” by incident wave $\hat{s}_+$ at frequency ω_0 and grows at the rate $\frac{1}{\tau_e}$, such that the frequency of the drive is $\omega = \omega_0 - \frac{j}{\tau_e}$. Therefore,

$$\hat{a} = \frac{\kappa \hat{s}_+}{\frac{2}{\tau_e}} \quad (3.38)$$

Further, since

$$|\hat{s}_+|^2 = \frac{2}{\tau_e}|a|^2 = \frac{2}{\tau_e}|\hat{a}|^2, \quad (3.39)$$

$$\kappa = \sqrt{\frac{2}{\tau_e}} \quad (3.40)$$

Since phase of κ can be neglected because phase of a with respect to s_+ can be defined arbitrarily,

$$\frac{da}{dt} = j\omega_0 a - a\left(\frac{1}{\tau_0} + \frac{1}{\tau_e}\right) + \sqrt{\frac{2}{\tau_e}}s_{+1} \quad (3.41)$$

For a linear system, s_- can be determined as proportional to s_+ and a , such that

$$s_- = c_s s_+ + c_a a \quad (3.42)$$

From Eq. 3.36,

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$$c_a = \sqrt{\frac{2}{\tau_e}} \quad (3.43)$$

where the phase factor of c_a is fixed at unity by choice of reference pane at which s_- is to be evaluated. Next, by energy conservation, the net power flowing into the coupling cavity has to be equal to the rate of energy buildup and the rate of energy dissipation

$$|s_+|^2 - |s_-|^2 = \frac{d}{dt}|a|^2 + 2\left(\frac{1}{\tau_0}\right)|a|^2 \quad (3.44)$$

From Eq. 3.41,

$$\frac{d|a|^2}{dt} = -2\left(\frac{1}{\tau_0} + \frac{1}{\tau_e}\right)|a|^2 + \sqrt{\frac{2}{\tau_e}}(a^* s_+ + a s_+^*) \quad (3.45)$$

Comparing Eq. 3.44 and Eq. 3.45,

$$|s_+|^2 - |s_-|^2 = -\frac{2}{\tau_e}|a|^2 + \sqrt{\frac{2}{\tau_e}}(a^* s_+ + a s_+^*) \quad (3.46)$$

Eliminating a from Eq. 3.46 by Eq. 3.42 and Eq. 3.43,

$$c_s = -1, \quad (3.47)$$

$$s_- = -s_+ + \sqrt{\frac{2}{\tau_e}}a \quad (3.48)$$

Therefore, for the coupling cavity with the four fold symmetry waveguide coupling branches, for the two degenerate modes with amplitudes a and b , the amplitude of outgoing waves are given as:

$$s_{-1} = s_{+1} + \sqrt{\frac{2}{\tau_a}}a + \sqrt{\frac{2}{\tau_b}}b, \quad (3.49a)$$

$$s_{-2} = \sqrt{\frac{2}{\tau_a}}a + \sqrt{\frac{2}{\tau_b}}b, \quad (3.49b)$$

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$$s_{-3} = \sqrt{\frac{2}{\tau_a}}a - \sqrt{\frac{2}{\tau_b}}b, \quad (3.49c)$$

$$s_{-4} = \sqrt{\frac{2}{\tau_a}}a - \sqrt{\frac{2}{\tau_b}}b; \quad (3.49d)$$

such that the transmittance T , crosstalk X , and reflectance R levels can be expressed as:

$$\frac{s_{-1}}{s_{+1}} \equiv R = -1 + \frac{\frac{2}{\tau_a}}{j(\omega - \omega_0) + \frac{4}{\tau_a}} + \frac{\frac{2}{\tau_b}}{j(\omega - \omega_0) + \frac{4}{\tau_b}}, \quad (3.50a)$$

$$\frac{s_{-2}}{s_{+1}} \equiv T = \frac{\frac{2}{\tau_a}}{j(\omega - \omega_0) + \frac{4}{\tau_a}} + \frac{\frac{2}{\tau_b}}{j(\omega - \omega_0) + \frac{4}{\tau_b}}, \quad (3.50b)$$

$$\frac{s_{-3}}{s_{+1}} \equiv X_L = \frac{\frac{2}{\tau_a}}{j(\omega - \omega_0) + \frac{4}{\tau_a}} - \frac{\frac{2}{\tau_b}}{j(\omega - \omega_0) + \frac{4}{\tau_b}}, \quad (3.50c)$$

$$\frac{s_{-4}}{s_{+1}} \equiv X_R = \frac{\frac{2}{\tau_a}}{j(\omega - \omega_0) + \frac{4}{\tau_a}} - \frac{\frac{2}{\tau_b}}{j(\omega - \omega_0) + \frac{4}{\tau_b}}; \quad (3.50d)$$

Here, it is noted that in the limit when the Q-factor becomes significant enough for increasing layers of rods surrounding the center cavity, this model tends to become a quantitative description of the system (since there is an approximate ten times increase in Q-factor for each progressive increase from the 1×1 to 3×3 and from the 3×3 to 5×5 cavity configuration). Hence, for decay rates of both modes being equal, such that $\frac{1}{\tau_a} = \frac{1}{\tau_b}$, crosstalk levels remain zero for all frequencies.

When this optimized condition is altered, such that $\frac{1}{\tau_a} \neq \frac{1}{\tau_b}$, crosstalk inevitably

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increases from negligible to decrease the transmittance levels as can be seen from Fig. 3.28, where the power of the system are distributed between the transmission and reflection port. From the figures, it can also be seen that as expected, a resonator with a lower decay rate such as (b) will have a sharper frequency response than its lower quality factor counterpart as in (a).

(a)

(b)

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Fig. 3.28 Coupled mode theoretical prediction of four port optical intersection characteristics for degenerate modes with (a) high decay rates, and (b) lower decay rates.

When the PhC optical intersection operating point moves away from such optimized condition, crosstalk levels, however, increase as no effective cancellation can occur, as can be seen from Fig. 3.29.

(a)

(b)

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Fig. 3.29 Coupled mode theoretical prediction of four port optical intersection characteristics for modes a and b with different decay rates with (a) one order of magnitude difference, and (b) two order of magnitude difference.

From Fig. 3.28, it can be seen that for degenerate modes with similar decay rates, the higher decay rates from the cavity results in correspondingly broader spectrums with lower Q-factors (Fig. 3.28a) while lower decay rates gave transmission and reflection spectrums which were much sharper with higher Q-factors (Fig. 3.29b). This scenario corresponds to the case for which the optimized PhC optical intersection had degenerate modes designed to have the same coupling efficiency with the connecting ports. On the other hand, for modes which do not have the same coupling efficiency with the connecting ports, incomplete cancellation gives rise to crosstalk, which increases from 3 % to 23 % for increase in difference of decay rates from one order of magnitude (Fig. 3.29a) to two orders of magnitude (Fig. 3.29b).

3.5 Design of Optical Coupling Structures

One of the most important design considerations for PhC research at the optical communication wavelength is the need to incorporate macro to micro optical experiments. As presented in Section 2.3, there are mainly two critical interfaces in optical coupling required for optical experiment; the first being the interface between the PhC device and the integrated waveguide; the second being the coupling between the integrated waveguide and the macroscopic probing medium (e.g. an optical fiber or a set of collimating lens coupled to an optical meter). Based on the many works reviewed in Chapter 2, the focus here will be mainly on the interfaces between optical

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fibers, integrated silicon waveguides and the PhC devices. While the interface coupling between fibers and the silicon waveguides were achieved via deep etched fiber grooves, the coupling between the silicon waveguides and the PhC devices need to be carefully designed.

Since the PhC devices are only a few micrometers in size, PhC and silicon waveguides need to be used in order to input optical signal into of the PhC devices, and also receive output signals from them. As the ideal conversion of the fiber mode to waveguide mode requires complex 3D lens systems - which are not easily fabricated using the top-down approach as presented in the previous chapter - the scope of this work is limited to coupling structures amenable to the integrated device process fabrication. Further improvements of the coupling results obtained may therefore be provided by discrete coupling devices such as lensed fibers; focusing systems and collimators etc.

3.5.1 Tapered Silicon Waveguides

In the HAR PhC rod type devices, the fiber mode has a similar mode size to the widened end of the PhC tapered input. In such devices, the PhC waveguide was used to gradually reduce the lateral size of the input signal via step taper structures [141]. However, due to the lack of confinement in the vertical direction, the input beam spot remains confined only in the in-plane direction of the PhC and diverges quickly out-of-plane as an expanding Gaussian beam in the vertical direction. On the other hand, for the case of the slab type PhC, which has a slab thickness of only 3 μm , an input fiber mode would have a mode size which is too large to couple properly into the silicon waveguide. Since all the light that manages to couple into the silicon waveguide may be confined both in and out-of-plane due to the mechanisms of PhC

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and index guiding respectively, meaningful measurements may still be obtained. The design for such tapered silicon waveguides were simulated in FDTD, as shown in Fig. 3.30, which exhibit both the designed structures together with the steady state simulation results. Here, designed tapered silicon waveguides were obtained for adiabatically converting larger fiber modes into suitable dimensions for the slab-type PhC waveguides.

Structure

Simulation results

(a)

(b)

(c)

(d)

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Fig. 3.30 On the left side, taper silicon waveguides (a) without photonic bandgap crystal; (c) with reduced radius photonic crystal line defect rods; (e) with photonic crystal lattice and line defect waveguide. On the right side, the FDTD simulation results corresponding to designs of (a), (c) and (e) are shown in (b), (d) and (f) respectively.

In Fig 3.30, the layout schematics are shown on the left side while the simulation results are shown on the right. For the case of a taper silicon waveguide in air, it can be clearly seen in Fig. 3.30b that an optical mode had been successfully converted to have a narrower beam width through the gradual tapering of the silicon waveguide. Here, as the mode leaves the confinement of the waveguide, it quickly diverges as can be seen from the electric field profile. If however, the tapered silicon waveguide was terminated, not in air but by a succession of reduced radius PhC waveguide rods (Fig. 3.30d), then some confinement after the beam leaves the silicon waveguide can be observed. Finally, if the tapered silicon waveguide is coupled to a PhC waveguide, the continuous to discrete waveguiding mechanism typically is accompanied by high reflections due to incompatibility between the two waveguide modes. In the case of Fig. 3.30f however, high coupling was obtained based on optimization of the waveguide structure [159].

3.5.2 Cut-Back Method Structures Design

These tapered silicon waveguides may therefore be used as input structures (Fig. 3.31).

(a)

(b)

(c)

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Fig. 3.31 Straight through test configurations with tapered input silicon waveguides (a) shortest at $15a$ length; (b) mid-length at $35a$ length; and (c) longest at $55a$ length.

Figure 3.31 gives the layout of tapered silicon waveguides for different propagation lengths. These test structures were used as normalizing references for similar PhC waveguides of varying lengths, which instead of free space is filled with 2D rod type PhC, as shown in the layout images of Fig. 3.32. Hence, instead of “cutting back” a longer waveguide after every measurement, the design of waveguides with different lengths enables non-destructive testing, and also the elimination of differences in coupling factors due to the changes in end facet quality, resulting from each cleaving action.

(a)

(b)

(c)

Fig. 3.32 Straight photonic crystal reduced radius waveguides with tapered input silicon waveguides (a) shortest at $15a$ length; (b) mid-length at $35a$ length; and (c) longest at $55a$ length.

Therefore, these designed PhC devices of 1D PhC resonant filters, single line defect waveguides, and crossing PhC optical intersections etc, were further investigated for – dynamic modulation possibilities, fabricated by development of nano-fabrication technologies and demonstrated experimentally – as will be presented in the subsequent chapters of this thesis.

3.6 Summary

In conclusion, this chapter presents the principles for the theory and designs of PhC devices. Specifically, the chapter began with the derivation of the transmission and reflection properties for the simplest PhC structure – a high index contrast, layered PBG structure that is periodic in a single direction. Progressing from 1D and 2D PBG structures were then investigated and presented. Here, the band structures composing the dispersion properties of 2D PhC unit cells described by the Bloch theorem was analyzed in detail. Insights from the analyses then resulted in the

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derivation of a novel record large bandgap structure design with a high symmetry square lattice configuration (which exceeds that found in literature through algorithm searches). These band structure studies are then followed through with device design for 2D PhC lattices, especially for design of embedded PhC micro-resonators, in single line; cascaded, and also orthogonally crossing waveguides.

Finally, the analyses of a four port PhC optical intersection was also carried out with coupled mode theory for the various designs of PhC optical intersections with degenerate intersection modes. Based on such theoretical formulations, predictions for the various cavity structures were made. Following which, the design of optical test structures for such PhC devices were also presented, specifically in the area of coupling by adiabatically tapered waveguides; and also propagation loss measurement structures by the cut-back method. All these theoretical and design works therefore lays the foundation for the next chapter, which will feature the demonstration of such PhC designs enabled through the development of deep sub-micrometer processing techniques, including critical fabrication modules such as sub-wavelength lithography and ICP etching techniques etc.

CHAPTER 4

OPTICAL PHOTONIC CRYSTAL FABRICATION

The objective of this chapter is to develop the fabrication technologies required to realize deep sub micrometer sized optical PhC devices, which are sensitive to the canonical communication wavelengths centered at 1550 nm. Especially, since the performances of PhC devices are heavily process dependent – and PhC fabrication technologies are not mature – it is therefore crucial to develop a flexible fabrication template suitable for realization of different PhC types (such as the 2D hole/ rod type PhC). Amongst the many processing steps required to fabricate working PhC devices, patterning and pattern transfer into device material are especially critical and challenging since PhC devices are typically sub-micrometer in size, and arranged in contrasting super-dense and nearly isolated densities of bulk and defect regions respectively. To successfully demonstrate working PhC devices, the difficulties attributed by these unique characteristics of PhC must be overcome. To do so, the issue of drastically reduced process window of DUV lithography, DRIE, and post processing modules for a super dense array of submicron size rods or holes features with typical diameters of 90-230 nm and spacing of 340 nm apart is specifically treated in this thesis.

This chapter begins with a presentation of the process flows designed for planar PhC structures. Following this, the OL process is introduced to initiate and explain the strategies taken to push the lithography process beyond its conventional limits whilst keeping photomask fabrication cost and system simulation time cost low.

With this foundation, the lithographic experiment set-up is presented and discussed to enable further presentations of the details involved to achieve high resolution PhC patterning. Here, rigorous design of experiments yielded necessary PhCs devices with precise lattice dimensions even near regions of “defect structures” designed for device operations.

Completion of the OL process manipulations then allows development of the etching process, and other post processing modules. Especially challenging in this phase, was the development of the etching module – where the stringent requirement of etch angle needed for successful realization of such super dense array of submicron size PhC lattice need to be satisfied before any working PhC device can be achieved. DRIE was the method of choice developed. Based on the developed methodology, etch sidewalls of high verticality, and record HARs with ultra-low scallop-depths was obtained.

4.1 Design of Fabrication Process Flow

In the experiments to achieve sub-lithographic wavelength OL, only conventional binary chrome-on-glass photomasks without phase shift features were used. Positive DUV chemically amplified resist (CAR) was coated atop a bottom anti-reflection coating (BARC) using a Tokyo Electron ACT8 wafer-track-system. A DUV Nikon S203B laser step and scan system was used for controlled 248 nm wavelength exposure [77]. The SOI wafers were first prepared using standard steps of cleaning, particle counting, and surface profiling before a blanket deposition of 5000 Å undoped silicate glass (USG) using a Novellus Concept Two Sequel plasma enhanced chemical vapor deposition (PECVD) system. Uniformity of hard mask and

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other characterizations were then checked for before commencement of lithography process.

To permit for independent manipulation of the lithographic and time-multiplex etch processes, different requirements for masking together with corresponding recipes are needed to realize drastically different mask openings and etch depths, for PhC array of rods ($\sim 13\ \mu\text{m}$ deep with $340\ \text{nm}$ wide openings) and for deep trenches required to couple standard SMFs (more than $50\ \mu\text{m}$ depth and $125\ \mu\text{m}$ wide openings).

A rigorous design of fabrication process for single crystal silicon wafers without any buried oxide layers is as follows. An initial mask for the deep-submicron size PhC structures were first defined through a thin layer of hardmask, using a similarly thin layer of photoresist spun on top of an anti-reflection coating. When the pattern was transferred onto the pre-deposited undoped silicate glass (USG) hardmask using magnetic resonance reactive ion etching (MERIE), Photoresist strip was then carried out for a refill of even thicker resist needed for the longer duration deep fiber grooves etching, exposed aligned to the first. When the required depth of the fiber grooves were achieved, any remaining photoresist was then stripped to reveal the PhC structures in the hard mask for final device etch. Upon achievement of sufficiently HAR, the PhC rod type 2D device was then formed. In another process, a thinner 2D PhC device comprising a slab of holes perforated SOI wafer may be obtained using the process flow of Fig. 4.1.

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Fig. 4.1 Fabrication process flow for two-dimensional hole type photonic crystal in silicon-on-insulator wafers.

Here, Fig. 4.1 also exhibits the design of process flow is a critical factor in the fabrication of PhC with other structures. Not solely for the effective development of

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each process module such that different requirements with corresponding recipes may be discovered through rigorous design of experiments; the proper sequence of processing steps also prevents elemental contamination of reaction chambers, material degradations, and process overruns et cetera. Here, the fabrication process flow for control of lithographic, deep etching processes with disparate requirements are shown as a schematic of the integrated fabrication process flow for PhC with optical testing structures, which may be described in four main parts: Integrated fabrication process flow for PhC with optical testing structures. Steps (a) - (c) describes the deposition of the metal electrodes and oxide hard mask layers. Steps (d) – (f) describes the PhC and comb drive CD pattern definition and transfer process. Steps (g) – (i) describes the opening of large alignment structures while steps (j) – (l) depicts the oxide release and also post processing modules.

Film material deposition processes was initiated with USG on cleaned SOI wafers. Following electrode pattern opening in hard mask (Fig. 4.1a), copper seed deposition and metallization plating (Fig. 4.1b). Planarization was then carried out using chemical mechanical polishing (CMP). To avoid contamination in subsequent steps, another layer of USG film was deposited to cover the defined electrode (Fig. 4.1c). The deposition of this protective USG layer therefore completes the first part of the thin film processes and lay foundation for the second set of steps necessary for CD definition. Here, PhC together with the optical testing structures were defined in photoresist on a layer of anti-reflection coating (Fig. 4.1d) prior to MERIE etching of PhC for good profile transfer of CDs onto the hard mask layer (Fig. 4.1e). Complete resist strip after this step (Fig. 4.1f) in the second phase then allows the third phase of OTS fabrication to begin.

