The Development of Novel Passive and Active Photonic-Crystal Devices

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Abstract

Photonic crystals are anticipated to have impact on large-scale photonic integrated-circuits by allowing the creation of compact and efficient devices such as waveguides, splitters, microcavity filters, light emitting diodes, and lasers. Previous experimental research has mainly focused on photonic crystals composed of a lattice of air holes etched into dielectric slabs. This thesis discusses the design, fabrication, and characterization of the “inverse” structure, a square lattice of dielectric-rods in air. Bandgap guiding of 1.5 μm light is experimentally demonstrated for a photonic-crystal waveguide created by introducing a line-defect of smaller-radii rods. To provide efficient optical coupling between input/output dielectric waveguides and the photonic-crystal waveguide, an adiabatic taper having two stages is employed.

Furthermore, the thesis investigates novel photonic-crystal devices and fabrication schemes. An expose-develop-etch (EDE) method is utilized to fabricate rod-based photonic-crystal devices in III-V and SOI material systems. The thesis also presents an electrically-activated linear-waveguide photonic-crystal laser. A compact microcavity is created by introducing a defect inside a one-dimensional photonic crystal. Electrical-activation and edge-emission are achieved by patterning microcavity waveguides into p-i-n-doped epitaxial heterostructures. The compact photonic-crystal laser is anticipated to have impact on the integration of optical devices on the same chip.

Thesis Supervisor: Leslie A. Kolodziejski
Title: Professor of Electrical Engineering
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I vividly remember the day I arrived at MIT, my first time in the US, as a young freshman on August 18, 1996. During the last eight years, I have learned a lot and have gotten the opportunity to explore the latest research efforts. MIT is a world-class institute that has many brilliant people with innovative ideas. I definitely enjoyed the daily intellectual challenge, and benefited from the people around me. I am very grateful to many people who contributed to my success during the amazing time I spent at MIT.

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Chapter 1
Photonic Crystals:

Background

1.1 Motivation

The last few decades have witnessed the transformation of telecommunication networks [1]. The development of high speed transistors, semiconductor lasers and detectors, and the enormous bandwidth provided by the large amount of fiber already installed (but yet to be fully utilized) have resulted in the increase of information transmission capacity. There is tremendous network traffic growth due to the current demand for high-speed data, and multimedia such as high-quality video [2].

However, the electronic circuits at network nodes which interconnect fibers only meet the current communication bandwidth demand and will soon become a limitation [3]. In the nodes, light is converted into electrons so that the electronic signal can be re-shaped, re-timed, and re-amplified (3R regeneration), routed, buffered, etc.; then, the electronic signal is converted back into light. This ‘electronic bottleneck’ at the nodes leaves the large bandwidth of the fiber underutilized. Furthermore, the numerous racks of electronics which consume a large amount of space and power make the nodes very expensive.
The network capacity can be increased, while lowering the cost, by packing functionality and intelligence into an optical-chip. Such chips, packed with optical devices, will be able to identify the contents of the individual wavelengths of light in a fiber, where each carries a specific video or voice data-stream. The chips will then route each wavelength to a particular location after performing packet error correction and 3R-regeneration. If realized, the integrated optical-chip will replace racks of electronics for a fraction of the cost [4].

A functionality required by the high-density photonic integrated-circuits is guiding light around a bend with a radius of curvature on the order of a wavelength [5, 6]. To make this possible, high-index-contrast waveguides need to be utilized to guide light on photonic chips. Though the radius of curvature to turn a corner is on the order of microns, thus allowing high-density integration in a small area, the waveguides are very susceptible to loss mechanisms such as scattering loss due to sidewall roughness introduced during fabrication [7-11].

Photonic crystals have been proposed as a potential solution to guide light around corners including 90° bends with near perfect transmission [12]. This will help reduce the large area in current photonic chips due to the large radius of curvature of waveguides, hence enhancing microphotonics device integration for high density optoelectronic circuits. However, the practical use of photonic-crystal waveguides is limited by the poor coupling efficiency between the photonic-crystal waveguide and conventional index-guided waveguides. The photonic crystal waveguide to conventional waveguide coupling poses a challenge because the photonic-crystal waveguide exhibits a
significantly different mode profile and propagation mechanism compared to traditional waveguides that use index confinement.

Furthermore, optical 3R regeneration and optical logic functionalities capable of performing header recognition and error correction have been demonstrated by combining various discrete optical components, by using delay lines, external laser sources, and lens assemblies that extend over many optical tables [13-17]. However, such assemblies are too bulky and too costly to deploy at network nodes. Optical integration would be more efficient, practical, and economically advantageous if compact enough to fit on an optical-chip. To this end, the implementation of all-optical 3R regeneration and logic will require laser sources that interact with the incident light carrying the information. Hence, photonic crystals can be utilized to create a compact and efficient optical source for photonic integration.