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Here, a different photoresist of higher viscosity was spun on thickly without first coating a BARC layer (Fig. 4.1g). Due to the shallow depths of the hard mask patterns defined in the previous phase, the resist coating recipe may be developed to successfully planarize the surface, enabling exposure of the second photomask after alignment to at least five underlying marks patterned during the first exposure (Fig. 4.1h). The testing structures exposed may therefore be sequentially etched for the: hard mask oxide, SOI device silicon, SOI buried oxide then SOI handle silicon again, till an etch depth of nearly 60 μm (Fig. 4.1i). This step completes the construction of OTS and the wafers undergo the final phase of PhC and optical testing structures etching and other post processing modules.

In Fig. 4.1j, photoresist strip and polymer cleaning was performed prior to device etching so as to enable simultaneous etching of both PhC structures and the OTS, using etch recipe developed to optimized etch quality of the PhC devices. After device sidewalls optimization, chemical buffered oxide etching (BOE) was then performed to release both the movable structures and the air bridge type PhC devices (Fig. 4.1k). In this step, not only was peeling of the metallic electrodes prevented, precaution was also taken to ensure no further rework in case of contamination arising from the exposed electrodes.

Next, Fig. 4.2 shows the fabrication process flow for rod type PhC fabrication on SOI wafers for buried oxide layer cladding. In this process, PhC rods realized in the device layer may be filled in between with silicon dioxide for waveguiding mode symmetry. Here, due to the introduction of an insulating oxide layer and reduced radius PhC rods waveguide, out-of-plane control of radiation was introduced and the PhC rods need not be etch for very HAR. For SOI wafers of device thickness 3 μm

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and reduced radius PhC rods radii less than 50 nm, special techniques are needed for sub-wavelength lithography, smooth etch sidewall profiles et cetera.

Fig. 4.2 Fabrication process flow for rod type photonic crystal in silicon-on-insulator wafers.

4.2 Sub-Wavelength Lithography

In the past, the most straightforward way to improve resolution was to decrease the wavelength of radiation, as illustrated in Fig. 4.4. However, reduction of wavelength beyond Argon Fluoride (ArF) lasers emitting at 193 nm would require a drastic redesign of lithographic system since shorter wavelengths are simply absorbed by the quartz lenses that direct source light in current systems with laser wavelengths between 193 to 432 nm. Alternatively, RETs [78-80] such as PSM, optical proximity correction (OPC), and off-axis illumination (OAI) may be used for exposure systems of specific wavelengths to improve their respective resolution limits (as indicated by the line marked with round symbols in Fig 4.3).

Fig. 4.3 Limits in resolution improvement through reduction of optical lithographic wavelengths.

Whilst each of these techniques improves baseline resolutions, they are limited mainly by their respective drawbacks, which for PSM (Fig. 4.4a) and OPC are the cost and computational efforts required for implementation, whilst for the various OAI schemes illustrated in Fig. 4.4b, it is the discrimination needed for varying pattern densities. Therefore, alternative approaches for achievement of sub-wavelength lithography resolutions have been widely investigated in recent years [81, 82].

Fig. 4.4 Illustration of (a) phase shift masking technique with use of shifters within glass mask. (b) Off axis illumination of the annular and quadrupole schemes.

To develop OL, it was a key consideration that out of the major components used in a set of optical exposure system, the radiation source cannot be easily changed as compared to the parameters of the condenser; mask; wafer; pattern design; resist chemistry; coating mechanisms et cetera. The various parameters of the imaging system such as the lens set numerical aperture (NA) and partial coherence of the condenser system design can also be varied for different lithographic performance.

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Whilst an ideal lithographic projection tool should be coherent with unity NA (a measure of how well a lens is able to collect diffracted light from a photomask and in turn project the image onto the wafer as illustrated in Fig. 4.5), real systems without immersion technology cannot provide unity NA, nor purely coherent illumination since the total image is the sum of all the intensity images from all source points. The degree of coherence factor is usually expressed as

$$\sigma = \frac{NA_c}{NA_p}, \quad (4.1)$$

where $NA_c = n \sin \theta_c$ and $NA_p = n \sin \psi_{\max}$ represents the NA of the condenser and the projection lens, which is in turn determined by n the refractive index at the image plane; $\psi_{\max}$ and θ_c which are the maximum cone angle of rays subtended by the maximum pupil diameter at the image and condenser plane respectively (see Fig. 4.5).

Based on the theoretical resolution limits of an otherwise ideal imaging system, the Rayleigh equation for resolution of imaging system is given by

$$R = k_1 (\lambda / NA), \quad (4.2)$$

where λ is the wavelength, and k_1 is the process-dependent constant. This equation not only provides the limits of OL as shown in Fig. 4.3, but also indicates the latitude of processing windows for different CDs. Hence, for 100, 200 and 300 nm resolution, the k_1 process constant needed can be calculated as shown in Table 4.1.

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Fig. 4.5 Schematic of an on-axis illumination lithographic system for depiction of maximum cone angles in the condenser and projection lens.

Since controllable processes typically operate in the range of $k_1 \cong 0.6$ to 0.7 , it can be deduced from the table that while resolution near 200 nm is difficult to achieve without high NA , RETs are essential for CDs below 200 nm . At the same time, while lens with higher NA would be able to collect more diffracted orders and consequently more information to correctly reproduce the required image, there would be an inherent trade off with depth of focus (DOF), since

$$DOF = k_2 \frac{\lambda}{NA^2}, \quad (4.3)$$

where k_2 is the second process constant. It is clear, therefore, that for high resolution, increases in lens NA quickly decreases the DOF , which should have preferably a large value (since tolerances for wafer flatness, resist coating etc should be more than

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a few hundred nanometers). Therefore, alternative control of photomask pattern densities and lithographic partial coherence factors should be used to achieve such similar resolution improvements. For partially coherent systems, the resolution of the imaging system can be described with some correction to Eq. 4.2 such that

$$R = k_1 \frac{\lambda}{(1 + \sigma)NA}. \quad (4.4)$$

Therefore, the increase of coherence factor can be used to derive improved resolutions.

Table 4.1 Theoretical resolution limits of line widths by deep ultraviolet optical lithography.

Numerical aperture	300nm	200nm	100nm
0.30	0.36	0.29	0.12
0.40	0.48	0.39	0.16
0.50	0.60	0.49	0.20
0.60	0.73	0.59	0.24
0.70	0.85	0.68	0.28
0.80	0.97	0.78	0.31
0.90	1.09	0.88	0.35
1.00	1.21	0.98	0.39

	Resolution enhancement techniques needed
	Typical optimized process parameters
	Process parameter without optimization
	Process constant beyond theoretical limits

4.3 Lithography Experiment Set-Up and Methods

The lithographic experiments were carried out using a resist track; a DUV scanner based on the KrF laser of 248 nm and a binary mask of four times

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magnification without phase shift features with positive DUV resist (Shipley UV210 and JSR 221). Prior to resist coating, it is important that wafers are cleaned and primed to minimize the effect of surface oxides, which form long range hydrogen bonds with water adsorbed from air (resist adheres to water vapor rather than to wafer surface) resulting in poor resist adhesion to wafer surface. Therefore, in the experiments, cleaning and priming with hexamethyldisilazane (HMDS) was carried out using the liquid priming process of spinning solvent-diluted HMDS. Resist can then be spun onto primed wafer surface with the target of greatest possible uniform thickness. Although the physics of spinning is complicated, it can be determined to be strongly dependent on the evaporation rate of the solvent used together with the assistance of spin speed charts. A pre-exposure bake then drives solvent from the resist enabling high quality profile when appropriately carried out whilst decreasing the sensitivity of process if over-done. Post exposure, another bake is needed to reduce standing waves on resist profiles. Development of resist was then carried out following a final post-develop bake to improve the resist's etch resistance.

4.3.1 Lithographic Parameters Manipulation

Whilst the resolution of the lithographic process is not a fixed number but depends on the factors of pattern type; resist thickness and wafer topography, it is generally easier to print an isolated feature than a dense pattern like that of a PhC structure. At the same time, it is important that the focus of a system is always checked and compensated for - prior to exposure by adjustment of lens to wafer distance. For projection method of lithography used, the "resolution" that determines the narrowest line/ space of a repetitive pattern that can be correctly reproduced is given by Eq. 4.2, while the other critical factor, DOF is given by Eq. 4.3. These

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factors effectively form the limiting determinants for the spread functions that control the size of isolated and dense patterns. When these parameters are not carefully controlled, typical failure modes that occur include uprooted resist (Fig. 4.6a) due to diffracting wave mis-focusing; missing patterns (Fig. 4.6b) due to illumination over-dose and distorted shapes of resist profile (Fig. 4.6c) due to overlapping wave-functions interference.

Fig. 4.6 Lithographic problems that arise from un-optimized process conditions include (a) uprooted resists, (b) missing patterns, and (c) distorted shapes.

According to Eq. 4.2, it is clear that for good resolution, the value of proportionality constant k_1 and λ should be the smallest possible whilst the value of NA is the largest possible. Technologically, the reduction of λ hits a barrier beyond 193 nm since shorter wavelengths are simply absorbed by the quartz lenses that direct source light onto the wafer and therefore cannot be used without a drastic redesign of lithographic systems. At the same time, because the DOF of Eq. 4.3 is inversely proportional to the square of the NA , increasing the aperture to improve resolution quickly decreases the DOF, which should have a value of greater than 500 nm since wafers cannot be perfectly flat and photoresist usually has thickness variation of several hundred nanometers. To increase the value of NA for better

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resolution, lens designs of larger diameters and greater lens element count are used to increase the amount of light collected through the photomask. On the other hand, to reduce the trade-off between R and DOF, k_1 can be reduced through improvement of the illumination coherence, anti-reflection coatings and also resist parameters. Hence, two-level, multiple two-factorial experiments were carried out by running the experiments with different levels of BARC and CAR thickness to yield results of process windows summarized by the focus exposure matrixes (FEMs) of Fig. 4.7.

From the plots, it can be seen that the poorest exposure latitude was obtained for the case of high level of CAR and low level of BARC (Fig. 4.7b) while an increase in level of BARC still resulted in slanted profiles of the process window (Fig. 4.7d). On the other hand, decrease in the level of CAR shown improvement in latitude of process window for both high and low levels of BARCs (Figs. 4.7a and 4.7c). The plot of the FEMs with low level of CAR and high level of BARC can be seen to yield the greatest exposure latitude and also focus range (Fig. 4.7c). Hence, the effect of CAR thickness can be significant and a smallest k_1 can be obtained for a lower level of CAR thickness and higher level of BARC. These results supported the fact that reduced aberrations result from minimum resist thickness whilst presence of BARC aids reduction of the effect of lithographic dimensional errors due to minimization of scattering from substrate material. Furthermore, it has also been identified that these two parameters have a minimum interaction effect as indicated by the non-twisting of their response surface when the results of Fig. 4.7 are plotted in 3D.

Fig. 4.7 Plots of focus exposure matrix for (a) low-, low-; (b) high-, low-; (c) low-, high- and (d) high-, high- level of resist thickness and anti-reflection coating respectively.

4.3.2 Optical Proximity Error Model

Beyond the improvement of Eqs. 4.2 and Eq. 4.3 as discussed, other methods for resolution enhancement include techniques such as OPCs, use of PSM and OAI systems to manipulate the amplitude, phase or propagation direction of the illuminating electromagnetic waves respectively. Whilst there are high computing powered programs available for OPC, these are often costly and in state-of-the-art IC layout tools. On the other hand, PSM is also relatively much more costly (as compared to a conventional binary photomask). Finally, whilst OAI of annulus, dipole and quadrupole types had been demonstrated to work well for dense areas of repetitive patterns, the technique faces limitation for isolated features, which will

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often be encountered in our application to PhC device in the form of tunneling defects and the likes.

In this study, a binary mask and non-shifted axis illumination exposure system were used for achieving required PhC defect structures within a dense matrix of otherwise similar sized PhC rods. Here, the achievement of designed tunneling defect size is critical for successful fabrication of PhC devices with useful properties. Current challenge in this area lies in the fact that PhC devices are super-dense arrays of periodic structures with feature size close to the lithographic wavelength. Hence, by the effect of diffraction, dense neighboring features illuminate to interfere with each other either constructively or destructively to print smaller and larger rods respectively as opposed to being isolated, to give rise to the OPE effects. This unavoidable phenomenon affects the fundamental dispersion characteristic of a designed PhC drastically as can be seen in Fig. 4.8, in a single line defect waveguide where the rods near the waveguide defects patterned (Fig. 4.8a) much smaller than designed (Fig. 4.8b), such that the originally single mode (Fig. 4.8d) waveguide becomes multi-modal within the bandgap frequencies (Fig. 4.8c).

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Fig. 4.8 (a) Top view scanning electron micrograph (SEM) of photonic crystal array with proximity errors along the periphery rods of the intersecting line defect waveguides, and (b) its corresponding multi-mode dispersion simulation result. (c) Photonic crystal after resolution enhancement by proximity correction and (d) the single mode dispersion property within the bandgap frequency range.

To overcome this problem of OPE between bulk, semi-isolated structure and isolated features, test patterns with mask biases of varying degrees and shapes were designed to yield CD measurements for varying exposure energy (E), focus (F), “correction factor” (CF) and “shape factor” (SF). Here, CF s were varied with different sizes of the periphery PhC rods and defined as their diameter ratio to that of

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the intended bulk rods' diameter as designed on the optical mask. The SF used corresponds to the circular and the square shape of the rods drawn with width of squares equated to the diameters of the circular rods needed (i.e. for the square shaped rods drawn, the same definition of correction factor applies with simply replacement of square width with circular diameter).

Based on these two designed experiment control parameters, the measured results are recorded as “experiment factor” (EF) giving the measured rods' diameter normalized by actual bulk PhC rod diameter. For the two sizes of rods diameters 300 and 360 nm investigated, two types of SF s (square and circular shape) and eight sets of CF s were tested using varying F and E between 0 - 0.2 and 18 – 22 mJ/cm² respectively. Each treatment combination of SF and PhC rod size was varied against the other parameters as described to yield 43 sets of measurements each, resulting in a total of 172 data sets.

By first studying the result of these experiments through scatter matrix plots, correlations of the experiment factors with respect to CD errors measured can be deduced. Therefore, based on initial hypothetical multi-linear models, with regressors of CF , E and F deduced accordingly, the OPE measured for the different structures can be used to obtain fitting parameters for each of the regressors such that prediction errors by the models are minimized. In this way, much-simplified OPC models were derived for both the semi-isolated and isolated structures, where the former was fitted with singular power factors of CF , E and F , while the latter was fitted with a double power factor for CF , and singular power factor for E and F .

In Fig. 4.9, the exaggerated effects of variations in CF s (as ratios of periphery PhC rod diameters to bulk ones) for values of 1.1 to 1.8 are shown as designed on the

photomask (with actual CF values used ranging from 1 to 1.07 in steps of less than 0.01).

Fig. 4.9 SEM of varying CF s (in dash-line boxes) along the periphery of bulk photonic crystal rods in exaggerated scale.

Also, variations in SF s were designed as different shapes of circles and squares drawn on the layout of the schematic. The micrograph photographs of the fabricated photomask with these SF s are given in Fig. 4.10. By plotting scatter plots of lithographic errors (LE) for each of these experiment conditions, trends for dependencies can be identified and expressed as a function of E , F and CF such that:

$$LE_k = a_0 + a_1 E_{k,1} + a_2 F_{k,2} + a_3 CF_{k,3} + \varepsilon_k, \quad (4.5)$$

where a_0 , a_1 , a_2 , and a_3 is a set of best estimate modeling parameter and ε is the error of estimation, which can be reduced [120] to:

$$\hat{\underline{a}} = (\underline{X}^T \underline{X})^{-1} (\underline{X}^T \underline{Y}), \quad (4.6)$$

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where $\underline{X}$ is a 43-row matrix of ones with the second and subsequent columns replaced by coefficients of E , F and CF respectively; whilst $\underline{Y}$ is given by the measured values of LE . The results of the regression model were therefore obtained and summarized by Table 4.2. Using these model parameters, the prediction errors for each treatment can be shown to have median errors of less than 1% and standard F-numbers of 14 to 67 indicating significance of regression at above 97.5% confidence level. This OPC model therefore allows for proximity corrected PhC device structures with appropriate defect sizes, and average measured deviations below three percent target value.

Fig. 4.10 Micrographs of fabricated photomask with chrome-on-glass patterns of photonic crystal rods (a) without shape factor correction, (b) with shape factor correction.

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Table 4.2 OPC regression model parameters obtained through minimization of regression modeling errors for different shape factors and photonic crystal rods diameters.

Shape factor / Model	Constant	Energy	Focus	Correction factor
Square ($w = 360\text{nm}$)	-0.4301	-0.0012	-0.0151	1.4711
Square ($w = 300\text{nm}$)	-1.1162	-0.0045	-0.0089	2.1917
Circle ($\varnothing = 360\text{nm}$)	-0.5868	-0.0001	0.0084	1.5873
Circle ($\varnothing = 300\text{nm}$)	-0.5901	-0.0203	-0.0143	2.0161

An OPC model was therefore developed based on such design of experiment for experimental compensations, which allowed for proximity corrected PhC device structures with appropriate defect sizes, and average measured deviations below three percent target value. Thus, mask bias corrections can be made in anticipation of OPE, improving resolution of near sub-wavelength DUV OL without use of expensive PSM or high-end computations to yield compensated results of Fig. 4.8c, where PhC device structures near defect structures are obtained with desired dimensions.