This thesis focuses on how photonic crystals can be used to enhance the performance of both active and passive devices, and allow the integration of photonic devices on a chip. The major section of the thesis demonstrates photonic-crystal waveguides created from a periodic arrangement of dielectric rods. The structures are used for optoelectronic integration by solving the problem of coupling from high-index conventional waveguides into low-index photonic crystal waveguides. The photonic crystals have been fabricated in both III-V and SOI structures. Furthermore, a key component that has been lacking from photonic crystals is their electrical activation. In the last section of the thesis, a novel electrically-activated photonic-crystal linear-waveguide microcavity laser is proposed. Various process sequences are assessed and results from preliminary fabrication of the front-end are presented.
1.2 **Photonic Crystals: Introduction**

Photonic crystals are composed of materials with their dielectric constant modulated in a periodic fashion. The periodic arrangement of high and low refractive-index materials gives rise to a stop-band in which a range of frequencies are prevented from propagating. Given the appropriate dimensions, the stop-band acts as a photonic bandgap in which photons are prevented from propagating [18]. This is analogous to the energy bandgap for electrons that is observed in electronic materials due to coherent Bragg scattering from the periodic variation in the electronic potential due to the electronic structure of the atoms [19]. Lord Rayleigh performed the first study on electromagnetic wave propagation in a material with one-dimensional periodicity in 1887, and Felix Bloch studied wave propagation in three-dimensionally-periodic media in 1928 [20]. The existence of a complete bandgap for electromagnetic waves in a photonic crystal was reported independently by Yablonovich [21] and John [22] in 1987.

![Fig. 1-1: Schematic illustration of photonic crystals a) one-dimensional (1D) b) two-dimensional (2D) c) three-dimensional (3D). In each figure, the index contrast is indicated by the difference in color.](image-url)
Photonic crystals can be classified as one-dimensional (1D), two-dimensional (2D), or three-dimensional (3D) [Fig. 1-1]. 3D photonic crystals are ideal because of their complete bandgap [23]. However, they are difficult to fabricate at small length scale due to the planar nature of the current semiconductor fabrication technology [24]. The best alternative to 3D photonic crystals is to emulate them with 2D photonic crystals combined with index confinement in the direction perpendicular to the plane of periodicity [25]. These structures, in which a photonic crystal resides in the high-index material surrounded by low-index material, are known as slab photonic crystals. In the plane of the photonic crystal, the confinement is due to the presence of a bandgap, while the confinement in the vertical direction occurs due to the existence of a high-index guiding layer surrounded by low-index cladding. The existence of the low index surrounding gives rise to a light-cone, a region in the dispersion diagram that contains the radiation modes guided by the background material. Even though these radiation modes exist in the bandgap, a mode is still guided as long as the guiding layer has a higher refractive-index with respect to the cladding layer.

Photonic crystals can be constructed in two main configurations as shown in Fig. 1-2. The first type consists of a periodic arrangement of high index dielectric material (pillars) in a low index surrounding, which gives rise to a bandgap for the TM-like (odd) mode where the E-field is polarized perpendicular to the plane of periodicity. The second type consists of a periodic arrangement of lower index dielectric material (holes) in a higher index slab, which gives rise to a bandgap for TE-like (even) modes where the H-field is polarized perpendicular to the plane of periodicity. Most experimental studies have focused on periodic holes etched into a dielectric slab, mainly due to the ease of
fabrication and testing. Other configurations that have been studied by many include opals, inverse-opals, and self-assembled colloidal structures [26-28].

Fig. 1-2: Schematic illustration of 2D slab photonic crystals. a) Square lattice of pillars. Each pillar has a high-index guiding layer surrounded by low index top and bottom layer. b) Triangular lattice of air holes etched into a high index dielectric slab.

Photonic crystals have useful applications in compact optical devices such as microcavities and waveguides. A photonic crystal microcavity is created by introducing a defect in the periodic array and localizing a mode inside the bandgap. Furthermore, a photonic crystal waveguide, which is created by introducing a row of defects, is useful for routing light within a photonic integrated circuit. While the periodic arrangement of dielectric material results in a photonic bandgap, the defect row functions as a waveguide by localizing a band of frequencies. As a result, these frequencies propagate within the defect row and are evanescent in the bulk photonic crystal. Perfect transmission through $90^\circ$ bends have been calculated in 2D simulations of photonic-crystal waveguides that are created by omitting a row of cylindrical rods in an otherwise perfect photonic crystal [29].
1.3 The Physics of Photonic Crystals