4.3.3 Partial Coherence and Pattern Density Control

Based on this, critical line width experiments may be carried out. Optimized resist coating recipe was applied, first with wafer surface priming by HMDS for adhesion preparation, followed by a layer of BARC (Shipley AR3) that was spun at a combination of rotation speeds between 1.5k to 4.5k rpm for 40 seconds before bake at 205 degrees for 60 seconds. Following which, the spun layer of BARC with thickness 600 Å was then baked at 130 degrees for 60 seconds. For application of CAR with thickness 4800 Å, the CAR was spun at rotation speeds between 1.5 krpm to 2.5 krpm for 40 seconds. After a pre-exposure bake, the wafers undergo a wafer edge exposure for removal of edge bead formed in the resist coating spiral stage (after

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approximately a thousand revolutions). Line widths experiments were then carried out using patterns of lines with widths 200 nm, and duty factors (line/space ratio) of 1:3 and 1:1, as shown in Fig. 4.11. CDs of each set of duty factor experiments were taken using a Hitachi 9200 CD Scanning Electron Micrograph (SEM) imaging system. Based on a lithographic imaging system with a calibrated zero focus and NA of 0.68; the designed line widths of 200 nm was used in OL experiments for values of coherence factors being 0.38, 0.45 and 0.51.

Fig. 4.11 Lithography experiment patterns with constant line-widths, and different pattern density of line/space duty factors (a) 1:3 and (b) 1:1 respectively.

The results of the partial coherence variation experiments were plotted as measured CDs with respect to the exposure dosage used, as shown in Fig. 4.12. From the CD plots of the line width experiments, it can be seen that the 1:3 density patterns are much more sensitive to coherence factor variations than that of the 1:1 density patterns. Especially, the 1:3 density patterns have measured line widths, which were drastically reduced for the exposure with coherence factor 0.51 as compared to the exposures with coherence factors 0.38 or 0.45. On the other hand, the higher density 1:1 patterns had similarly reduced line widths for all three coherence factors used. From further such experiments, it was obtained that reduction of original line widths

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to less than 200 nm allowed for further reduction of CDs obtained. However, such progressive reduction of designed line widths for corresponding reduction of CD approaches its limit at a drawn line width of ~ 130 nm. This is due to the reduced process window of the smaller CDs, where small deviation in exposure energy or focus leads to lithographic failures.

(a)

(b)

Fig. 4.12 Critical dimension plot for lithography experiments with a constant numerical aperture of 0.68, and varying coherence factors of 0.38; 0.45; and 0.51 for line patterns with duty factors of (a) 1:3 and (b) 1:1 respectively.

Examples of typical exposure failures, brought about by such constraints are as shown in Figs. 4.13 and 4.14, where in Fig. 4.13a, unresolved features results from insufficient exposure dosage in spaces between dense line patterns; and in Fig. 4.13b, resist peeling occurs at narrow ends of line patterns due to over-exposure. In Fig. 4.14, there is the necking effect, where biasing of patterns near line terminations are required in order to prevent neck breakages at line ends. The layout and exposure lithographic variations are shown for a narrow line end (Fig. 4.14a and 4.14b) where there is the pull-back mechanism and in a connected line end (Fig. 4.14d and 4.14e) where there is the flaring mechanism at the end of the connected lines. Combined together, these two effects constitutes the mechanisms for necking such that pull-back coupled with flaring in the mild case leads to patterns of critical line widths with constricted 'neck' interfaces as shown in Fig. 4.15a. In the unbridled case of necking, extreme constrictions leads to critical line breakages at line-base interface as shown in Fig. 4.15b.

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Fig. 4.13 SEM images of sub-lithographic wavelength exposure failures for (a) unresolved dense structures, and (b) lifted off resist.

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Fig. 4.14 From left to right, (a) schematic illustration of layout, followed by (b) lithographic variations, then (c) SEM example due to pull-back mechanism at line end; and similarly, (d), (e), and (f) respectively for flaring mechanism at end of connected lines, combined to cause 'necking'.

Fig. 4.15 (a) Patterns of critical line widths with constricted 'neck' interfaces. (b) Extreme constrictions leading to critical line width breakages at structure interface.

4.3.4 Chemically Amplified Resist Deactivation

DUV radiation exposure on the CAR results in formation of minute catalytic amounts of acids in the exposed areas of CAR as determined by the openings on the chrome photomask. Subsequent processing by acid chemical-amplification processing then allows the CAR to become soluble in the alkaline-developer solution, allowing the removal of the exposed resist. If, however, the minute acid formed during exposure is unintentionally quenched by base impurities on the wafer or in the environment, chemical amplification can be deactivated, causing erroneous patterning where CAR are not effectively removed by the developer where an opening should be. This type of “resist poisoning” is illustrated in Fig. 4.16a, where a PhC lattice of holes was patterned and some holes are not properly developed to result in positions of missing holes.

Fig. 4.16 (a) Square photonic crystal holes array patterns with areas of resist poisoning (missing holes in a uniform holes array). (b) Unintended resonators form within the photonic crystal holes lattice.

Such defects install optical states within bandgap frequencies, which can become micro-cavities that act as unintended resonators (Fig. 4.16b). To deter the formation of such deactivated CAR, the presence of weak base pyrimidine ($C_4H_4N_2$) resulting from treatment with solvent should be avoided with minimization of resident time after solvent cleaning process for successful lithographic patterning [107]. It is important to avoid such instances of resist poisoning since reworks are not only complicated but also often ineffective.

4.3.5 Photoresist Trimming for Critical Dimension Reductions

Beyond the many RETs presented so far, there is still an overriding need to decrease the size of the smallest feature printable using OL. While the development of shorter wavelength lithography together with its accompanying lens systems, resist chemistries and mask material etc are continuously being explored, developmental progressions take considerable time. Hence, it is very useful to make use of the technique of dry plasma etching in order to further reduce the size of the smallest feature printed by resolution enhanced OL. Such a method, known as “photoresist trimming” (or “photoresist ashing”, “oxide lateral etching”, and “resist thinning”) [137], makes use of oxygen based plasmas to etch photoresist polymers isotropically. Halogens or fluorocarbon gases are also added to provide control over the ratio of the lateral and vertical etch rates.

In this work, the resist trimming recipes were developed for a thin layer of CAR, deposited atop a layer of organic BARC. An ICP etcher was used to generate CF_4 and O_2 plasma in this process. While the O_2 plasma was used mainly to isotropically etch a developed resist pattern, CF_4 fluorocarbon was used mainly as a polymerizing gas to ensure vertical resist profile after trimming. In such photoresist

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trimming process, the key parameters to be controlled are gas composition; wafer temperature; bias voltage; chamber pressure; source power; and total gas flow.

First, in terms of gas composition, an initial addition of polymerizing CF_4 gas helps accelerates the hydrogen extraction process from the resist pattern, which therefore increases the trim rate. However, this trim rate increment effect saturates with further supply of CF_4 gas, since the increased concentration of polymerizing gas deposits around resist patterns, hindering the etch process by the reduced concentration of O_2 plasma. Second, trim rate increases as wafer temperature increase as can be expected since higher temperature enhances chemical reaction rates and reduces sidewall polymer deposition. Third, lateral trim rate on the other hand generally decreases with increases in bias voltage; since with higher bias voltages, the ions are more energetic and are less likely to be deflected laterally to aid the trim chemical reaction. Fourth, increasing the chamber pressure serves to decrease ion energy since increased number of collisions arises. However, it also increases the scattering of reactive species onto resist sidewall and therefore enhances trimming reaction. Further, increases in pressure also increase the neutral chemical flux which also serves to increase the trim rate. Fifth, trim rate also increases with source power since enhanced dissociation of O_2 plasma reactive species aids the resist etching process. Finally, the effect of increasing total gas flow only increases trim rate as much as it is possible to increase the number of chemical reactions around the photoresist pattern surfaces.

An optimized resist trimming recipe has high uniformity across the wafer, and maintain good pattern integrity (e.g. no line bending etc). This can be obtained using only O_2 and Ar gas, with flow rate of 5, and 45 sccm respectively. For chamber pressure of 2 mT, platen power of 25 W, and coil power of 600 W; a trim rate of 400

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$\text{\AA}/\text{min}$ was obtained in the vertical direction, together with a trim rate of $500 \text{ \AA}/\text{min}$ in the horizontal direction for isolated resist patterns. For highly dense PhC resist patterns however, trim rate tends to be correlated with the pattern density. For PhC resist patterns (created in a stack of $600 \text{ \AA}$ BARC (Shipley AR3) and $2800 \text{ \AA}$ CAR (JSR M221), and exposed using the same track and DUV OL techniques), the uniformity and quality of the trimming process were measured using test patterns with varying CDs and densities. Fig. 4.17 shows the trim result of PhC resonators with radius ranging from 100 to 250 nm, subjected to trimming process time of 55 s.

Fig. 4.17 Critical dimension measurements of resonators with radius ranging from 100 to 250 nm, before and after the trimming process.

For each CD resonator, placed within a similar single resonator structure surrounded by bulk PhC rods such as that shown in Fig. 4.18b, five measurement points were taken at the middle, left, right, top and bottom positions of the wafer. These readings were plotted on the vertical axis of Fig. 4.17 for each corresponding

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point of measurement (plotted along the horizontal axis). Based on these readings, it was shown that an average radius trimmed was $256 \text{ \AA}$ – corresponding to a lateral trim rate of $559 \text{ \AA/min}$ for each PhC rod CD. Although very similar trim rates were obtained for PhC resonators of different CDs, placed within a similar bulk PhC lattice; it was found that trim rates were varied by surrounding structures (such as that of single line defects shown in Fig. 4.18a, bulk PhC of an unperturbed lattice, or single resonators of Fig. 4.18b).

Fig. 4.18 (a) Single line reduced radius rods within a line defect photonic crystal waveguide. (b) Single resonator rod surrounded by bulk photonic crystal rods.

Figure 4.19 shows the results of patterning and trimming found for different PhC pattern densities, specifically of the single resonator and bulk PhC lattice rods. While bulk rods patterned to become much larger than their reduced size counterparts drawn within a single resonator pattern on the photomask, they trimmed down by nearly the same amount to give similar CAR etch rates. This is in contrast with the trim bias, found for PhC rods, patterned in a single resonator versus a single line

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defect pattern, as plotted in Fig. 4.20. Here, it can be seen that while the differences in pattern density did not result in significance differences in the initial lithographic process, the line defect PhC rods were trimmed down to a smaller size than those found in a single resonator configuration. Hence higher corresponding etch rates were found for the single line structures rather than that of the resonator ones. This may be attributed to the increased opening size along a ‘line’ rather than a ‘point’ defect, which would enable greater transport of trim reactants towards the trim sites.

Fig. 4.19 Comparison of trim result for photonic crystal rods of the same critical dimension, placed within the bulk lattice and within a single resonator structure.

Fig. 4.20 Difference in trim rate for varied pattern densities of single line and resonator structures.

Figure 4.21 shows SEMs of the CAR pattern in a single line PhC waveguide before and after the trimming process. Here, it can be seen that the isotropic trim process not only reduces the CDs of the PhC rods laterally, but also serves to etch away vertically, the BARC up to a thickness of 60 nm. From the profiles of the patterned photoresist as shown in Fig. 4.20a (which are tapered from the base up) and the FEMs of Fig. 4.22 (where small exposure latitudes were found), it can be seen that the limits of the process would impede further reduction of CDs using lithographic RETs. Hence, to obtain sub-100 nm CDs, resist trimming is an important technique. Figure 4.23 shows the top down SEM image of some PhC optical intersections, with single line reduced radius PhC rods; resonator rod and the surrounding PhC bulk crystal prior to and after the optimized trim process. Figure 4.24 shows the cross-sectional counterpart to Fig. 4.23b.

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Fig. 4.21 SEM of line defect rods flanked by bulk photonic crystal lattice. (a) Photoresist patterned by deep ultraviolet lithography (b) Trimmed photoresist with sub-100 nm critical dimensions.

Fig. 4.22 Focus exposure matrix for reduced radius photonic crystal critical dimensions.

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Fig. 4.23 Top view SEM of photonic crystal optical intersections with critical dimensions (a) before, and (b) after trim processing.

Fig. 4.24 Cross-sectional SEM of trimmed photonic crystal rods resist pattern, with the reduced radius line defect rod flanked by two bulk rod pattern.

4.4 Post Lithographic Processing

After achievement of high-resolution PhC lattices in lithography, development of etching formulations are necessary to yield derivation of acceptable etch process window, for very deep etching of PhC lattices of HAR deep-submicron size rods (aspect ratio beyond 50) previously unattainable by the DRIE method for such length scale. Together with the suppression of etch sidewall “scallop” - a critical shortcoming of time multiplexed etching - in the form of sidewall undulations causing surface roughness; an atypically low value of scallop depth, being only 12 nm was obtained.

Using a STS deep etcher with ICP sources for plasma generation (coil) and biasing (platen), DRIE was carried out using the Bosch process [108] where time multiplexed scheme of etching and passivation enabled by well-controlled gas inputs, facilitate the achievement of vertical sidewalls in deep etching that consumes relatively lesser protection material. This is due to the switching between etching and passivation steps that are repeated as necessary. First, a silicon opening unprotected by masking material is etched using fluorinated gas chemistry comprising mainly of sulphur hexafluoride (SF_6) to give a slightly isotropic profile (caused by lateral physical etch effect of impacting ions at etch surface). The action of reactive ions results mainly by the formation of ion and radical species, by electron impact dissociation

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so that the ion-assisted fluorine radicals then react with silicon openings to form a volatile silicon by-product gas, which is then removed. Here, by mixture of oxygen (O_2) in the etching gas chemistry, suitable sidewall passivation can be formed

even during the etching phase such that the passivation layer derives from the formation of SiO_n , which adsorbs onto the surface of exposed silicon as an oxide layer (with passivation properties since subsequent etching reaction requires its removal prior to action by F). Therefore, after the etching phase, the chamber is pumped out and passivation gas octafluorocyclobutane (C_4F_8) is applied for deposition onto the wafer (coating both base surfaces and also sidewalls of trenches and other openings).

These two steps are then repeated as necessary to obtain the required amount of etch and passivation cycling. Generally, due to the assistance of platen power for the vertical etch direction; the directionality of reacting ions in the vertical direction is high, compared to the rate at which fluorine radicals are bombarded onto laterally exposed surfaces due to impact scattering and also chemical reactions. Hence, the vertical etch component is much more significant such that of the etch rate in the lateral direction, which is often considered negligible. At the same time, formation and removal of passivation compounds together with the etching of silicon must be designed to act in balance so as to maintain etch profile anisotropy. Otherwise, dominance by passivation would lead to low etch rates or even etch termination by surface residue build-up. On the other hand, insufficient passivation leads to loss in anisotropy and increased lateral etching occurs.

4.4.1 Unique Considerations for Photonic Crystal Rods Etch

General RIE etch concepts that are established for standard micrometer size devices have to be applied with much more stringent requirements since reduction in feature size results in a corresponding decrease in process window and tolerance. Hence, due to the reason that PhC used at the optical communication wavelength of $1.55\ \mu\text{m}$ has CDs of only a few hundred nanometers, stepwise isotropy and lateral etch rates need to be carefully monitored to prevent fabrication failure as shown in Fig. 2.1.

At the same time, etch scallops of undulations in sidewalls are inevitably formed during the etch/passivation cycling process due to the existence of isotropy in etch species bombardment phase. Past results of DRIE [109] has demonstrated scallop depths ranging between 50 to 300 nm. However, such depths of undulations on PhC rods can be unacceptable, as diffused scattering caused by such drastic scalloping can obliterate precisely designed Bragg reflections (of the designed PhC lattice structure) that constitutes the PBG effect. Therefore, to ensure that PhC properties are preserved, it is important that etch scalloping (resulting in etch profile undulations) be kept at a minimum to reduce the effect of diffused scatterings.

4.4.2 Development of Deep Reactive Ion Etching

The time multiplexed action of etching and passivation gases applied with independent bias control of the substrate was studied using an initial recipe of manual pressure control at 50 %; etching chemistry comprising of C_4F_8 , SF_6 and O_2 gases and passivation chemistry comprising only the C_4F_8 gas. The coil power was maintained at 600 W for both passivation and etch phase, while platen power was

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applied only for the etch phase. For dominating passivation processes, a re-entrant etch sidewall profile was obtained with a lower etch rate, often resulting in self-induced etch stops. This is due to the reason that plasma polymerization reactions require relatively high ion bombardment energies of several hundred electron volts (eVs) for their complete removal. At the same time, besides termination by surface residue built up, dominance of passivation also results in the incomplete removal of passivation polymers that leads to the formation of grass-like residues that is commonly known as “black silicon” (Fig. 4.25). Conversely, insufficient passivation causes loss in anisotropy such that lateral etching increases to result in the PhC rods being severed (Fig. 4.26). Often, such lateral etch effect can easily take dominance with the small diameters of the PhC rods, such that rods severed along their length leads to “runaway etching”, such that the etch openings become extended and etch species take over etching in the entire area that was previously filled with rods to result in a “released hard mask” situation (Fig. 4.27).

Fig. 4.25 Formation of “black silicon” in areas of etch openings, due to a passivation phase over-dominance during time multiplexed, etch/ passivation cycling.

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Fig. 4.26 SEM image of fabrication failure by effect of etching isotropy caused through inappropriate reduction of passivation.

Fig. 4.27 SEM image of runaway etch over entire area that was previously a lattice of photonic crystal rods.

To overcome such undesirable defective etch situations, etching gas flow rates and durations can be reduced while the corresponding values increased for the

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passivation phase. At the same time, other methods of reducing the dominance of etch include the decreasing the chamber pressure and also the platen power applied. Such processes and their respective parameters are compared in Table 4.3. Through balance of etch and passivation dominance and a reduced platen power, an acceptable process window for survival of deep-submicron size rods can be found, based on an etch chemistry of, SF_6 (100 sccm), C_4F_8 (30 sccm) and O_2 (10 sccm) at pressure of 50 % using platen power of 23 W together with a passivation chemistry of C_4F_8 (160 sccm) at the same plasma power but without application of platen bias to yield results of Fig. 4.28.

Fig. 4.28 SEM image of surviving photonic crystal rod array, without catastrophic fabrication failures but with rough sidewalls due to etch scallops undulations.

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Table 4.3 Process parameters of etch and passivation phases for the DRIE processes with different etching profiles.