1.3.1 Maxwell’s Equations

The propagation of waves in dielectric media is governed by Maxwell’s equations. Photonic crystals are created using materials which can be modeled as isotropic and low loss, wherein the dielectric constant is approximated as having a negligible imaginary component [18]. Using these facts, Maxwell’s equations can be summarized as follows:

\[ \nabla \cdot \vec{B}(\vec{r}, t) = 0 \quad \text{(EQ-1.1)} \]
\[ \nabla \times \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t} \vec{B}(\vec{r}, t) \quad \text{(EQ-1.2)} \]
\[ \nabla \cdot \vec{D}(\vec{r}, t) = 0 \quad \text{(EQ-1.3)} \]
\[ \nabla \times \vec{H}(\vec{r}, t) = \frac{\partial}{\partial t} \vec{D}(\vec{r}, t) \quad \text{(EQ-1.4)} \]

The time dependence in the equations can be eliminated by using time-harmonic fields. Time-harmonic fields are useful because they cover the whole spectrum of the electromagnetic waves, and Fourier analysis can be used to understand the time-domain phenomena. Furthermore, any solution can be built by combining the time-harmonic solutions through Fourier analysis [30]. By eliminating the time dependence, EQ-1.2 and EQ-1.4 can be re-written as follows:

\[ \nabla \times \vec{H}(\vec{r}, t) = -i\omega \varepsilon(\vec{r}) \vec{E}(\vec{r}) \quad \text{(EQ-1.5)} \]
\[ \nabla \times \vec{E}(\vec{r}, t) = i\omega \vec{H}(\vec{r}) \quad \text{(EQ-1.6)} \]
By decoupling the two equations, the final equation is expressed in terms of $H$ as follows:

$$\nabla \times \left( \frac{1}{\varepsilon(r)} \nabla H(\vec{r}) \right) = \omega^2 H(\vec{r}) \quad \text{(EQ-1.7)}$$

EQ-1.7 is the master equation for photonic crystals [18]. After solving for the magnetic field at a given frequency, EQ-1.5 can be used to obtain the electric field.

1.3.2 Bloch States in Photonic Crystals

Analogous to quantum mechanics, electromagnetism in photonic crystals can be stated as an eigenvalue problem in the frequency-domain approach by using $H$ as the eigenfunction and $\omega^2$ as the eigenvalue. In quantum mechanics, a Hermitian operator $\Omega$ acting on two field vectors $A$ and $B$ has the property that $(A, \Omega B) = (\Omega A, B)$, where $(A, B)$ is the inner product of normalized vector fields $A$ and $B$. A Hermitian operator implies that the eigenfunctions are orthogonal and they have real eigenvalues. EQ-1.7 can be simplified by defining an electromagnetic operator as follows:

$$\Pi = \nabla \times \left( \frac{1}{\varepsilon(r)} \nabla \right) \quad \text{(EQ-1.8)}$$

This operator can be easily proven to be a Hermitian [18]. Because $H$ is an eigenfunction of $\Pi$, it can be expressed as a linear combination of eigenmodes. For two-dimensional photonic crystals, the equation can be written as follows:
\begin{align*}
H_{k_x,k_y}(r) &= e^{i k_y y} e^{i k_x x} u_{k_x}(x,z)u_{k_y}(y,z) 	ag{EQ-1.9} \\
u_{k_x}(x,z) &= \sum_m c_{k_x,m}(z)e^{imb_{x,x}} 	ag{EQ-1.10} \\
u_{k_y}(y,z) &= \sum_n c_{k_y,n}(z)e^{imb_{y,y}} 	ag{EQ-1.11}
\end{align*}

\(k_x\) and \(k_y\) are the in-plane wavevectors. \(b_x\) and \(b_y\) are the primitive reciprocal lattice vectors, while \(m\) and \(n\) are integers. \(c(z)\), which is the expansion coefficient, is calculated by using the frequency domain approach; \(u(x,z)\) and \(u(y,z)\) are known as Bloch states.

### 1.3.3 Bandgap Formation

By using the operator defined above in EQ-1.8, the master equation for photonic crystals, EQ-1.7, can be written as follows:

\[\prod \tilde{H}(\vec{r}) = \omega^2 \tilde{H}(\vec{r})\]  

\(\text{(EQ-1.12)}\)

Bloch’s theorem can be applied towards photonic crystals by utilizing the analogy to Schrodinger’s equation from quantum mechanic and the periodicity of the refractive index. The photonic bandgap results from coherent interference of light scattered from periodically placed dielectric scattering centers (as an electronic band gap is the result of coherent interference of electron waves scattered from periodically positioned atoms in space). The degeneracy at the symmetry points \(\Gamma\), \(M\), and \(X\) is broken and the density of optical states in the bandgap is zero.
For an infinite stack of dielectric layers with all of the layers having the same dielectric constant (i.e. a dielectric slab), the dispersion relationship gives two straight lines with slope $\frac{\Delta \omega}{\Delta k} = 1$ in the extended zone representation. In the reduced zone, the folded bands meet either at the zone center or the zone edges. As a result, there is no bandgap with a range of forbidden frequencies for photons. The effect of index contrast on the bandgap can be seen from the electromagnetic variation theorem. The functional energy $E_f$ is given as [18]

$$E_f = \frac{(H, \Pi H)}{2(H, H)}$$

(EQ-1.13)

By considering the effect of a small perturbation, we finally find that [18]

$$E_f = \frac{1}{2(H, H)} \int \frac{1}{\varepsilon} \left| \frac{\omega}{c} D \right|^2$$

(EQ-1.14)

The equation gives the dependence of the energy bands on the refractive index. As $\varepsilon$ increases, $E_f$ decreases, and vice versa.
The bandgap is formed because the low energy modes are concentrated in the high-index dielectric layer and the high energy modes are concentrated in the low-index dielectric layer. While a uniform dielectric layer does not have a bandgap (Fig. 1-3 (a)), a dielectric composed of alternating layers with $\varepsilon_1=12$ and $\varepsilon_2=13$ results in the formation of a small bandgap [Fig. 1-3 (b)]. Finally, changing the contrast to $\varepsilon_1=1$ and $\varepsilon_2=13$ results in a larger bandgap as in Fig. 1-3 (c) [18]. The existence of a bandgap implies that photons with a frequency in the bandgap will not propagate. The modes that have frequencies within the bandgap become evanescent, such that their wave vector becomes imaginary in the direction of periodicity. As a result, the transmitted Poynting vector ($S_t$) becomes complex and the real part in the direction of propagation becomes zero, implying that the time-average power transmitted in that direction $<S_t>$ is zero.
1.3.4 Symmetry of Photonic Crystals

An electromagnetic mode $\Psi$ in a photonic crystal can be characterized by its mirror symmetry. For a mirror reflection $\mathbf{M}$, the mode is defined as odd if $\mathbf{M} \Psi = -\Psi$ and even if $\mathbf{M} \Psi = \Psi$. For the two-dimensional photonic crystal, the plane of periodicity is the x-y plane, and the axis of symmetry is the z-axis. The x-y mirror plane, called $\mathbf{M}_z$, transforms $z$ into $-z$. If $k$ is parallel to the plane $\mathbf{M}_z$, reflection through the plane gives back the wavevector itself. The modes are classified as TE (EQ-1.15) and TM (EQ-1.16) respectively as follows:

$$\vec{E} \cdot \vec{z} = 0 \quad \text{(EQ-1.15)}$$
$$\vec{H} \cdot \vec{z} = 0 \quad \text{(EQ-1.16)}$$

1.3.5 Computation Methods

Field propagation in photonic crystals can be analyzed using a frequency-domain approach or a time-domain approach. In the frequency-domain approach, Maxwell’s equations are decoupled using plane waves. The approach utilizes the periodicity of the dielectric constant, and expands it into a plane wave basis. The transverse magnetic field is expanded into transverse plane waves and summed over the reciprocal lattice vector $\mathbf{G}$ as follows [25]:

$$H(r, z) = \sum_{\mathbf{G}} H_k(G, z) e^{i(k+G) \cdot r} \quad \text{(EQ-1.17)}$$

The expansions are substituted in EQ-1.12 and the $\Pi$ matrix is diagonalized for each wavevector in the Brillouin zone. Then, the band structure is calculated using techniques.
such as the preconditioned conjugate gradient method, which are useful for solving Hermitian eigenvalue problems [31-35].

The finite difference time domain (FDTD) method can be employed to study the evolution of fields in photonic crystals [36]. For TM waves with the electric field pointing in the direction perpendicular to the plane of periodicity, the wave equation can be written as follows:

\[
\frac{\partial^2 E(x, y)}{\partial x^2} + \frac{\partial^2 E(x, y)}{\partial y^2} = \varepsilon(x, y) \frac{\partial^2 E(x, y)}{\partial t^2} \quad (\text{EQ-1.18})
\]

This can be transformed into a difference equation by dividing space \( s \) and time \( t \) into discrete \( \Delta s \) and \( \Delta t \) respectively [37]. By making centered difference approximation at each lattice point, EQ-1.18 can be re-written as follows:

\[
\frac{E^n_{i+1,j} - 2E^n_{i,j} + E^n_{i-1,j}}{(\Delta s)^2} + \frac{E^n_{i,j+1} - 2E^n_{i,j} + E^n_{i,j-1}}{(\Delta s)^2} = \varepsilon_{i,j} \frac{E^{n+1}_{i,j} - 2E^n_{i,j} + E^{n-1}_{i,j}}{(\Delta t)^2} \quad (\text{EQ-1.19})
\]