Condition	Process cycles	Gas flow (sccm)			Power (watts)		Process time (s)
		C ₄ F ₈	SF ₆	O ₂	Coil	Platen	
Re-entrant etch profile	Etch	30	100	10	600	23	8
	Passivation	160	0	0	600	0	5
Lateral etch dominant	Etch	30	100	10	600	23	9
	Passivation	110	0	0	600	0	5
Continuous etch	Etch	90	40	0	800	20	-

As can be seen, although surviving PhC rods are obtained, the sidewall profiles of this etch process has rough surfaces due to large undulations arising from etch scalloping effect. Here, it can be measured from cross-sectional SEM that the scallop depth is 106 nm while the scallop height is about 150 nm. Intuitively, removal of etch-passivation cycling in DRIE process should result in minimization of sidewall scallops. However, it was found that although a continuous etch with simultaneous plasma polymerization yields consistently smooth sidewalls, it was achieved at the expense of isotropic sidewall angles leading to lateral under cutting, which once again led to etch failures of Figs. 4.26 and 4.27.

Therefore, to optimize the recipe for reduction of scallop depths so as to achieve smoother sidewalls, a further reduction of etch isotropy was carried out to balance both reduction of etch dominance and increase in etch duration. Based on this principle, tremendous improvement in sidewall etch profile was indeed obtained as can be seen from Fig. 4.29, where scallop depths of only 12 nm was obtained for a drastic improvement from an initial 106 nm. Further, the development of such ICP etch processes may be developed to yield the conditions of sloped, retrograde or vertical sidewall profiles. Here, with an optimized RIE condition, the etch profile can

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be moderated to obtain nearly vertical sidewalls as shown in the cross-sectional SEM of the etched PhC rod lattice in Fig. 4.30.

Fig. 4.29 SEM image of comparison between (a) previous scallop depth of 102 nm and (b) smoothed scallop depth of 12 nm.

Fig. 4.30 SEM cross-sectional image of fabricated photonic crystal lattice with controlled parameters, yielding nearly vertical sidewall profiles.

At the same time, from the experiments, it was found that as opposed to conventional assumption that lateral etching of DRIE structures are negligible beyond typical scalloping effects, progressive etch durations of deep-submicron size rods (unlike for larger structures) consistently resulted in reductions of PhC rods CDs, especially near the surface of the wafer. Based on this, it can be deduced that the size reduced geometries resulted from a significant etch action, which is more dominant for the parts of the structures nearer the surface of the wafer, then deeper into the wafer as the etch process progresses. Such phenomenon can be attributed to the trapped nature of the etch species along the narrow etch paths of the PhC that resulted in the sidewalls being further etched laterally. Consequently, incorporation of mask design bias in addition to that for OPC derived in Section 3 is required for successful realization of targeted devices, which would otherwise turn out smaller.

4.4.3 Dense Deep Sub-Micrometer Critical Dimensions Etching

In the experiments to develop DRIE conditions that allow realization of the super dense PhC arrays, coil power of the RF source was maintained at 600 W while varied platen power was applied for bias of ions energetic in the vertical direction, normal to the wafer surface. For a chemistry dominated by passivation, a sloped sidewall profile tend to result in gradually reduced etch openings that often results in eventual self-induced etch stops.

Conversely, insufficient passivation causes loss in anisotropy such that lateral etching increases to result in retrograde sidewalls. To avoid such sidewall profiles, etch and passivation process parameters can be delicately balanced in such high density deep sub-micrometer CD arrays to give conditions of sloped, retrograde or vertical sidewall profiles. Therefore, the etch profiles of the CD structures can be

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moderated to obtain nearly vertical sidewalls as shown in the cross-sectional SEM of the etched PhC holes lattice as shown in Fig. 4.31.

(a)

(b)

Fig. 4.31 (a) Top view SEM image of photonic crystal holes lattice with dash line showing where cross-section was taken to yield, (b) cross-sectional SEM of photonic crystal with controlled etch/ passivation parameters yielding vertical sidewall profiles.

4.4.4 RIE Lag and Notching at Buried Oxide Interface

For etch patterns with different opening sizes, etch rates vary according to the effect of aspect ratio resulting in RIE lag. For etch openings of different line widths, the etch rates vary drastically. This can be seen from the cross-sectional SEM image of Fig. 4.32, where the most drastic difference in etch depth was obtained for the OTS structures with ultra-wide etch area, while for the more narrow line patterns on the left, correspondingly increased etch depths were observed with progressively increasing line widths. Such variations in etch rates with respect to aspect ratios and etch opening sizes arises as a result of several etch mechanisms. Some of which includes the ion and kinetic neutral shadowing effect; the transport of etch reactants toward, and transport of etch reactants away from the etch surface; and the effect of electrical charges on etch surface.

One of the most prominent of which would be the transportation of etch reactants, which becomes progressively inhibited for narrower trenches. This is similarly so for the charge effect on etch surface, where charge distribution on the etched surfaces tends to be more highly concentrated in smaller etch surface opening areas than larger ones. Hence, higher charge density at the bottom of smaller trenches results in higher probabilities of incoming charged reactive species being repelled away, which acts to reduce or even prohibit further etch actions eventually.

Fig. 4.32 SEM of reactive ion etch lag by aspect ratio dependent effects in plasma etching as shown for the high density pattern on the left and the large optical testing structures opening on the right.

Such charge accumulation effects also comes into play in another circumstance – notching of device silicon at the device and buried cladding oxide interface. This critical RIE effect is an important consideration in SOI device etching. A SEM of this type of etch problem is as shown in Fig. 4.33a. Here, there is severe undercut of the silicon PhC near the bottom of the device, at the interface of the buried oxide layer. This is due to the accumulation of positively charged reactive ion etching species, pulled down deep onto the etch surface by the vertical platen bias power.

Such residual charge accumulation on etch surfaces acts to deflect further incoming positive species when etching proceeds until the etch stop buried oxide charge insulating layer. This results in the lateral etch of the PhC structures near the device-cladding interface, as the etch species are deflected onto the sidewalls, as can be seen in Fig. 4.33b. In the case of mild notching, the performance of the fabricated

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PhC structures would be adversely affected. However, if notching due to over-etching was allowed to become extensive, then total destruction to the designed device would result.

To prevent this problem, this process was therefore designed as described in Section 2 such that only similar etch opening sizes and etch depths are required for each etch step. In this way, drastic etch lag effects would not result in the undercutting of larger etch features at the etch stop layer due to the over etch time required to complete etching for the narrowest openings. Otherwise, the use of periodic discharging technique to remove accumulated charges leading to side walls deflected etch species is another tool related method to ameliorate notching effects.

Fig. 4.33 Notching of a silicon-on-insulator wafer, as shown in the (a) SEM of photonic crystal holes array etched into silicon and ‘etch-stopped’ at the cladding buried oxide interface. (b) Schematic illustration of charge build-up effect causing further incoming ions to be deflected onto etch sidewalls.

4.4.5 Etch Post Processing

In the post processing process of the PhC and OTS devices, thermal oxidation was performed to improve the optical quality of device sidewalls through smoothening of sharp edges. To enable the high temperature furnace process, total strip of CAR was necessary to avoid organic contamination of the oxidation chamber. Through a wet clean recipe of piranha bath consisting of sulfuric acid (H_2SO_4) and hydrogen peroxide (H_2O_2) at high temperature of 130 °C, the polymers and remaining photoresist left over in the lithographic and etch process was removed and inspected under a defect review SEM with energy dispersive x-ray analysis to ensure complete stripping. The cleaned wafers were then oxidized in the furnace at 1050 °C for 90 minutes, consuming silicon at a rate of about 0.4 times the rate of oxidation. For oxidation of 1000 Å thickness, the sidewall edges of the time multiplexed DRIE etched sidewalls (Fig. 4.34a) were then rounded with reduced scallop depths (Fig. 4.34b). Therefore, the optical quality of the fabricated device was improved and optical scattering due to sidewall roughness was reduced.

Next, in the integration of electrode metallization, copper (Cu) seed deposition was first carried out using physical vapor deposition (PVD) for a conformal film of 250 Å Tantalum (Ta) before deposition of Cu on top of the Ta layer which proceeded until a conformal coating was formed. Following seeding, actual Cu film thickness required was then applied by electrochemical plating (ECP). In the plating cell, Cu plating process was carried out with a copper sulphate (CuSO_4), H_2SO_4 , and distilled (DI) water solution bath. After plating, the wafer surface was cleaned by DI water spray in the post plating module. Post annealing at 200 °C was then carried out before the Cu film undergoes CMP to achieve planarized stack thickness required and

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also to remove unwanted Cu over areas that should not be coated. This planarizing step therefore enables subsequent processing of high resolution lithography after another USG deposition was carried out for cover over the metal electrodes (thereby preventing subsequent process elemental contamination).

Fig. 4.34 Post processing for (a) device sidewalls with undulating time multiplexed sidewall scallop roughness. After thermal oxidation, (b) sharp edges of roughness on device sidewalls are visibly reduced.

Upon completion of subsequent clean room processes, the defined Cu electrodes were exposed in the final phase using BOE release which removes silicon oxide at a rate of 2500 Å/min. The wafers released with the wet etch bath (comprising ammonium fluoride and hydrofluoric acid) are then cleaned with DI water. For clean wafers spun dry at standard qualified recipe of 1800 rpm, peeling of the thinner metal electrodes with less area of adhesion to the underlying device silicon results (Fig. 4.35). To prevent such defects, two approaches may be taken, namely to reduce the spin speed of the dryer to 300 rpm or to alternatively allow the wafers to be evaporated dry after an isopropyl alcohol (IPA) bath rinse, without undergoing spin

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dry. Although the latter method was more time consuming and less precise, its advantage over spin drying is the reduced likelihood for the occurrence of stiction (the permanent sticking of released movable structures).

Fig. 4.35 SEM of peeling of electrode copper metallization after buffered oxide etch and spin drying.

Therefore, following sidewall optimization and buried oxide release, the movable structures, PhC air bridge structure and OTS were realized. A final FIB milling was then carried out on the CD of a monorail PhC waveguide such as that shown in Fig. 4.36a. Here, the FIB system uses liquid metal ion sources to form very small probes with high current densities. Where such high density ion beam strikes the required points on the silicon air bridge, silicon material was removed through a physical sputtering process. To carry out FIB milling on a CD structure, it was important that surface oxide was removed prior to the processing so that the effects of charging can be minimized for sharper scanning electron imaging and therefore more precise spatial milling. Optimized conditions were found for magnification of 35 k times, and beam duration of 8 seconds for each PhC hole milling. For higher order of

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magnifications used, greater imaging precision was adversely affected by increased specimen charging effect that reduced the resolution of the PhC holes patterned. The FIB etched PhC holes on monorail waveguide structure are as shown in Fig. 4.36b, completing the synthesized processing of disparate PhC structures & etch depth process.

Fig. 4.36 (a) Photonic crystal of dense holes array together with fine waveguide structures prior to sidewall optimizations. (b) Released monorail structure with focus ion beam etched photonic crystal holes.

4.5 Summary

Based on the identified advantage of batch processing in OL and DRIE, insights into the optimization of these techniques have been presented. In the first part of the process, an alternative method for achievement of sub-lithographic wavelength line width patterning, not commonly used in RETs such as PSM, OAI and OPC was derived. Using low lithographic system requirements of a DUV scanner

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working at wavelength of 248 nm, CAR with BARC, and conventional chrome-on-glass photomasks, without expensive phase shift features or OAI systems, the sub-lithographic wavelength CDs were obtained using pattern and partial coherence control. Here, based on the key factors of pattern density bias and imaging system partial coherence variations, smallest resolution of 36 % that of mask value can be obtained for resolution of 75 nm using a 200 nm binary photomask pattern. Whilst limit in the reduction of design line widths and types of pattern together with constricted patterning at line/ base interface by line end necking are the limitations of this developed technique; the advantages of this method are its simplicity and cost effectiveness for enhancement of resolution without use of expensive or high-end peripherals, through simplified mask making requirements and reduced demand on exposure hardware sophistication. Such derived method therefore may be used not only for PhC, but also for applications such as metal-semiconductor-metal photo-detectors, nano-electromechanical structures etc.

At the same time, the etch lag effects, notching of devices at interface of device silicon and buried oxide layer was also presented for the simultaneous implementation of PhC with optical testing structures. The techniques of FIB milling in the finalization step of the processing following buried oxide release for PhC structures on CD structures enabled a wide processing window for both lithography and etch phases, avoiding severe loading effects caused by disparate pattern dimensions (such as lag and notching). Besides realization of deep etching TMRIE for the wide OTS grooves, PhC structures were optimized, through the delicate etch and passivation multiplexing balance, and also through thermal oxidation. By careful development of each experiment process module, high resolution tunable PhC for use at optical communication wavelength of 1550 nm was yielded such that

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monolithically integrated tunable PhC was fabricated simultaneously in mixed densities of super dense PhC holes; dense line patterns; isolated waveguide structures; and ultra wide OTS grooves that were defined aligned to the deep submicron size PhC devices with sub-100 nm resolution CDs. Such experiments of DRIE revealed many interesting effects, which were previously un-emphasized since they were quite negligible for larger dimensioned structures (such as that of the amplified etch angle; process time effect on lateral etch and sidewall scallops etc). By careful consideration of such experimental effects, HAR (45-57) deep-submicron size rods with small scallop depths (12 nm) are the deepest and smoothest PhC by far achieved by DRIE technique used at the optical communication wavelength of 1.55 μm .

To conclude, in the fabrication of PhC structures with disparate patterns & device etch depths; many techniques were developed to overcome the unavoidable challenges. The foremost include the design of a feasible processing flow that allowed for both PhC CD definition and etch together with metallization and also suspended released structures. Through investigation of each process module to satisfy the demands of the device operating specifications (such as critical dimension needed for the PhC to operate at the canonical optical communication wavelengths), insights derived were applied to each processing module. Here, apart from the development of solution towards the resist poisoning issue, the author of the thesis takes full ownership of all other fabrication developments carried out, from layout to measurements.

CHAPTER 5

PRINCIPLES OF PHOTONIC CRYSTAL MODULATION

The objective of this chapter is to establish the theories and techniques required to realize optical modulation for the deep sub-micrometer scale rod-type PhC devices described in the earlier chapters. This was based on the identification of many benefits in optically induced modulations – such as ultra-fast switching; low power thresholds; immunity to electromagnetic interference etc – and its fundamental compatibility with PhC integration, permitting strategic implementation of optically induced signal modulations on appropriately designed PhC optical devices. These include the study of both static and dynamic optical device/ material modulation principles. First, in terms of the dynamic optical processes required, it is well known that the electrical properties of semiconductors are greatly affected by the presence of charge carriers into otherwise empty bands of energy levels. Although such carriers are typically thermally excited, a beam of laser radiation may induce real populations of charge carriers temporarily onto excited states. In optical terms, the extent of excitation depends upon the balance between the rate of absorption of energy and the corresponding relaxation mechanisms.

Although there are still many different types of mechanisms involved with laser irradiation onto a semi-conducting material – such as third harmonic generation, optical Kerr, Pockel and Raman effects etc – these effects are not directly relevant to the experiments carried out in these work and would therefore be referred to only in reference. In this work where the material of choice was silicon, saturation conditions

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were found to be varied from as low as 1 W/cm^2 to as high as 1 GW/cm^2 [138]. Also, the range of induced carrier densities relevant is between 10^{14} to 10^{22} carriers per cm^3 .

This chapter begins with the physical studies of the dynamic properties of silicon material processes. This is followed by a discussion of the quantum mechanics involved in silicon absorption processes. Based on these, the nonlinear free absorption properties of silicon are presented together with the saturation effects – governed by the scattering; diffusion and recombination processes. With these, the basis concepts and challenges involved in the application of free carriers' absorption for modification of PhC device silicon refractive index based on the simplified Drude Model are then presented. Especially, the effects of optically generated plasma and thermal effects of optical excitation are discussed and analyzed before a summary.

5.1 Physics of Dynamic Processes in Silicon

Any real, physical oscillating system will exhibit a nonlinear response when it is overdriven. In an optical system, a nonlinear response can occur when there is sufficiently intense illumination [139]. The nonlinearity is exhibited in the polarization ($\vec{P}$) of the material, which is often represented by a power series expansion of the total applied optical field ($\vec{E}$)

$$\vec{P} = \epsilon_0 \chi^{(1)} \vec{E} + \epsilon_0 \chi^{(2)} \vec{E}^2 + \epsilon_0 \chi^{(3)} \vec{E}^3 + \dots \quad (5.1)$$

where $\chi^{(1)}$ is the linear susceptibility representing the linear response and $\chi^{(2)}$, $\chi^{(3)}$ are the second and third order nonlinear susceptibilities respectively. This macroscopic expression describes the expansion of components in the polarization of the material, which in turn, may be further categorized for effects, in terms of susceptibility and frequencies, as given in Table 5.1 and 5.2 for the passive and active

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processes respectively [138]. The passive process are associated with the real parts of $\chi^{(1)}$, $\chi^{(2)}$, and $\chi^{(3)}$. Since second order effects are always passive, only first and third order process may be active, associated with the imaginary parts of $\chi^{(1)}$, and $\chi^{(3)}$.