In the equation, \( n \) is the time index, \( i \) and \( j \) are the space indices, \( E^n_{i,j} \) is the discrete field, and \( \varepsilon_{i,j} \) is the discrete dielectric constant. Boundary conditions, such as Mur’s second order absorbing boundary condition or Perfectly Matched Layers (PML), are utilized in order to minimize back reflection into the computational cell [38-42]. The time-domain approach is useful in determining the transient properties and the quality factor of localized modes. In this thesis, time domain simulations were the key tools in analyzing the challenges of coupling into photonic crystal waveguides.
1.4 The Development of Photonic crystals

1.4.1 Advances in Fabrication Techniques

The ability of 3D photonic crystals to create a complete bandgap, and guide light without radiation loss makes them ideal for optoelectronic applications. A great deal of research has been devoted to their development ever since Yablonovich created a 3D photonic crystal structure (called ‘Yablonovite’) by drilling holes in a dielectric slab and demonstrated the existence of a complete bandgap in the microwave regime [43-48].

Significant advances in building 3D photonic crystals for the optical wavelength regime have been made by utilizing the planar fabrication technology developed for microelectronics devices. The wood-pile structure is one type of photonic crystal created by the layer-by-layer fabrication approach [49, 50]. The process sequence required to make the wood-pile structure includes depositing and patterning SiO₂, filling the etched area with polycrystalline silicon, and polishing to achieve planarization. This sequence is repeated many times until the desired number of layers is obtained. Finally, the index contrast of the structure is enhanced by removing the oxide, which leaves behind the photonic crystal shown in Fig. 1-4 (a) [51-53]. A metallic version of the structure [Fig. 1-4 (b)] has been demonstrated by depositing tungsten on the previous structure and selectively removing the silicon [54]. Also, a similar structure [Fig. 1-4 (c)] has been fabricated by using wafer fusion, which involves creating each layer on a different substrate and then bonding the layers together [55].

Recently, a face-centered cubic structure that has a wide complete bandgap has been designed by Steven et al. [56]. The structure, currently being fabricated at MIT, reduces the required number of process steps [57, 58]. Some of the other innovative
approaches that are being investigated include glancing angle deposition (GLAD) [59], auto-cloning [60], and micromanipulation [Fig. 4d] [61].

(a)

(b)

(c)

(d)

Fig.1-4: SEM images of  
(a) woodpile structure made by layer by layer processing  
(b) structure in a after tungsten deposition and silicon removal  
(c) wood-pile structure made by wafer-fusion  
(d) individual layers that will be stacked on each other by micromanipulation.

Furthermore, there is a simpler and cheaper approach of creating 3D photonic crystals by using the self assembly of colloidal micro-spheres [62-67]. The technique utilizes the tendency of micro-spheres dispersed in a solution to spontaneously self-assemble and form face-centered-cubic (fcc) structures. Fig. 1-5 (a) shows an opal structure that has been formed from silica micro-spheres. In order to enhance the index contrast, a semiconductor material is infiltrated into the self-assembled opal structure, and the opal template is selectively etched away. Fig. 1-5 (b) shows the remaining
inverse-opal structure which has formed a 3D photonic crystal with periodic air spheres embedded in the semiconductor material. The disadvantages of colloidal structures, however, are that have a very small bandgap formed between higher bands and they mostly suffer from unintentional defects [68, 69]. One approach to reduce the defects is by controlling the colloid crystallization by adjusting the capillary force between the wafer and the solution containing the colloids by slowly sweeping the meniscus across the substrate [70-72].

![SEM images](image1.png)

**Fig. 1-5:** SEM images of a) opal colloidal photonic crystal composed of silica spheres b) inverse-opal structure after silicon infiltration and removal of the silica spheres.

Moreover, various 3D lithographic micro-fabrication approaches have been researched in order to form 3D photonic crystal templates. In two photon absorption, atoms or molecules are excited from a lower quantum state to a higher quantum state of the same parity with two photons absorbed simultaneously. The two photon absorption depends quadratically on the intensity; hence, under tight focusing conditions the absorption is limited to the focus and 3D structures can be formed with ~130nm resolution control as shown in Fig. 1-6 (a) [73-77]. However, further investigation has not yet been carried out on how to increase the index contrast and demonstrate the existence of a bandgap. The other 3D lithographic approach is holographic lithography,
in which four-beam laser interference is used to expose thick resist and create 3D periodic structures [78]. Fig. 1-6 (b) shows the structure in resist after the exposure and development, and Fig. 1-6 (c) shows the structure after metal infiltration in order to increase the index-contrast. However, the devices still suffer from unintentional defects and they have yet to be perfected and optically characterized.

Fig. 1-6: SEM images of 3D photonic crystals a) created in resist by two-photon absorption b) patterned in resist by holographic lithography c) the inverse of the structure in (b) after metal evaporation and removal of the resist template.

To summarize, the above review of various fabrication techniques has shown the development of creative approaches (self-assembly, two-photon absorption, and holographic lithography) to make 3D photonic crystals; however, these structures have a very small bandgap and they suffer from unintentional defects during fabrication. The layer-by-layer approaches, adopted from silicon microelectronic device fabrication techniques, produce defect-free devices over a large area; nevertheless, the fabrication of each layer involves many process steps, making the approach inefficient and time consuming. Finally, it is quite difficult to introduce intentional defects (for applications such as microcavities and waveguides) in all of the above approaches. These problems can be solved by using 2D slab photonic crystals.
1.4.2 Advances in Slab Photonic Crystal Waveguides

Slab photonic crystals, which are the combination of 2D photonic crystals with index-confinement in the vertical direction, provide a simpler method for achieving three-dimensional confinement of light [25]. The fabrication scheme of these structures utilizes the planar nature of the current fabrication technology in a much simpler way than 3D photonic crystals.

Because slabs lack translational symmetry in the vertical direction, the modes are not purely TE or TM polarized; instead, they are classified as TE-like (even) or TM-like (odd). Due to the finite height of the slab, the wavevector in the vertical direction introduces a light-cone, which consists of radiation modes or states that extend infinitely in the region outside the slab. Truly guided modes which do not couple to background radiation modes exist only outside of the light cone. The bandgap of the slab is the range where no slab-guided modes exist; it is not truly a bandgap since there are still radiation modes at these frequencies [25].

There have been many demonstrations of the existence of a bandgap in slabs patterned with a triangular lattice of holes [79]. Moreover, linear defects have been introduced in the photonic crystals to create waveguides that confine and gap-guide frequencies within the bandgap. For example, Fig. 1-7 (a) and (b) show photonic crystal waveguides where one and three rows of holes are removed respectively [80-82].

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A useful aspect of photonic crystals is the ability to guide light around sharp corners. The earliest demonstration of these waveguides was illustrated for the microwave regime by first setting up alumina rods (of aspect ratio 1:50) in a square lattice, and then removing perpendicular rows to create the 90 degree bend [83]. The very tall alumina rods allowed the approximation of the photonic crystal as a 2D system. A follow up paper by Chow et al [80] suggested that it “is difficult to make this structure at optical wavelength” in slabs, and demonstrated photonic crystal bends by patterning a dielectric slab with holes. For example, Fig. 1-8 (a) shows a waveguide with a 60 degree bend [80, 84-86]. Furthermore, 90 and 120 degree bends have been demonstrated as shown in Fig. 1-8 (b) and (c) [84, 85]. Finally, coupled cavity waveguides (CCW) and coupled-resonator optical waveguides (CROW) have been theoretically presented [87, 88]; even though there has been experimental demonstration of the waveguides in the microwave regime [89].
1.4.3 Advances in Photonic Crystal Coupling Approaches

To utilize photonic crystal waveguides for applications in photonic integrated-circuits, light needs to be efficiently coupled from fibers, lasers, or conventional dielectric waveguides. However, coupling is difficult, because the photonic-crystal modes are different from conventional waveguide modes that use total internal reflection [90]. Mode-size transformation allows independent optimization of the mode profile for efficient input and output coupling [91]. For conventional dielectric waveguides, mode transformation is achieved through adiabatic tapering of the waveguide, which is analogous to adiabatic transformation of a potential well in quantum mechanics [92, 93]. By slowly and continuously transforming the waveguide parameters as the optical mode propagates, the required condition for adiabatic transformation will be achieved [94-96].

While the adiabatic transformation for conventional waveguides is straightforward, it is quite complex for photonic-crystal waveguides [90, 94-97]. Conventional waveguides have continuous spatial translation symmetry along the mode propagation direction. However, photonic crystals possess only discrete translational
symmetry for which the optical confinement is achieved by multiple Bragg reflections. Hence, the refractive index of the dielectric medium and the optical modes usually change within the unit cells such that slow transformation of the modes, in order to fulfill the adiabatic condition [96], is difficult.

Furthermore, most active devices have extended modes while photonic-crystal waveguides have a small and controllable number of modes [98-100]. For strongly confined modes in ridge waveguides, an adiabatic taper can be implemented. However, this would not work for buried heterostructure and ridge-waveguide lasers, since a coupling mechanism is required if the laser is to be integrated on a chip to build more complex photonic circuits.