Table 5.1 Passive polarization effects in terms of susceptibility and frequencies

	Frequencies of incident fields	Frequencies of fields generated by the polarization of the medium	Susceptibility	Process
First order	ω_1	ω_1	$\chi^{(1)}(\omega_1, \omega_1)$	Linear dispersion
Second order	ω_1, ω_2	$\omega_3 \omega_3 = \omega_1 + \omega_2 $	$\chi^{(2)}(\omega_3, \omega_1, \omega_2)$	Sum mixing
	ω_1	$\omega_3 \omega_3 = 2\omega_1 $	$\chi^{(2)}(\omega_3, \omega_1, \omega_1)$	Second harmonic generation
	$\omega_1, 0$	ω_1	$\chi^{(2)}(\omega_1, \omega_1, 0)$	Electro-optic linear Kerr effect
	ω_1	$\omega_2, \omega_3 \omega_1 = \omega_2 + \omega_3 $	$\chi^{(2)}(\omega_2, -\omega_3, \omega_1)$	Difference-frequency mixing
	ω_1	$\omega_2 \omega_1 = 2\omega_2 $	$\chi^{(2)}(\omega_2, -\omega_2, \omega_1)$	Degenerate difference-frequency mixing
Third order	$\omega_1, \omega_2, \omega_3$	$\omega_4 \omega_4 = \omega_1 + \omega_2 + \omega_3 $	$\chi^{(3)}(\omega_4, \omega_1, \omega_1, \omega_1)$	Third harmonic generation
	ω_1, ω_2	$\omega_3, \omega_4 \omega_1 + \omega_2 = \omega_3 + \omega_4 $	$\chi^{(3)}(\omega_3, -\omega_4, \omega_1, \omega_2)$	Four-wave difference-frequency mixing processes
			$\chi^{(3)}(\omega_4, -\omega_3, \omega_1, \omega_2)$	
	ω_1	$\omega_2, \omega_3, \omega_4 \omega_1 = \omega_2 + \omega_3 + \omega_4 $	$\chi^{(3)}(\omega_2, -\omega_3, -\omega_4, \omega_1)$	
	ω_1	ω_1	$\chi^{(3)}(\omega_1, \omega_1, -\omega_1, \omega_1)$	Intensity-dependent refractive index
	$\omega_1, 0$	ω_1	$\chi^{(3)}(\omega_1, 0, 0, \omega_1)$	Quadratic Kerr effect

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Table 5.2 Summary of active first and third order nonlinearity polarization effects

	<i>Susceptibility</i>	<i>Process</i>
First order	$\chi^{(1)}(\omega_1, \omega_1)$	Linear absorption
Third order	$\chi^{(3)}(\omega_2, \omega_1, -\omega_1, \omega_2)$	Raman scattering
	$\chi^{(3)}(\omega_1, \omega_1, -\omega_1, \omega_1)$	Intensity-dependent absorption

For indirect bandgap semiconductor like silicon, the energy minimum of the conduction band and the maximum of the valance band occur at different wave-vector (k) values. In which case, optical absorption from above bandgap radiation results from the additional interaction of a long wave-vector phonon allowing momentum conservation to be satisfied. In the transition diagram of Fig. 5.1, an electron excited by a photon in a virtual transition requires a phonon scattering off it to compensate for the energy mismatch. Like two-photon absorption, this is a two particle interaction and absorption is difficult to evaluate since all possible combinations of intermediate and final states must be summed and the electron-phonon interaction changes considerably with k -value.

Fig. 5.1 Indirect electronic bandgap structure of silicon with wave-vector mismatch.

5.1.1 Quantum Mechanical System

While the real and imaginary components of the linear susceptibility $\chi^{(1)}$, are associated with refraction and absorption, the real and imaginary parts of $\chi^{(3)}$ describes nonlinear refraction and nonlinear absorption. The conservation of energy dictates that both annihilation and generation of photons involve atomic and/or molecular transitions from one state to the other. Transition diagrams may be used to illustrate such processes in Fig. 5.2.

Fig. 5.2 Illustration of time ordering photon transitions in third order mechanisms of (a) absorption-emission-absorption-emission sequence, (b) absorption of two photons followed by emission of the two photons.

Here, the energy level $|g\rangle$ is the ground state while $|a\rangle$, $|u\rangle$, and $|b\rangle$ are intermediate states of the system in a sequence of transitions involving photons with frequencies ω_i , ω_j , ω_k and ω_l (where $i, j, k, l = 1, 2, 3, 4$) such that $\pm \omega_i \pm \omega_j \pm \omega_k \pm \omega_l = 0$. Energy conservation [138] is strictly obeyed upon the completion of the interaction but may be violated in the time frame of intermediate

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state transitions. This is allowed by the Heisenberg's Uncertainty Principle [140]. In many cases, an intermediate state is a “virtual” state – which implies that a real, intermediate state of the system does not exist to support the transition of a photon at the selected wavelength.

The virtual intermediate state allows for energy conservation in transition diagrams, but a physical description of the optical interaction using quantum mechanics involves only real eigen-states of the system. In particular, there may be a dipole-allowed transition between the initial state $|g\rangle$ and a real state “associated” with a virtual state. The timescale and strength of the interaction is partly determined by the energy mismatch between the virtual, intermediate state and an associated real, electronic state. This means a system can absorb a photon of energy $E = \hbar \omega$ (where $\hbar$ is the Planck's constant and ω is the frequency of the radiation) and make a transition from the ground state $|g\rangle$ to a real intermediate state $|a\rangle$ even though there is insufficient photon energy to bridge the gap, i.e. there is an energy mismatch $\Delta E = |\hbar \omega_i - E_a + E_g| > 0$.

This is possible provided the interaction occurs in a time faster than the observation time $\Delta t \sim \hbar / \Delta E$ permitted by the Uncertainty Principle. Transitions of this type are called virtual transitions as opposed to real transitions where energy is conserved. In the former case, Δt is known as the virtual lifetime of the transition. If the entire sequence of transitions comprising the third-order interaction is not completed within the virtual lifetime, the intermediate state collapses back to the ground state and no nonlinear interaction occurs. In other words, all the required particles must be present in the system during the virtual lifetime. Hence, the longer the virtual lifetime, the greater will be the probability that the required photons appear,

allowing the multi-particle interaction to run to completion. Further, the availability of the appropriate states within the bands, described by the Fermi's golden rule [139] also determines whether the transitions may take place successfully.

5.2 Free Carrier Absorption and Non-Linear Properties

In the limit of high laser fields; multi-photon absorption; laser-induced impact ionization and tunneling, optical generation of plasmas occur as the result of nonlinear mechanisms. Otherwise, at frequencies below the threshold for interband transitions and exciton absorption, silicon has a continuous absorption spectrum due to intraband transitions, also known as Cerenkov radiation [140]. While the time scales of interband transitions are typically in the nanoseconds range (with that of silicon taking as long as milliseconds), the time scale of intraband transitions typically are in the picoseconds range. In general, absorption is approximately proportional to the number of electrons (or holes) in the band and therefore can be varied by doping. When a free carrier absorbs a quantum of energy $\hbar\omega$, it must change its k such that it can make a transition to an empty state at higher energy within the same band. As the photon wave-vector is small, this is only possible if the lattice takes up the momentum in a similar way to indirect absorption. Hence a phonon must be emitted or absorbed in the free carrier transition. The absorption thus depends on the phonon scattering process involved.

Before delving into the area of non-linear properties of free carriers, the simpler case of free carriers, with linear optical properties can be expressed in complex dielectric constant as

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$$\varepsilon = 1 + \frac{4\pi Ne^2}{m} \frac{1}{(-\omega^2 - i\Gamma\omega)}, \quad (5.2)$$

where m is the mass of the carriers, N is the electron-hole pair density, e is the electronic charge, and Γ represents the line-broadening effects of scattering processes on the zero frequency resonance of free carriers. Separating the real and imaginary parts of ε , the refractive and absorptive effects can be expressed as

$$\varepsilon' = n^2 - k^2 = 1 - \frac{4\pi Ne^2 / m}{\omega^2 + \Gamma^2}, \quad (5.3)$$

and

$$\varepsilon'' = 2nk = \frac{4\pi Ne^2 \Gamma / m \omega}{\omega^2 + \Gamma^2}. \quad (5.4)$$

When both electrons and holes are excited by the incident laser beam, by some process, such as interband transitions, two photon absorption (TPA), phonon assisted indirect transition etc, the electron-hole plasma have an average number of carriers excited are

$$N = \frac{I}{\hbar \omega} \alpha_{\text{effective}} \tau_R, \quad (5.5)$$

where I is the laser intensity, $\alpha_{\text{effective}}$ is the part of the absorption coefficient responsible for carrier generation, $\hbar$ is the reduced planck constant, and τ_R is the recombination lifetime. Substituting Eq. 5.5 into Eqs. 5.3 and 5.4 then gives the expressions for the non-linear, intensity dependent free carriers' effects.

For free carriers' refraction, when the frequency is sufficiently high such that $\omega^2 \gg \Gamma^2$, and

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$$\Delta n = \frac{1}{2n_0} \cdot \frac{4\pi e^2}{m_e \omega^2} \sum \frac{N_0}{m_j^* / m_e} \quad (5.6)$$

where m_e is the free mass of electrons, m_j^* / m_e is the appropriate mass ratio for the band extremum and

$$n_2 \cong \frac{2\pi e^2 \alpha_{\text{effective}} \tau_R}{\hbar \omega^3 m^* n_0} \quad (5.7)$$

where e is the electronic charge, n_0 is the unperturbed index, for the case of one dominant carrier of mass m^* . Absorption coefficients can therefore be calculated as

$$\gamma = \frac{2\omega k}{c}, \quad (5.8)$$

through substitution of N from Eq. 5.5 to obtain the intensity dependent absorption.

As free carrier absorption depends explicitly on the scattering processes through Γ in Eq. 5.4, the frequency dependence can be more complicated than the expression suggest, since Γ is a frequency dependent and can vary considerably in differing semiconductor bands. The scattering is related to the carrier mobility and is dominated in electron hole plasma by those with the smallest mobility, e.g. the heavy holes. Theoretically, appropriate summations would therefore need to be formulated for this purpose. Here, since the intraband scattering processes occur on a picosecond timescale, the redistribution of electrons are also considered for the dynamics on such a timescale.

5.2.1 Saturation Effects of Free Carriers Generation

An implicit assumption for all the formulations is based on the premise that the induced carriers' population in the conduction states is negligible. However,

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when the optically induced population with the associated depletion of the lower states is not negligible, the absorption will be altered due to finite population. This intensity-dependent process is called saturation since in the high intensity limit in the steady state, the net absorption coefficient tends to saturate to a specific level. Such saturation effects however, can be observed before this limit is reached. In silicon where two-level models of saturation may not be applied, saturation of optical absorption between bands is mainly described by the phenomenon of ‘state-filling’ and ‘band-filling’.

Strong, direct optical transitions between bands in which states coupled optically are effectively those of the same k -value in the different bands (as the photon momentum is negligible). Thus, as far as direct optical interactions are concern, absorption characteristics are similar to that of a collection of two-level systems, one for each k -value so the system appears like an ‘inhomogeneous’ absorber. This type of saturation is known as ‘state-filling’ as only a small fraction of the states in a band is saturated, specifically those directly excited optically. Alternatively, ‘band-filling’ involves the strong transfer of excitation between states resulting in the progressive filling of an entire band. This occurs when the scattering within the band occurs much faster than the recombination between the bands. Thus populations created in bands are scattered rapidly usually towards quasi-equilibrium thermal distributions of excited carriers within each band and these distribution relax more slowly through interband recombination.

The time constants associated with electronic scattering, diffusion and recombination are very important for saturation dynamics. For these processes, consider the electrons to be excited by some arbitrary excess energy ΔE above the

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bottom of the conduction band so that the following scattering, diffusion and recombination processes may take place.

5.2.2 Scattering, Diffusion and Recombination of Carriers

First, in scattering, electrons after excitation scatter very rapidly to some other conduction band states. In general, scattering times are short with the result that very high intensities are needed to observe state-filling saturation. Second, in diffusion, the spatial distribution of optically generated carriers through a crystal becomes inhomogeneous unless the thickness of the crystal is much less than an absorption length (reciprocal of absorption coefficient). In particular, the interband absorption above the fundamental edge creates carriers within a depth of only a few micrometers [103].

Diffusion on the other hand is characterized by coefficient D , which relates the number of carriers, n_d crossing a unit area per unit time to the concentration gradient are expressed as

$$n_d = -D \frac{\partial n}{\partial x}, \quad (5.9)$$

where D the diffusion coefficient is determined by the mobilities of the carriers through the Einstein relation

$$D = \frac{\mu k T}{e}, \quad (5.10)$$

where k is the Boltzman constant, e is the electronic charge, T is the temperature and μ is the magnitude of the mobility, which depends on the scattering process. When the numbers of electrons and holes are approximately equal as in the case of laser generated electron-hole plasmas, the diffusion of both carrier types is described

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by an ambipolar diffusion coefficient D_a , which is related to the coefficients for the electrons and holes, D_e and D_h respectively by

$$D_a = \frac{2D_e D_h}{D_e + D_h}. \quad (5.11)$$

Since any separation of charge would create a Coulomb field between the electrons and holes, the two carriers must diffuse at the same rate. Finally, in the recombination process, excess electron-hole pairs typically recombine on larger timescales than the average scattering event. The life time of optically generated excess carriers may be set by one of several competing recombination routes depending on such parameters as the band structure; lattice temperature; crystal defects and carrier concentration. The energy of an electron-hole pair can be transferred to EM radiation; phonons and other carriers. Electrons can recombine with holes by making a single transition between the conduction band or exciton level and the valence band.

For indirect bandgap silicon, the transitions include the simultaneous emission or absorption of a number of phonons instead of a photon. This is however very inefficient because large number of phonons are required to take up the energy of the electron. The lifetime of electron-hole pairs is usually dominated by the existence of states near the middle of the forbidden gap due to impurities or lattice flaws. The electron de-excites in a two stage process via these deep traps. The recombination is completed when an occupied trap captures a hole. However, the capture rate for holes are quite different from that of electrons.

Energy may be given up in the form of radiation; phonons; or carriers heating. One of the most efficient of which, is through the interaction with the lattice. This process in which the electron cascades down through the excited states of the trap

emitting phonons between levels has the highest probability. Special account needs to be taken for localized flaws near the surface of a semiconductor. Electrons and holes may diffuse to the surface and recombine at these traps; the surface recombination time can often be higher than in the bulk necessitating special surface treatment to control this.

5.3 Design of PhC Modulation Device

Optical absorption effect may be used to modulate the device output levels through free charge carriers' plasma generation. When photons with sufficient energy are absorbed in a dielectric material, electrons in the valence band are promoted to the conduction band. The optically-excited electron-hole pairs increase the free carriers' density within the material and therefore alter its optical properties as described by the Drude model [104]. Such behavior is, however, dependent on the intensity of the incident radiation. For silicon, optical absorption at low incident power density levels scale linearly with intensity I as αI , where α is the linear absorption coefficient of silicon (which tends to zero for photon energies less than its band-gap energy E_g). At high incidence intensity, an additional nonlinear TPA effect becomes significant, scaling with optical intensity as βI , where β is the two-photon absorption coefficient of silicon, which vanishes for photon energies larger than half the silicon material's electronic band-gap energy.

In the optical experiments, high intensity pump radiation of photon energies greater than the silicon bandgap energy 1.1 eV, was used to excite the free charge carriers of electrons and holes in the optically pumped material. Low intensity signal at the telecommunication wavelengths, may then be used as optical probe input for

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which the lattice length scale of the PhC structures was designed to be sensitive to. In this case, since the optical absorption effect is mainly linear, the Drude model can be used to describe well the changes in dielectric index for the silicon material [148, 149] (for induced charge carriers density not exceeding 10^{22} - corresponding approximately to 10 % of the total valence-band population [105]). In such circumstance, the lifetime of these additional carriers is much influenced by surface recombination, which is process dependent. To characterize such carriers' effect, the change in real dielectric constant [106] may therefore be expressed as

$$\Delta\epsilon = -\frac{Ne^2}{m^* \epsilon_0 (\omega^2 + \tau_d^{-2})}, \quad (5.12)$$

where N is the free electron concentration, e is the electron charge, m^* is the optical reduced mass, ϵ_0 is the optical frequency dielectric constant, ω is the frequency, and τ_d is the Drude damping time.

Thus, the induced change in refractive index via change in dielectric constant is directly determined by the optically induced free charge carriers' density. Here, to enable effective modulation of material and device properties, the minimum activation dimensions need to be less than the carrier absorption length [103] for the excited free carrier plasma, which is given as:

$$l_{abs} = \left(\frac{\omega}{\omega_p} \right)^2 \tau_d c; \quad (5.13)$$

where c remains the speed of light, and the plasma frequency is given by

$$\omega_p = \sqrt{\frac{Ne^2}{m^* \epsilon_0}}. \quad (5.14)$$

The corresponding carrier density profile expanded from is given by

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$$N(z) = \frac{I(z)\tau_{pump}}{\hbar\omega_{pump}} \left[\alpha + \frac{1}{2}\beta I(z) \right], \quad (5.15)$$

where ω_{pump} is the pump laser frequency, τ_{pump} is the pump pulse duration; the factor of half before the TPA coefficient indicates the need for two photons to be absorbed before the generation of an electron-hole pair; and the intensity depth profile is given by

$$I(z) = \frac{I_0 e^{-\alpha z}}{1 + (\beta I_0 / \alpha)(1 - e^{-\alpha z})}, \quad (5.16)$$

where I_0 is the intensity at the interface, and z is the displacement.

Figure 5.3 derives from Eq. 5.13 to illustrate the exponentially inverse relationship between pump beam intensity and the carrier absorption length. Here, it can be seen that the absorption length is more than $8\ \mu\text{m}$ for an incident pump power of $20\ \text{mJ}/\text{cm}^2$, corresponding to an induced carrier density of $5.36 \times 10^{20}\ \text{cm}^{-3}$.

Fig. 5.3 Absorption length relationship with intensity of applied pump beam inducing free carriers plasma.

The absorption length is critical for the experiments as the progressive decrease in absorption span affects the limitation and effectiveness of the method. Figure 5.4 shows the intensity depth profile for the different linear absorption and TPA absorption coefficients. In Fig. 5.4a, only linear absorption mechanism is present and the intensity of the incident radiation onto the material decreases by 3 dB at less than a unit length. In Fig. 5.4b, where the linear and TPA coefficients are equal to 0.5, slightly longer absorption depth is obtained. Finally, the best scenario for absorption penetration depth is obtained for the case whereby TPA is dominant as shown in Fig. 5.4c.

(a)

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Fig. 5.4 Intensity depth profile for (a) only linear absorption; (b) linear absorption and two photon absorption coefficient equal to 0.5; and (c) dominantly two photon absorption.

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To quantify the relationship between the absorption coefficients and the pumping homogeneity, critical for assessing the limitations and effectiveness of such optical modulation techniques, a homogeneity length as the span for the carrier density remaining within 10 % of its surface value can be defined as

$$l_{\text{hom}} \cong \frac{0.1}{f} \times \left[\frac{1}{N(z)} \frac{dN(z)}{dz} \right]_{z=0}. \quad (5.17)$$

where f is the filling factor of the silicon as compared to a bulk material, and $N(z)$ is the carriers' density as a function of the incident displacement. Since f is always smaller than unity for PhC as compared to bulk material, the homogeneity length increases correspondingly. For instance, the l_{hom} of the PhC system is greatly increased, by the low f of the rod-type structure. For an estimated mean free path (MFP) length of 63 unit cells, at the frequency of 5000 cm^{-1} , absorption length of 116 unit cells, the homogeneity length spans 4.1 unit cells. Hence, the smaller the lattice filling parameter, the greater the homogeneity length may be. Also, considering the extinction of pump light due to the random scattering inside the PhC material, the homogeneity length of light for the PhC becomes

$$l_{\text{hom}} = 0.1 \left(\frac{1}{l_{\text{abs}}} + \frac{1}{l_{\text{mfp}}} \right)^{-1}, \quad (5.18)$$

where l_{mfp} is the MFP length of the scattering mechanism and l_{abs} is the absorption length. Figure 5.5 gives a surface plot of the l_{hom} for varied absorption and l_{mfp} , the latter arising from the scattering mechanisms within the PhC material.