Initially, most researchers bypassed the problem of coupling by stating that “measuring qualitatively the optical properties of a 2D photonic-crystal etched through a planar waveguide can prove awkward with external light sources” [101]. Instead, the characterizations used a light source at constant wavelength internally created by photoluminescence [100-105]. As shown in Fig. 1-9, an external light source is utilized to excite the embedded quantum wells so that the light emitted throughout the plane will be incident on the photonic crystal. At the output, light is simply collected from the cleaved edge with a detector. This procedure eliminated the need for input and output conventional dielectric waveguides.
The coupling between photonic-crystal waveguides and ridge-waveguide lasers, which have a weaker refractive-index confinement of light, has been investigated by Happ et al [97]. To couple the mode in the ridge waveguide [shown in Fig. 1-10 (a)] into the photonic crystal waveguide created by a missing row of holes, the photonic crystal is tapered as shown in Fig. 1-10 (b).

Fig. 1-9: Schematic of coupling from embedded active region into the photonic crystal [101].

Fig. 1-10: Schematic of a) the mode of the ridge waveguide  b) the mode coupling into the tapered photonic crystal waveguide.
Progressively varying the diameter of the etched holes has also been proposed [106-112]. As shown in Fig 1-11 (a), the 1.1µm input ridge waveguide is coupled to a photonic-crystal waveguide which is created by removing three rows of holes (called W3 waveguide). Then, the W3 waveguide is tapered into a photonic-crystal waveguide wherein one row of holes is removed (called W1 waveguide) by slowly introducing holes over 10 periods. Also, a similar approach is utilized to couple two different photonic-crystal waveguides [113].

![Fig. 1-11: Schematic of (a) coupling from a ridge waveguide into a photonic crystal waveguide by introducing holes progressively and (b) using the same procedure to couple two photonic crystals of different width.](image)

### 1.4.4 Summary

The above review demonstrates most of the reported experimental studies have focused on photonic crystals composed of periodic holes etched into dielectric slabs. In this thesis, photonic crystals composed of square array of dielectric rods are simulated, fabricated, and optically characterized. Furthermore, various schemes for coupling from a conventional dielectric waveguide into the photonic-crystal defect waveguide are investigated.
Chapter 2

Square Lattice of Dielectric Rods: Design

2.1 Overview: Why Use Dielectric Rods?

The previous chapter has introduced applications such as linear waveguides, splitters, and sharp-bend waveguides implanted by utilizing photonic crystals composed of air holes in a dielectric slab. Photonic crystals composed of a square lattice of dielectric rods are useful for similar, as well as other unique applications.

The periodic dielectric rods have some unique properties that differentiate them from their air-hole counterparts. First of all, their photonic bandgap exists for the TM-like (odd) modes. Second, the modes in the defect rods are delocalized, because the radius of the defect rods is reduced compared to rods in the surrounding cladding layer. The mode delocalization has useful application in coupling between devices that are monolithically integrated. Third, the small size of the bandgap creates small-bandwidth, flat defect bands. The resultant low group velocity is useful for applications requiring slow-light enhancement and to achieve pulse self phase modulation [114].

Finally, the disconnected structural topology of the rods is very advantageous for various mechanical-oriented applications. For example, it is possible to fabricate sensors by flowing fluids and gases around the rods to induce a change in the index contrast (which alters the bandgap and the defect band). Also, the array of rods can be integrated
with micro-electro-mechanical-system (MEMS) devices that move or bend the rods, hence creating a tuning of the bandgap or the guided mode.

Nevertheless, engineering the array of dielectric rods is challenging. Their fabrication is difficult due to the required high aspect-ratio etching. Furthermore, the coupling mechanism is quite different from that of waveguides that are made by eliminating rows of holes. For hole-based waveguides, light is coupled from a high-index conventional waveguide into a high-index photonic crystal waveguide. For the array of rods, however, reducing the radius of a row of rods creates a low-index defect waveguide; hence, the coupling occurs between the high-index conventional waveguide and the low-index photonic-crystal waveguide. The coupling challenge is discussed in detail in Section 2.4.

2.2 Bandgap Engineering

2.2.1 Simulation Techniques

To obtain the band structure of the photonic crystal, the simulation is performed by establishing periodic cells and by using a plane wave-basis for preconditioned conjugate-gradient minimization of the Rayleigh quotient [115-117]. In this arrangement, the slab photonic crystal which has two-dimensional periodicity forms periodic cells in the plane; periodicity is achieved in the vertical direction (perpendicular to the plane) by placing the aforementioned cells in a periodic sequence. The cells are separated by thick background regions so that they do not affect each other [118]. Then, the light cone, which indicates all the background radiation modes, is calculated and overlaid on the band diagram [25]. Only the lowest boundary (called the light-line) is
required, because all the higher frequencies are automatically included. If the background is uniform, the light-line is simply the wave vector divided by the index. If the background is periodic, the light-line is the lowest band of the corresponding two-dimensional periodic system.