Fig. 5.5 Homogeneity length of free carriers from the surface of incident radiation, plotted with respect to both absorption and scattering mechanisms.

From Fig. 5.5, it follows that the more extended the l_{mfp} for the free carriers within the PhC material, and the longer the l_{abs} , the larger the l_{hom} . These formulations therefore lay the foundation for the experiments and provide a guide for the limitation and effectiveness of the method.

5.3.1 Basis Concepts & Key Challenges

The optical modulation mechanisms described by Eqs. 5.12 and 5.13 can be effectively implemented in many PhC devices; particularly those with small isolated cavity structures since the application of the high energy and intensity laser source may be localized for greater pump efficiency and lower thresholds in smaller switching volumes.

Fig. 5.6 Illustration of high intensity pump radiation onto center of photonic crystal optical intersection, inducing localized material property changes in the center resonator rod.

Figure 5.6 depicts the probe beam at longer wavelengths may be applied through side-coupling to the PhC device, while the pump beam at shorter wavelength and higher photon energy may be beamed from the top of the device. By applying an optical pump beam at the center of the PhC intersection cavity's center resonator rod, localized application of optical pump radiation may be directed through a focusing lens onto the entire center resonator rod (since it has diameter of only a few hundred nanometers) to induce effective refractive index modulations in the cavity rod. To

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demonstrate such PhC resonator modulations experimentally, many finer nuances need to be addressed. First, there is the requirement to develop deep sub-micrometer sized PhC device fabrication processing techniques. Second, coupling of probe radiation into the sub-wavelength sized optical intersections is critical in order to enable characterization of the PhC optical intersections. Finally, optical focusing and level control of high power pump beam radiation precisely onto the center cavity rod of the optical intersection is also a non-trivial issue.

The issues for application of localized pump radiation onto the specific center resonator rod of the PhC optical intersection is mainly concerned with the diffraction limits imposed on the focusing of the pump beam, and also the temporal and spatial differentiation between the pump and probe beam. While the current experiments do not seek to distinguish between the spatial (i.e. to contain the probe beam within the pump beam) and temporal (i.e. to have determinate time delays between the pulses of the pump and probe beam) differences relative to the pump and continuous wave probe beam, the resolving power of the lens for localized application of pump beam onto the PhC resonator is critical.

5.3.2 Spatial Localization of Pump Beam with Diffraction Limited Focusing

The resolving power of any lens is fundamentally limited by diffraction, as already described in Chapter 4. The aperture of a lens acts like a 2D ‘single slit’, such that light passing through a lens aperture inevitably interferes with itself, to create a diffraction pattern, known as an Airy disc. This empirical diffraction limit, also known as the Rayleigh criterion is given by

$$\sin \theta = 1.22 \frac{\lambda}{D_{lens}}, \quad (5.19)$$

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where θ is the angular resolution, λ is the wavelength of light, D_{lens} is the diameter of the lens; and 1.22 denotes the position of the first dark ring in the diffraction pattern in the Airy disc. This value coincides with the first positive zero of the Bessel function of the first kind, of order one, divided by π . For an ideal lens of focal length FL , Eq. 5.19 yields a minimum spatial resolution as

$$\Delta l = 1.22 \frac{FL \cdot \lambda}{D_{lens}}, \quad (5.20)$$

which states the smallest spot radius that a focused laser beam can be collimated onto.

Hence, the shorter the wavelength of pump light used, the smaller the corresponding focused beam spot can be. This is simulated for the 100 times objective lens used in the experiment with focal length of 2 mm, for wavelength range of 0 to 2 μm . As shown in Fig. 5.7, the spatial resolution is linearly proportional to the wavelength range of interest. Here, it is also noted that for a telecommunication wavelength of 1550 nm, the minimum spot size that can be obtained is 108 nm. For a Titanium: Sapphire (Ti:Sa) laser output at 780 nm, the smallest spot size that can be obtained is reduced to 50 nm. Finally, for the Neodymium: Yttrium Aluminium Garnet (Nd:Yag) laser used in the experiments with 532 nm output, the smallest spot size that can be obtained is as low as 36 nm. This is much smaller than the size of the PhC resonator rod and hence the diffraction limit of light in focusing does not limit the application of Nd:Yag pump beam for optical modulation in this work.

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Fig. 5.7 Spatial resolution for different optical wavelengths as limited by the diffraction limit of light.

Yet, even though the application of pump radiation onto the PhC resonator rod is not diffraction limited, the focusing of the pump beam was difficult to achieve since the peak intensity of the pump beam should be targeted for the middle of the resonator rod height instead of at the surface of the device, which is easier to observe from the microscope. Hence, during the experiment, the vertical focus of the device needs to be adjusted for largest effect contrary to observations in the sharpness of the beam spot at device surface. Also, once the optical alignment of the probe beam was secured in place, it was critical to ensure that further alignment of the pump beam to the PhC device was carried out without altering the side-coupling of the optical fibers to the devices.

5.4 Photonic Crystal Device Effects of Optical Modulation

For optically controlled optical PhC response, the index modulations induced by the absorption of optical pump radiation in the center cavity rod results in the lowering of refractive index in the affected silicon material. To characterize such effects within the miniature size PhC devices, both HAR and slab type configurations were investigated in both static and dynamic measurements. These include the variation of altered cavity conditions, induced by the changes in resonator rod sizes; application of continuous wave and pulsed radiation to produce effects of carrier-plasma and thermo-optic operations etc. For an applied pump beam at wavelength 532 nm, from a Nd:Yag laser, the quantum energy of the photons is 2.3 eV, which is much greater than the silicon optical energy gap of 1.1 eV at room temperature of 295 K. As a result free-carrier plasma can be generated by the laser beam which can in turn alter the optical properties and establish an optical nonlinearity of the material. Here, there is a resonant effect which primarily depends on the physics of the second step, i.e. the influence of the free carriers' on the optical properties.

Two mechanisms have been found in the past to be relevant for silicon. Firstly, the free-carrier plasma gives rise directly to a change in the optical absorption and refraction which can be described by the classical Drude model. Based on this model, excellent agreement between prediction and experiment can be found in literature. Experimentally, this type of optical nonlinearity has been observed using short optical pulses from a Q-switch laser system to study phenomenon such as four-wave mixing; free-carrier gratings; self-modulation etc [140]. Secondly, the thermo-optical properties also play an important role, especially when the measurements are performed by a continuous wave laser. In which case, the lattice of the semiconductor

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silicon is heated up by the recombining charge carriers. The resulting change of the refractive index then leads to optical bistability in silicon. In this section, the physical mechanisms for the optical plasma effect and the thermo-optic effects are detailed.

5.4.1 Optically Generated Plasma

Optical generation of stable plasmas is readily obtained in semiconductors, through cascaded linear processes in the formation free electron-hole pairs that are generated by bandgap excitation with incident photons. The optically produced carriers augment the background electron-hole density and the free carriers' plasma remains electro-statically neutral. If the generation of an excess amount of plasma exceeds the rate of loss (by recombination or diffusion) on the timescale of interest, the plasma modifies the linear optical properties of the material. This effect is well modeled by the classical Drude model, where the refractive index of the material is given as

$$n = n_0 \sqrt{1 - \frac{\omega_p^2}{\omega^2}}, \quad (5.21)$$

where ω is the angular frequency of the light, n_0 is the linear index in the absence of significant free carrier density, and ω_p is the density-dependent plasma frequency given by Eq. 5.14.

With increasing pump power, the carriers' density increases as

$$N = \frac{\alpha P_{pump}}{\hbar \omega}, \quad (5.22)$$

P_{pump} is the optical pump power, α is the absorption coefficient, and $\hbar$ is the reduced Planck constant. This is as shown in Fig. 5.8, where the densities of the induced free

carriers increase proportionally with the power of the applied pump beam, based on the Drude formulations [103].

Fig. 5.8 Photo induced carriers' density with 532 nm pump laser being directly proportional to the applied pump power, based on the Drude formulations.

Hence, as the carrier density increases, the plasma frequency increase, which leads to a corresponding decrease in the material's refractive index as described by Eq. 5.19. Figure 5.9 plots the effect of increasing pump power on the real and imaginary indices of the silicon PhC material.

Fig. 5.9 Induced free carriers effect on silicon refractive index by optical pumping.

Directly proportional to the density of the free charge carriers' plasma generated by the absorption of pump radiation onto the PhC material, the increasing optical pumping power applied reduces the dielectric constant of the center cavity rod correspondingly, as shown in the plot of Fig. 5.9. As can be seen, the increase in real index is also accompanied by a corresponding increase in the imaginary component, which indicates greater absorption of the material. Such trade-off therefore brings about a direct consequence onto the l_{abs} of the excited carrier plasma which as described in Section 5.3.1 needs to be carefully managed in order to prevent inhomogeneous device modulation

The time scale for such processes are determined by the cavity charging time and the carrier relaxation time, which according to the rate equation, is typically 80 picoseconds approximately for silicon. Figure 5.10 shows for example the transmission spectrums of a 3×3 PhC optical intersection when the refractive index

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of the center resonator rod is reduced by optical pumping. For the case whereby the index contrast of the PhC optical intersection compared to air was 2.65, the FWHM was 17 nm. This was reduced to 15 nm for PhC resonator rod index contrast reduced to 2.55, and to 13 nm for index contrast reduced to 2.45.

Fig. 5.10 Simulation results of decreased full width at half maximum for photonic crystal resonator rod refractive index reduced by carriers' plasma effects.

Such optical modulation becomes ever greater in sensitivity for optimized resonator rod dimensions. In the case where the thermo-optics effects become dominant; the reversed effects are to be observed, except for the additional phenomenon of resonant wavelength shifting arising from the effects of larger area

modulations. The details of these differences will be described in the following section.

5.4.2 Thermal Effects of Optical Excitation

Linear absorption of light must result in energy deposition in the irradiated material. If the rate of energy deposition significantly exceeds its rate of removal, thermo-optics effect takes place through the heat generated with the optically produced carriers. As the energy of a collection of atoms and molecules increases, their macroscopic optical properties will be altered. The physical interpretation of the thermo-optic effect arises from the induction of refractive index changes which are proportional to the total energy deposited in the medium – in the form of the integral of the absorbed intensity. The energy per unit volume absorbed in the silicon material which may be converted to heat is represented by

$$\frac{\partial E}{\partial V} = \alpha \tau_E I, \quad (5.23)$$

where α is the linear absorption coefficient, τ_E is the thermal diffusion time in the steady state, and I is the intensity of incident radiation.

To quantify the thermo-optic effect, two main material characteristics must first be considered. First, the polarizability

$$\rho = \frac{\vec{p}}{\vec{E}}, \quad (5.24)$$

which denotes how easily an electric field is able to distort the material's electron cloud, such that the dipole moment $\vec{p}$ is a fraction of the applied electric field $\vec{E}$. Generally, higher polarizability is accompanied by correspondingly higher refractive

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index of the material. Secondly, a material's density decreases with respect to temperature increases so that

$$\vec{P} = \frac{m}{V} \rho \vec{E} = \epsilon_0 \chi_e \vec{E}, \quad (5.25)$$

where m is the total mass, V is the total volume, ϵ_0 is the electric permittivity and χ_e is the electric susceptibility. Substituting $\chi_e = n^2 - 1$, we can obtain the refractive index as a function of density, and polarizability such that

$$n = \sqrt{1 + \frac{m\rho}{V\epsilon_0}}. \quad (5.26)$$

By substituting the terms in Eq. 5.26 as functions of temperature, the thermo-optic coefficient of silicon may be obtained as

$$\frac{dn}{dT} \cong 1.8 \times 10^{-4} + 3.47 \times 10^{-7} T - 1.98 \times 10^{-7} T^2. \quad (5.27)$$

By neglecting the higher order terms of the thermo-optic coefficient, it is clear that the thermo-optics effect is linearly and positively proportional to temperature T for silicon. The relationship between changes in refractive index with respect to changes in temperature of single crystal silicon may therefore be plotted as shown in Fig. 5.11.

Fig. 5.11 Thermo-optic effect of silicon, with change in refractive index plotted against change in temperature.

While the carriers' plasma effect is ultrafast, the timescale for the thermo-optic effects are much slower, typically eight order of magnitudes slower than that of the carriers' plasma effect, in the time scale of milliseconds. At the same time, due to the conduction effect of the thermo heating induced, not only the center resonator rod will undergo refractive index modulation, but also the surrounding rods. With increasing heating, the index contrast between the PhC resonator rod and the surrounding rods will increase [148, 149] to result in the reverse effects compared obtained in Fig. 5.10. This is illustrated by the simulation result of Fig. 5.12, whereby not only the center resonator rod index was modulated, but also the surrounding partially reflecting PhC rods. In which case, not only does the increase in refractive index contrast brings about a corresponding increase in bandwidth, the center wavelength was also shifted towards the longer wavelengths to result in a red shift.

Fig. 5.12 Simulated effect of thermo-optic modulation on the optical photonic crystal intersection with conduction resulting in the alteration of surrounding rods refractive index.

5.5 Summary

This chapter presented the physical, architectural and phenomenological effects of silicon dynamic processes – by method of free carriers' inducement – in the especially chosen position of the resonator rod within a PhC optical intersection device structure. The indirect bandgap and small non-linear coefficient of silicon as the material of the PhC was taken into consideration for the selection of free carriers' modulation method, which is capable of inducing refractive index changes to the PhC resonator rod that is proportional to the density of free carriers' generated by optical means. In this chapter, not only were the limitations of absorption and homogeneity lengths studied; the main challenges for spatial localization and high resolution focusing were also analyzed and presented in context of the PhC optical intersections

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of concern. Finally, the two most critical effects for such optical modulation experiments, namely the optical plasma and the thermo-optic effects were distinguished. While the former induce instantaneous modulations, the latter as a consequence of accompanied lattice heating have a much longer process time. Finally, while the former induces an inverse decreasing effect in the refractive index of the silicon PhC material with application of increasing pump optical radiation, the latter instead induces a proportional increase in the material index. Hence, it can be expected that the two described phenomenon would induce distinct and opposite modulation effects, probed and demonstrated in experiments as to be recorded in the following chapter of experimental measurements, which seeks to demonstrate the effects studied in this chapter. To do so, the challenges of coupling, fabricated device parameters calibrations, together with the static and dynamic optical measurements will be presented.

CHAPTER 6

OPTICAL MEASUREMENTS OF PHOTONIC CRYSTAL

The objective of this chapter is to present and develop the necessary experimental principles and techniques required to realize optical measurements for the fabricated deep sub-micrometer length-scale PhC devices. These include the study of measurement techniques; experiments design; and also the methodology of measurement equipment set-ups. This chapter begins with the discussion of designs for the various PhC integrated circuit devices fabricated – including test structures, coupling schemes and methodologies etc. Following which, the experimental set-ups and techniques employed are presented. Based on such, the various aspects of static and dynamic optical measurements are then described. Especially, the results of cavity manipulations and also different testing procedures leading to various outputs and optical modulations for each specific design are recorded. Finally, the experimental results of the measurements for the deep sub-micrometer size optical PhC devices are analyzed and discussed before a summary concludes the chapter.

6.1 Experiment Methods and Techniques

Based on the theory, design, fabrication and principles of PhC device operations, experimental set-ups specific for PhC testings are necessary. Experimental arrangements applicable to single-line embedded resonators and crossing PhC waveguide systems enable characterization measurements at the optical wavelengths. Through the use of appropriately designed testing structures, the

various device performances, such as bending loss, propagation coefficients etc may be probed to obtain new bench marks not currently available in literature.

6.1.1 Experiment Set-Ups

In the experiments with base-line set-ups depicted schematically as in Fig. 6.1, the input signals (falling within the C- and L- band wavelengths in the optical communication spectrum) were obtained using a Lightwave LDX-3412 continuous-wave laser source and an ANDO AQ4321 tunable laser system (TLS). For these two types of input sources, the output from the PhC optical intersection devices were then probed using a Newport 1835C optical meter and the TLS synchronized ANDO AQ6317 optical spectrum analyzer (OSA) respectively. In addition, broader band measurements were also made, using a super-luminescent light emitting diode (SLED) DenseLight DL-BD9 which was similarly measured using an OSA.

Fig. 6.1 Schematic of experiment set-up, where the two-dimensional photonic crystal device was optically coupled to the input tunable laser source and output probing measurement apparatus with observations made from the top plane with a charge coupled device.

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To apply the input laser and also probe the output signals from the very small PhC devices, optical fibers were used as the interconnecting medium for its excellent optical (attenuation of less than 0.2 dB/km) and mechanical properties. To perform side coupling of the optical fibers to the PhC optical intersection devices (Melles Griot NanoMax-TS alignment stages were used). For the coupling of the optical fibers with cladding diameter 125 μm , core diameter 8.2 μm , and mode field diameter of 10.4 μm , to the HAR PhC device (with device height 13 μm), alignment of the input and output optical fibers was achieved via physical guiding of the optical fibers along the monolithically integrated optical testing fiber grooves, which were aligned (in-plane) to the PhC device with high lithographic accuracy. Tilt of the fibers was also minimized through alignment to the etched sidewalls, which was optimized to have etch angles ~ 90 degrees. Figure 6.2 shows the coupling fiber grooves, with and without fibers in groove, together with the probe needles during experiment. Out-of-plane, microprobe needles with tips of 2 μm diameters were used to ensure alignment of fibers to the lower surface of the fiber grooves so that vertical alignment between the core of the optical fibers and the PhC device was achieved (see Fig. 6.3).

(a)

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(b)

Fig. 6.2 (a) SEM of integrated fiber grooves without fibers in grooves, and (b) top down microscope image of fibers aligned in grooves.

Fig. 6.3 Optical microscope image of probe needles used to apply fibers in grooves.

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Figure 6.4 depicts the experiment set-up designed to enable dynamic optical modulation experiments as opposed to simpler static measurements, with coupling alignments, device search with imaging and also spatially localized focusing of high intensity pump beam onto the center of the optical intersections. Using such a set-up, both static and also the dynamic properties of the PhC optical intersections may be probed. Specifically, in the static experiments, properties of PhC optical intersections with different center cavity rod sizes were characterized. Based on this first set of experiments, the center cavity rod modulations principles as described in the previous chapter was tested for its dynamic properties through optical excitation for inducement of changes in refractive index via optically induced free charge carriers plasma effect.

Fig. 6.4 Schematic of experiment set-up, where the pump beam was focused into high intensity onto the resonator from the top, while the weaker, longer wavelength probe beams were applied and detected laterally.

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For such experiments where localized material property change effected by high intensity pump laser needs to be induced in conjunction with application of the side coupled probe signal laser inputs; a laser focusing system such as that illustrated in Fig. 5.6 allows for independent manipulations of each laser source. Here, the pump laser being a Q-switch Nd:YAG based 532 nm direct-coupled system consisted of a laser head containing the optical pump and resonator components with a closed-loop chiller. At the output of the laser head, a half-wave plate was used to rotate the polarization of the linearly polarized pump beam such that a rotation of θ degree by the wave plate about the beam axis would rotate the polarization of the beam by 2θ . In addition to the wave plate, a polarizer was used in combination to form a first attenuator. The pump beam was then directed (by steering mirrors) through a second discrete variable attenuator and beam splitter to reach the top plane of the PhC device under test. Through a 100 times aberration corrected Mitutoyo objective lens, the pump laser beam spot was then focused onto the center cavity rod of the PhC optical intersection, to a beam spot size of less than a micrometer.

The spatial application of such localized pumping was enabled through alignments made with the sample stage, and observation of the pump beam (adjusted to low power level) through a charge coupled device camera fed to a display card on a computer which outputs the feedback image. When the pump laser power was adjusted to a high level, the resulting pump intensity on the PhC optical intersection's center cavity rod becomes very high since the beam was focused into a very small spot size. Therefore, through optical absorption of the pump beam by the PhC intersection's center cavity rod, high density of free charge carriers' result in the PhC material, which induces modulations in the device. These effects are measured with a low intensity probe laser (for which the PhC structures were designed to be sensitive

to). Since the linear absorption of the low intensity probe beam at 1550 nm wavelength is considered negligible for the PhC material (as the photon energies is lower than the band-gap energy of silicon), modulations detected by the probe beam may be attributed entirely to the effect of the localized high intensity and high photon energy pump beam. At the same time, the crosstalk levels measured were also verified to be free from pump radiation through monitoring of readings, while toggling the application of pump laser power was carried out with the probe laser switched off.

6.1.2 Photonic Crystal Test Structures

Besides the experiment set-ups, another important factor for consideration in PhC demonstrations at the optical communication wavelength is the need to incorporate macro to micro coupling testing structures. As presented in Section 2.3, there are mainly two critical interfaces in optical coupling required for PhC testing; the first being the interface between the PhC device and the integrated waveguide; the second being the coupling between the integrated waveguide and the macroscopic probing medium (e.g. an optical fiber or a set of collimating lens coupled to an optical meter). Based on the works described in Chapter 2, the focus here will be mainly on the interfaces between optical fibers, integrated silicon waveguides and the PhC devices. First, integrated fiber grooves were fabricated as presented in Chapter 4. Figure 6.5 gives the cross-sectional SEM image of the monolithic integration scheme involving both the PhC device with the deeply etch optical fiber grooves.

Fig. 6.5 Cross-sectional SEM image of (a) deeply etched fiber grooves with the deep sub-micrometer scale photonic crystal devices; (b) blown up view of photonic crystal device.

Here, the optical fibers were designed to have their cores placed at the same level as the micro scale PhC devices in both vertical and lateral directions. While careful control of etch rates – which differs greatly for varied etch conditions – are required to ensure vertical coupling; lateral alignments were ensured with a series of search and alignment marks made around the periphery of the optical mask. Figure 6.6 shows the overlay marking which indicates how well the PhC devices were aligned to the optical fiber grooves. According to the measurements obtained, the average misalignment in the x and y directions were 0.085 and 0.157 μm respectively. Although such alignment accuracies would still need to be improved for multiple layer stacked 3D PhC fabrications, nanometers scale accuracy is sufficient for good optical coupling between the silicon waveguides and optical fibers.

Fig. 6.6 SEM image of deeply etched fiber grooves with the deep sub-micrometer scale photonic crystal devices.

At the same time, beside the vertical and lateral alignment of the fiber mode field with the micro-scale PhC devices, appropriate coupling between the two well aligned optical modes is also critical. For this purpose, the waveguide taper structures as described in Section 3.5 are necessary. As can be seen from Fig. 6.7, a singular taper at the interface near the PhC waveguide would not be sufficient to enable coupling between macroscopic fibers with modes of $\sim 10\ \mu\text{m}$ to sub-micrometer widths PhC waveguides. Hence, two tapers are required, for slab type PhC devices, a bigger one near the fiber tip, and a smaller one to connect to the PhC optical intersections, as shown in Fig. 6.7b and 6.7a respectively.

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Fig. 6.7 Micro and macro tapered silicon waveguides for coupling between (a) silicon waveguide and photonic crystal; and (b) fiber and silicon waveguide.

At the same time, on top of such taper waveguide structures, it was also necessary to make use of curve waveguide structures to avoid the occurrence of straight through optical paths. In this way, optical leakages that occur, either under or over the PhC devices (through the substrate or over through the upper cladding of air, respectively), can be eliminated. To quantify the wave propagating characteristics of such curved waveguides, many similar curved waveguides were connected in tandem and tested. Figure 6.8 exhibits the microscope image of two such test structures with two and four curved waveguides respectively.

The results of all the above-described test structures measurements will be presented next in the following section, with discussions based on principles similar to the cut-back method employed for the quantification of the very small scale optical waveguide propagation coefficients as presented in Section 3.5.2.

Fig. 6.8 Optical microscope image of test structures with two tapered input waveguides and varied number of curved waveguides.

6.2 Basis Calibrations and Measurements

Determination of the guiding and coupling interfacing components characteristics then allows for subsequent calibration and measurements of the PhC devices, in both HAR and slab type configurations.

6.2.1 Photonic Crystal Line Defect Waveguides

In the experiments, the high aspect ratio (HAR) PhC devices were fabricated as described in Chapter 4 to obtain the high density rod-type PhC square lattice patterns of period 570 nm and rods radii 115 nm – with high resolution and optical proximity corrections (OPCs) along the line defect waveguides. Record HAR etching of PhC rods with ultra-smooth etch sidewall scallop depths of 12 nm were fabricated

in the intersection configuration with different center cavity rod sizes, as shown for example in the SEM image of Fig. 6.9.

Fig. 6.9 High aspect ratio photonic crystal rods SEM images (a) top view with coupled mode analyses ports notations; (b) plane view.

At the same time, slab type PhC of much thinner device silicon thickness was also fabricated similarly. As described in Section 2.3, these two configurations are differentiated mainly by their aspect ratio and also their out-of-plane guiding mechanism. Figure 6.10 shows the top- and orthogonal- view SEM images of the slab type PhC with reduced radius line defect waveguide to confine the optical beam in the vertical direction. Fabricated in 8" SOI wafers; of device thickness 3 μ m; buried oxide thickness of 1 μ m and handle silicon layer of 725 μ m, the bulk PhC array has lattice constant of 517 nm; bulk rods diameter of 223 nm, and sub-100 nm reduced radius line defect rods diameter of 89 nm. These line defects not only confine optical radiation in-plane via PBG action, but also use index assistance for out-of-plane waveguiding.

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(a)

(b)

Fig. 6.10 SEM of slab type photonic crystal intersection device with reduced radius rods waveguide in (a) top view, and (b) orthogonal view.

For the fabricated PhC devices with the monolithically integrated fiber grooves, Fig. 6.11 illustrates how the buried oxide layer acts as the lower cladding; while optical coupling was achieved via fibers side coupled to the devices through deeply etch fiber grooves. In the slab type PhC, tapered silicon waveguides were used for mode size conversion instead of the PhC tapers used for the HAR PhC devices. In this way, optical alignment of the macro size fibers and the sub-micrometer size PhC waveguides may be achieved in both lateral and vertical directions.

Fig. 6.11 Schematic diagram of slab type photonic crystal (in rod configuration), implemented in silicon-on-insulator wafers and coupled with optical fibers.

6.2.2 Silicon Waveguides – Coupling and Bending Losses

The spectrum response of the PhC optical intersections were obtained using the OSA synchronized tunable laser sweeping wavelengths 1520 to 1620 nm in steps

of 0.05 nm. The transmission spectrum of the HAR PhC optical intersection with center cavity rod of radius 300 nm as measured by the OSA when synchronized to the tunable laser was obtained as shown in Fig. 6.12.

Fig. 6.12 Transmission spectrum measurement of the photonic crystal optical intersection with center cavity rod radius of 300 nm, measured using an optical spectrum analyzer synchronized to a wavelength sweeping tunable laser source.

Here, as expected from the simulation results, it was observed that the reflection from this PhC optical intersection with designed center cavity rod was lower than the case for which there was no center cavity rod in the PhC optical intersection. Next, characterization of a simple straight PhC waveguide property was carried out using the FP Resonance method. In Fig. 6.13, the reflection spectrum was measured with changing wavelength in the telecommunication range.

Fig. 6.13 Reflection spectrum measurement of straight photonic crystal waveguide for Fabry-Perot resonance method evaluation of propagation characteristics.

For this FP resonance method, a constant power input light was used and the output end of the waveguide was butt coupled directly by another cleaved single-mode fiber. From the spectrum obtained, the propagation loss coefficient is given by

$$\alpha = -\frac{1}{L} \ln \left(\frac{1}{R} \cdot \frac{\sqrt{I_{\max}/I_{\min}} - 1}{I_{\max}/I_{\min} + 1} \right), \quad (6.1)$$

where L is the waveguide length, R is the facet modal reflectivity, $I_{\max}$ and $I_{\min}$ are the peak and bottom intensities of each resonances respectively. Compared to the conventional cut-back method, the use of the $I_{\max}/I_{\min}$ ratio, which is independent of coupling condition of input and output light, makes the evaluation of such high index waveguides more precise. Here, the effective index is given by

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$$n_{eff} = \frac{\lambda^2}{2L\Delta\lambda}, \quad (6.2)$$

where $\Delta\lambda$ is the FSR, indicating the band width between neighboring resonance peaks. Based on such calculations derived from the measured peak/ bottom intensities of each resonance, together with the FSR, the propagation loss coefficient of the HAR PhC waveguides may be estimated at 0.032 dB/ μm .

Next, for the slab type PhC structures, which allows for vertical confinement and therefore better waveguiding properties over longer propagation distances, the propagation loss coefficient may be obtained based on the cut-back test structures as described in Section 5.3.2. Here, instead of the destructive method of reducing the waveguide length after each measurement set, many waveguides with exactly the same input coupling and output probing conditions were tested for their propagation loss sustained from different waveguide lengths. Using similar input powers, PhC waveguides with different propagation distances were fabricated as shown in the SEM images of Fig. 6.14.

(a)

(b)

(c)

Fig. 6.14 Photonic crystal line defect waveguides of varying length (a) shortest at $15a$ length; (b) mid-length at $35a$ length, and (c) longest at $55a$ length.

The propagation loss coefficients obtained for single line defect slab type PhC waveguides with and without reduced radius waveguides were $0.46 \text{ dB}/\mu\text{m}$ and $0.72 \text{ dB}/\mu\text{m}$ respectively. The higher rate of propagation loss in the devices without reduced radius waveguides may be attributed to the lack of vertical confinement, otherwise present in the index assisted reduced radius PhC line defect waveguides.

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Here, the waveguide propagation loss seem greater than that of the HAR case since the HAR throughput was measured without isolation structures such as bends etc. Hence, the straight through path of the measurement resulted in greater transmission coefficients. At the same time, even though the slab structure has index guiding in the out-of-plane direction, coupling with TE-like modes from the symmetry-breaking substrate will result in such waveguides being leaky too.

Based on these results, to obtain the losses incurred by each 90 degrees waveguide bends, similar test structures were used as shown in Fig. 5.13. Based on the differences in transmission levels for the two 90 degrees bend and four 90 degrees bend test structures, the loss incurred by the addition of each 90 degree bend may be estimated to be ~ 3 dB. This loss may be attributed to both the small bending radius and also multimode nature of the silicon waveguides, which promotes mode scrambling at the tight bends that result in losses through coupling to the radiative modes.

Here, it was noted that the coupling loss per port for the HAR was much lower than that of the slab type PhC devices. While the total coupling loss was only 2.7 dB for the HAR PhC devices, the total coupling losses for the slab type PhC devices were ~ 50 dB. This was due to the incompatible optical mode sizes between the fiber and the much thinner silicon waveguides in the slab configuration. Although this loss is high, the cause of it was due to the lack of an appropriate mode converter between the very large optical fiber mode and the slab type silicon waveguide. This type of losses due to incompatible mode sizes had been shown to be effectively circumvented with many methods, as discussed in Section 2.3.1, where it had been shown experimentally that an adiabatic mode connector [136] may be used to achieve connection loss as low as 0.8 dB per port [123] for slab type PhC with dielectric claddings. Yet, since

such adiabatic mode connector does not work as well with PhC slabs with air claddings, further design and investigation is needed.

Therefore, the many characteristics of the testing structures, such as the propagation loss coefficients, coupling losses, and bending losses were measured using many dies, and the PhC devices may then be measured and evaluated with these foundations.

6.3 Static Photonic Crystal Device Experiments

Having established the optical properties of the OTS assistance devices, and also the basis properties of the PhC waveguide propagation characteristics, the various functionalities of the 1D and 2D PhC optical intersection devices are then measured, first in the static configuration.

6.3.1 Measurement of One-Dimensional Photonic Crystal Fabry-Perot Filter

Figure 6.15 shows the fabricated 1D PhC FP filter device. As the devices were fabricated via the same mask as the optical intersection devices, and the processes were targeted for the latter devices, the 1D filters do not have ideal dimensions.

Fig. 6.15 SEM image of one-dimensional photonic crystal implementation for Fabry-Perot resonator filters structure.

Hence, the partially reflecting mirrors formed by the layered 1D structure were a few tens of nanometers off-target CD and therefore had low reflectance. This fabrication short-coming therefore as expected resulted in low Q-factor measurements made for the device, as shown in Fig. 6.16, where the measured transmission spectrum is scaled in arbitrary units and plotted along with the theoretical calculation. For further enhancement of device properties, out-of-plane structural symmetry with refill of oxide post device etching would also be useful.

Fig. 6.16 Optical experiment measurements of the one-dimensional photonic crystal Fabry-Perot filter transmission spectrum compared against simulation results for fabricated dimensions.

6.3.2 Verification of Photonic Crystal Optical Intersection Designs

For both single line resonators, and two orthogonally intersecting single line defect PhC waveguides (forming small form factor optical intersections), the cavity modes can be controlled by the size of the coupling cavity rod at the intersection, even for the case of the 1×1 resonator. To unveil the relationship between the size of the center cavity rod and the performance of the HAR PhC optical intersections, transmission measurements were repeated for different PhC optical intersection devices fabricated with different center cavity rod sizes (see Fig. 6.17) at wavelength 1550 nm.

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Fig. 6.17 SEM images of photonic crystal optical intersections with progressively larger center resonator rod dimensions.

For HAR optical intersections with center tunneling cavity rods of varying radii (normalized to the lattice pitch of the PhC), the crosstalk and transmission level measurements were made as shown in Fig. 6.18 (a) and (b) respectively. In the plots, the experimental results are indicated by filled symbols while the FDTD simulation results are plotted in a continuous line. In the plots, the abscissa indicates the normalized radii of the center cavity rods (expressed as a ratio of the PhC lattice period), while the ordinate axis represents the measurement levels in dB.

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(a)

(b)

Fig. 6.18 Optical experiment measurements (filled-symbols) and FDTD simulation results (smooth line) for (a) crosstalk, and (b) transmittance levels, of the photonic crystal optical intersection devices with progressively increased center cavity rod size.

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Here, measurements of PhC optical intersections with center rod radius of less than 200 nm (i.e., normalized radius less than 0.35) cannot be realized due to limitation in fabrication resolution. Hence, the normalized radius of the tunneling cavity cannot be tested for small values ranging between 0 and 0.35 times the lattice period of 570 nm (i.e. between 0 to 190 nm due to limit in fabrication process resolution). For the other tunneling cavity sizes of PhC intersecting waveguide measurements, both the measured crosstalk and transmission results corresponded well with the FDTD simulation results with good repeatability. From the experiments, the modulations of the transmission and crosstalk levels, by the different cavity sizes were measured to be greater than 16 and 12 dB respectively. Here, it is to be noted that since the optical path of the crosstalk measurement was not a straightforward one (unlike that of the transmission branch); the crosstalk measurements made can be attributed solely to the effect of PhC wave guiding and not from stray leakage radiations.

Further, for similar PhC intersections in the slab type configuration instead, where missing rod waveguides were replaced by reduced radii PhC rods, higher Q-factor resonators were tested with presence of vertical confinement mechanism. Here, Fig. 6.19 exhibits the Lorentzian response of the single line configuration 3×3 PhC optical resonators with one surrounding PhC bulk rod around the center cavity resonator.

Fig. 6.19 Measured optical spectrums of single line resonators with varied center resonator rod sizes.

For resonator sizes varied as 0, 84, and 136 nm, the expected blue shift of the optical responses for increase in resonator rod radius size from 0 to 84 nm was found to be 19 nm. At the same time, increases in transmission spectrum levels were also observed for optical intersections with radii 0 and 84 nm as compared to that of radii 136 nm. For the a range of center resonator rod dimensions and their corresponding effects, Fig. 6.20 shows the steady state normalized transmission levels of a 5×5 slab type PhC optical intersection at the telecommunication wavelength of 1550 nm, plotted with reference to resonator rod radius. Here, the filled symbols in Fig. 6.20 represent the optical measurements while the unfilled ones represent the 3D finite deference time domain simulation results.

Fig. 6.20 Photonic crystal optical intersection with two bulk rods on each side of the resonator and its simulated and measured transmittances for varied center resonator sizes.

Hence, both HAR and slab type PhC structures have been experimental measured to demonstrate the predicted characteristics of sensitivity towards the center cavity resonator rod sizes. At the same time, as expected, Lorentzian responses were observed for PhC intersections with order higher than the 1×1 configuration, as demonstrated in the slab type PhC optical intersection measurements. Although the slab type PhC suffered from high coupling losses due to the incompatible coupling between the input fibers and the slab type waveguide mode, much higher quality optical intersections were successfully demonstrated due to the improved confinement in the out-of-plane direction. Hence, with these static measurement results, the next section will present the dynamic modulation aspects of the fabricated PhC devices.

6.4 Dynamic Modulation of Photonic Crystal Intersection

The unique structure of the orthogonally intersecting line defect photonic crystal waveguides with optical characteristics dependent on the center resonator rod properties is useful for dynamic optical modulation purposes as described in Section 5.3. This is due to the enhanced optical nonlinearity imposed by the PhC optical intersections. The experiments realized for these modulation principles and designs will be described in greater details in the following sections.

6.4.1 Optically Generated Plasma Effects for Ultrafast Modulations

As evaluated in Chapter 5 of this thesis, the application of an optical pump beam onto the center resonator rod of the PhC intersection is capable of effectively modulating the optical responses of such devices. A demonstration of this prediction is shown for a center cavity rod size of 0.53 times the PhC lattice period for a HAR PhC optical intersection. Figure 6.21 shows the modulated response of the crosstalk levels in the HAR PhC optical intersection when the power of the pump beam was decreased progressively through increasing attenuation. Here, the abscissa axis gives the intensity of the pump laser while the ordinate axis plots the normalized changes in crosstalk levels. The measured crosstalk levels are plotted as round symbols in the figure while the FDTD simulation results are plotted as a solid line.

Fig. 6.21 Normalized crosstalk level modulated by optical pumping.

For pump beam radiation of intensity less than 60 MW/cm^2 , the measurements of the modulated signals were well repeatable. However, for pump beam radiation of more than 75 MW/cm^2 , the PhC material began to show signs of damage, which under SEM inspection revealed melted material within the altered intersection. Such damage to the PhC device material being irreversible therefore changes the cavity property of the optical intersections permanently (effect remaining even after removal of the optical pump beam). Hence, based on these experiments, an effective modulation range of normalized crosstalk being 15 dB was therefore found for the HAR PhC optical intersection devices with applied pump radiation kept below 60 MW/cm^2 (where reversible modulations of the PhC optical intersections are possible). To explore the possibility of improving these results, higher Q-factor PhC optical intersections in the slab type configuration was tested.

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Similar to the procedures used for the HAR PhC optical intersections, the slab type PhC intersections were also modulated dynamically with a pump laser applied with spatial localization from the top onto the center resonator rod. For a 3×3 slab type PhC optical intersection, it can be seen that the Lorentzian spectrums were shifted in magnitude instantaneously with the on and off toggling of the applied continuous wave pump laser. Figure 6.22 gives the transmission spectrums of such a 3×3 slab type PhC optical intersection, with and without application of optical pump power. From the spectrums, it can be seen that the modulated spectrum peak was increased by $\sim 57\%$ while the FWHM was decreased from 40 to 36 nm. When this same device was melted down, the transmission signal was indeed lost as shown in the measured spectrum of Fig. 6.22.

Fig. 6.22 Experimental results of instantaneous photonic crystal output modulation by the on/ off toggling of the high intensity applied continuous wave pump laser.

Here, the optical power required to achieve such modulations were much reduced in such slab-type PhC optical intersections of higher order configurations

than in the HAR 1×1 configuration; so that the power applied was only 0.318 MW/cm^2 for the case of instantaneous modulations demonstrated in Fig. 6.22. This is due to the higher Q-factors in such cavities as compared to the HAR case without partially reflecting PhC rods surrounding the center cavity resonator. As an accompanying consequence, much lower power was observed for the meltdown thresholds ($\sim 1.06 \text{ MW/cm}^2$), since higher order cavities are better capable of retaining radiation for a longer life-time. Hence, the free carrier-plasma effect was observed and the time scales of such operations are limited mainly by the relaxation time of the carriers as described in Section 5.1. When the application of optical pump radiation was used to heat up the lattice, through fast energy exchange between the optically excited electronic sub-system and the lattice, thermo-optic effect modulations were instead measured as will be presented in the following section.

6.4.2 Thermal Modulation Effects

Thermo-optic switching operations may be derived using a similar experiment set-up as shown in Fig. 6.4. For pump laser pulses with repetitive frequency of 50 kHz, the effect of increasing the thermo levels of the PhC intersection devices can be shown to yield both expected red shifts in the resonant spectrums (towards the longer wavelength) and also corresponding bandwidth increases, in the much slower thermo modulation effect. The thermo-optic effect arises from excessive circulating optical flux within the lattice of the PhC silicon material, which gets heated up by the recombining charge carriers. Typically, continuous-wave laser beams used for optical pumping are more prone to the thermo-optic effects, due to the continuous bombardment of photons onto the material. However, as the continuous wave laser used in our experiments had much lower intensity than the Q-switched pulsed mode

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of the pulse-type laser output, we were able to induced thermo-optic effect modulations, only via the pulsed pumping mode. Figure 6.23 gives the thermo-optic modulation effect on the bandwidth of the 3×3 PhC slab-type optical intersection device as increasing optical pumping power was applied onto the center cavity resonator rod. For incident pump power increased from 0 to 0.110 mW, the bandwidth of the PhC device was increased by up to 3 nm. Bandwidth modulations of such magnitude indicates that the induced refractive index increase was larger than 0.2, as simulated in Fig. 5.12 for the PhC intersection device. This would indicate that sample melting due to temperature increase of over a thousand degrees as predicted in the result of Fig. 5.11 may be justified since melting of sample prevented further experiments towards the end of the last few readings.

Fig. 6.23 Progressive bandwidth change to a photonic crystal optical intersection resonator as it was thermo-optically modulated by progressively higher pump power.

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At the same time, the bandwidth widening was also accompanied by a corresponding red-shift in the center wavelengths of the Lorentzian transmission spectrums as shown in Fig. 6.24. Figure 6.24 plots the resonant wavelength shifts of the 3×3 slab-type PhC optical intersection device under thermo modulation, as progressively increasing optical pumping power was applied. From the experiment, with applied optical power up to 0.11 mW, the center wavelengths was increased by 2.2 nm for increasing optical pump power applied. From the measurement, it may be observed that fine shifts of 0.1 nm was observed for such modulation effects with applied pump power increased in steps of ~ 0.01 mW. Based on the FDTD simulation results presented in Section 5.3, center wavelength red-shifts of 2 nm would therefore correspond approximately to refractive index changes of nearly 0.2, which is corroborated by the induction made based on the bandwidth widening effect. Such index changes in turn corresponds to large increases in temperature which therefore causes localized melting of the device under test, as shown in Fig. 6.25.

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Fig. 6.24 Corresponding center wavelength shifts for the 3×3 photonic crystal optical intersection resonator as it was thermo-optically modulated by progressively higher pump power.

Therefore, from the experiments, the effects of the carriers' plasma and thermo-optic type modulation were very easily and clearly distinguished. In the carriers' plasma modulation effect, the changes made to the device spectrum returned instantaneously to its original position once the pump laser beam was switched off. On the other hand for the thermo-optics induced effect, the modulated device spectrum took a relatively much longer time in order to return to its original spectrum position. This may be attributed to the much slower rate of material cooling in the thermo-optic effect (required to return the device to room temperature after getting heated up by the pump laser) as compared to the fast recombination and relaxation processes in the former carriers' plasma process.

While the thermo-optic effect provides an alternative means of optically induced modulation for the PhC devices, its distinctively longer time scales makes it suitable mainly for state changing applications, and not optical switching operations which requires as short a switching time as possible. At the same time, as expected, the modulation of refractive index by the carriers' plasma effect was larger than that of the thermo-optic induced refractive index change. Also, the use of thermo-optic effect for modulation would also require the careful application of laser irradiance onto the PhC device, since any occurrence of melting in the silicon PhC material is irreversible. Figure 6.25 shows not only how well the pump beam laser may be focused onto the center of the resonator rod to cause localized melting (Fig. 6.25a), but also how the unbridled application of laser irradiance can lead to melting of the silicon material (Fig. 6.25b) at the PhC resonator rod.

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(a)

(b)

Fig. 6.25 SEM of extreme effect in localized high intensity optical pumping; (a) photonic crystal intersection device prior to complete melt down, but slightly deformed after pumping. (b) Photonic crystal after excessive pumping, inducing cavity rod melting and collapse onto a nearby neighboring rod.

6.5 Summary

The optical experiment set-up, techniques, and methods for measurement of PhC devices sensitive at the optical communication wavelengths centered at 1550 nm were presented. Based on these, the optical characteristics such as the coupling loss; waveguide propagation coefficients etc of the various structures such as the tapered waveguides; the isolation bends were calibrated. These allowed progression onto the measurement of the PhC devices, such as the 1D PhC FP filter and also the 2D PhC optical intersections. In the static measurements of the PhC optical intersections with varying center resonator rod dimensions, the sensitivity of the intersection resonators to the center cavity rod as predicted in Chapter 3 was verified. Following which, in the dynamic optical modulations of such PhC optical intersections, the effect of free carriers' plasma induction for modulation of cavity rod index to demonstrate light-tuned-light effects were achieved without homogeneity issues due to the advantage of small area volume of the center cavity rod.

Hence, the effectiveness of PhC tuning was demonstrated for fabricated high resolution 2D PhC optical intersection devices. The potential of such modulation scheme as a practical means of device property modulation points to many exciting opportunities for further development of tunable PhC devices. This work is not only significant for its precedence, but also for its implications to potential applications in both tunable and also ultra-fast switching deep sub-micrometer size optical PhC intersection circuits.

CHAPTER 7

CONCLUSIONS

7.1 Conclusions

Three main aspects of the novel PhCs meta-material have been developed. First, in the area of PhC nano-fabrication, record high resolution and aspect ratio PhCs with sub-micrometer length scales applicable for use at the optical communication wavelengths were realized based on critical process flows and various dependent modules development. Second, in the area of theoretical analysis and design, a large complete photonic bandgap structure has been theoretically analyzed and designed together with other nano-cavities; single line resonator; spatially shifted; cascaded and optical intersection PhC resonators. Third, optical experiments of the sub-100 nm scale PhC circuit devices were successfully designed and implemented such that both static and dynamic measurements were yielded at the optical communication wavelengths. The major conclusions arrived at are as follows:

In the nano-fabrication aspects of PhC, first in the optical lithographic development of the high density deep sub-micrometer length scale PhC structures useful for the optical communication wavelengths, sub-lithographic wavelength OL can be used to derive high density PhC rods array without typically expensive resolution enhancement techniques of PSM and OAI etc. Here, highly dense PhC rods array with sub-100 nm reduced radii PhC defect rods with diameters of only 38% the wavelength of irradiation at 248 nm was obtained. At the same time, OPE

corrections was developed based on regression modeling arising from a multiple factor design of experiment to yield OPC experimental compensations. In the etch module of the 2D rod type PhC structures fabrication, record HAR (~ 50) etch of the 115 nm radii, super dense PhC array with orthogonal air spacing apart of only 340 nm can be achieved with mask bias and also critical etch/ passivation balance. This is unprecedented since previously, such HAR etchings were always almost exclusively realized only with macroporous silicon etching. Record low scallop depth of 12 nm as opposed to typically reported low values of 50 -300 nm can be obtained through optimization of the recipe with reduction of etch isotropy carried out to balance both reduction of etch dominance and increase in etch duration. Monolithic integration of disparate opening sizes and depths of etching required to enable macro optical fiber assisted coupling to the micro-scale PhC, together with wide and independent process window development can be implemented through fabrication process flow that allows for independent module development.

In the design aspects, both bandgap and device application designs for 2D PhC integrated circuits have been presented in detail. First, large complete bandgaps can be designed based on the optimization of respective TE and TM bandgap conditions using structural and empirical deductions. Improved configurations of embedded microcavities system can be designed based on the Q-factor and multiple resonances interaction principles. Tunability to device operation can also be implemented based on time domain simulations of dielectric properties variations. Due to the small size of PhC optical resonators, and the isolated nature of rod type PhC resonators, effective optical modulations of PhC integrated circuit devices can be effected.

In the optical experiments with these sub-micrometers scale PhC optical intersection circuits etc, coupling between macroscopic optical source and detectors,

to the microscopic scale PhC circuits were achieved. The experimental results of the fabricated PhC devices have shown that the PhC devices is capable of achieving integrated circuit level performances such as compact size, large tuning range, and high tuning accuracy.

Next, in the optical modulation experiments making use of excited carriers' plasma to affect the material optical properties within the sensitive resonator cavity volume, it was shown that light-tuned-light signal modulations of more than 12 dB can be implemented in the native optical form with spatial homogeneity based on localized free carriers' injection on small PhC devices with times limited by the relaxation times of the carriers. Here, both thermal and instantaneous modulation optical throughput was demonstrated, as described in Chapter 6. In addition, an additional benefit of such methods is that batch fabrication enables easy IC integration to other electronic or photonic circuit device and applications, which would not only reduce cost of implementation, but also broaden the application areas. Moreover, the miniaturization possible makes it advantageous to construct very small size optical modulation circuits of the sub-wavelength dimension, which advances the state of the art for optical length-scale PhC devices capable of high-density integration.

Hence, the design and fabrication of high resolution PhC devices of HAR and slab type PhC PIC were achieved with optical measurements and modulation demonstrations. As a first demonstration of HAR PhC waveguide and optical intersection in the optical communication wavelengths, these works provide: proof of concept for the devices designed and simulated; developed fabrication techniques in DUV lithography for sub-100nm patterning; realized ultra high aspect ratio (~50) etching of highly dense sub-micron length-scale lattice array of PhC rods etching with reactive ion etching; optical measurements of static parametric variations and also

optical modulations of PhC optical resonators with top down application of optical pump beam. Based on these results, much insight into the workings and intricacies of PhC devices at the sub-micrometer length scale were obtained.

However, as discussed, the main limitations of these devices lie in the areas of optical losses and the efficiency of the plasma modulation processes. While the former is brought about, mainly by the non-optimized device properties such as the incompatible mode sizes and lack of out-of-plane confinement etc, the latter is a consequence of the small interaction volume, and is often further impeded with the occurrences of nonlinear absorption which results in significant thermal effects. While coupling inefficiencies arising from incompatible mode sizes may be improved upon with further optimizations in the design of mode couplers (such as those described in Section 2.3), lack of out-of-plane confinement may be circumvented with the use of HIC waveguiding within the device, so that in-plane confinement may be better achieved. Further to this, the group velocity of the PhC device may be further optimized so that greater enhancement in light-matter interaction may be allowed for within a small interaction volume. To prevent excessive nonlinear absorption and unnecessary thermal damage to device, shorter pulse durations for the pump laser may be used.

To further allow these works to be further developed for application in large scale integrated photonic circuits, the above discussions on the improvements needed should be carried out in future works with relevant recommendations for such efforts described in the following section.

7.2 Recommendations

Recommendations for future research are summarized as follows:

First, it is significant to develop on-chip PhC optics to further improve the specifications of the PhC devices. In this respect, there are a few foreseeable methodologies. Large scale 3D PhC circuits' fabrication using two photon interferometric lithography or HL are recently researched intensely and have since obtained promising fabricated device results. Further optimization of current 2D PhC device circuits are also a viable option in this respect. Such efforts may be directed towards advances to be made in the area of further RETs in sub-lithographic wavelength lithography and also etch sidewalls optimization in reactive ion etching to yield ever smoother and greater verticality in the PhC cross-sectional profiles.

Second, further efforts in the area of macro to micro level coupling are needed for greater ease of PhC optical measurements. This issue of disparate length-scale between the micrometer size PhC devices and optical coupling fibers, if not addressed properly, prevents the proper interrogation of fabricated PhC devices and results in unnecessarily high coupling loss. Although much progress has been in this area, for example with 3D couplers described in Section 2.3, such designs cannot be applied for all cases of PhC systems (for example it is non applicable for non-top clad PhC systems). Therefore, further works in design and simulations are needed to obtain greater efficiency optical fibers to integrated PhC device interactions. For such purposes, gratings and evanescent wave coupling are two good candidate methods which show good potential for research [6].

Third, further improvements may be made to the integrated PhC device optical performance, namely in the area of propagation coefficients in the waveguides and also optical modulation power efficiency in the optical intersection resonators. The critical parameter of concern in both these factors lies in the improvement to

confinement of optical power, in the waveguide and in the resonator. Greater confinement in the waveguide leads to lower propagation loss coefficient while greater confinement in the resonator leads to a longer decay time for greater resonator quality factor, which in turn results in the reduction of optical power required for optical modulations. As described in Section 7.1, such improvements may be sought based on improvements to the number of dimensions in confinement as obtained with the introduction of reduced radii defect waveguide rods within missing rods line defect waveguides. Further to this, greater precision in the deep sub-micron fabrication of such devices, especially in the obtainment of accurate critical dimensions and smooth device sidewalls are needed to obtain close to ideal device performance. Another area for future work includes the procurement of a set of pump probe equipment setup, which will allow for accurate time domain switching measurements of the devices during modulations with very short pulse durations to prevent undue sample heating.

Next, apart from the improvements to the current device demonstrations, in the greater picture of PhC device, greater flexibility in the implementation of integrated PhC circuitries would also be of great value to the advancement of this field since current designs and implementations are strictly implemented on a case by case basis of time domain simulations. Libraries of optical PhC components that can be implemented in various connections would reduce design time and aid large scale integration efforts.

Finally, there is still room for greater sensitivity in the optical response of the PhC devices. A possible candidate to achieve such improvement may be through the use of electromagnetically induced transparency material, which would theoretically be able to reduce the optical modulation power threshold, to a discrete number of

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photons. However, as such material is currently still rather exotic, a corresponding re-development for fabrication processes amenable for such material would be necessary.

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