2.2.2 Slab Photonic Crystal Design

This section emphasizes the design of slab photonic crystals composed of a square lattice of dielectric rods. Some of the possible configurations are shown in Fig. 2-1. The first configuration in Fig. 2-1 (a) has high-index periodic rods that are sandwiched between solid low-index substrates. If the substrate is several wavelengths thick, the substrate is considered to have infinite thickness because the intensity of the guided modes decays exponentially outside the rods. The index contrast between the rods and the substrate provides confinement in the vertical direction. The design is symmetric and the modes in the rods can be classified as TM-like (odd). The major disadvantage of the design is the difficult fabrication. The first design considered had a symmetric background [Fig 2-1 (a)]. If all the layers are deposited first, then it will be difficult to fabricate the rods by processing only the middle layer. Also, the symmetric structure can be created by depositing the lower substrate and the guiding layer first, then defining and etching the rods, and finally depositing or bonding the top substrate. However, the size scale of the rods (needed for operation near 1550nm) is not capable of supporting the thick overlaying substrate. The second design considered was similar to the first, but with the background substrates patterned as shown in Fig. 2-1 (b).
The final design is shown in Fig. 2-1 (c). The structure has a guiding layer, which is sufficiently separated from the substrate by low index “stilts.” The mirror symmetry is lost due to the asymmetric nature of the structure. However, in order to classify the guided modes as even or odd, it is only necessary to preserve mirror symmetry where the guided modes have non-negligible amplitude.

Fig. 2-1: Various configurations of a photonic crystal consisting of rods a) the low index substrate below and above the rods create symmetry b) low index cap and stilt surrounding the rods create symmetry c) asymmetric structure with low index stilt.

The thickness of the slab plays a crucial role in the design of the structure. If the slab is too thick, higher-order modes will exist very close to the lower-order modes and will cause the bandgap to disappear. On the other hand, reducing the slab thickness will cause the modes to become weakly guided residing very close to the light cone. If the slab thickness is less than half a wavelength, the confinement of the mode is very small. The optimal thickness is roughly half the two-dimensional gap-bottom wavelength [25].

In the design shown in Fig. 2-2 (a), the high-index slab was GaAs (n=3.37) and the low-index layer was Al₅O₇ (n=1.6). Simulations were performed using a photonic crystal with lattice constant (a) that range from 450nm to 650nm. The simulated heights were varied from 1.36ₐ to 1.66ₐ while the diameter d was varied from 0.4ₐ to 0.6ₐ. From the simulations, the optimal thickness for the structure was chosen to be 0.83 μm.
The lattice constant was chosen to be 500nm and the rod diameter was chosen to be 300nm, which resulted in a dielectric filling factor of 28%. The structure also included 0.6 μm thick AlₓOᵧ stilts and 0.9 μm thick AlₓOᵧ layer on a GaAs substrate. Fig. 2-2 (b) shows the simulated band structure. This configuration yields a photonic bandgap for frequencies between 0.29 and 0.32 (c/a) with a gap-to-midgap ratio of 10%. Other simulations have shown that the band structure of the asymmetric structure is 90% similar to the band structure of the symmetric structure given in Fig. 2-1 (b). Finally, the transmission through the structure, shown in Fig. 2-2 (c), clearly shows the bandgap for TM-like modes, while no gap exists for the TE-like modes.
Fig. 2-2: a) Schematic of the simulated structure consisting of 0.83μm GaAs guiding layer, 0.6μm AlₓOᵧ stilts, 0.9μm AlₓOᵧ spacer layer, and GaAs substrate. b) The simulated band structure indicates a bandgap from 0.29 to 0.32 (c/a). c) The simulation of transmission through the structures a bandgap for TM while there is no gap for TE.
2.3 Waveguide Engineering

2.3.1 Simulation Techniques

The calculation of the projected band diagrams for the waveguides is similar to the calculation performed for the photonic crystal without any linear defect. Additional cells are used in the direction perpendicular to the waveguide in such a way that the waveguide modes in each cell are well localized so that they do not influence the nearby cells [118]. Then, the bands from the photonic crystal without the waveguide are projected onto the Brillouin zone of the line defect to indicate the photonic crystal slab modes. Finally, the light cone is calculated and projected on the diagram to indicate radiation modes. The modes guided by the linear defect are only those outside of both the slab bands and the light cone [118].

2.3.2 Waveguide Design

There are three constraints when designing a photonic crystal waveguide [118]. First, the waveguide needs to have truly guided modes (not resonances). These modes require well defined Bloch wave number, obtained only through periodicity in the direction of propagation [119]. Second, the waveguide needs to be singlemode at the operation frequency in order to minimize reflections during coupling [119, 120]. Finally, the truly guided mode needs to be inside the bandgap. If the mode is not well inside the bandgap, the transmission will decrease and reflection will increase [119, 120]. Note that conventional waveguides fulfill the first two requirements, but suffer from loss at sharp bends since they don’t fulfill the last requirement [121-123].
Two different approaches were initially considered in designing the defect waveguides. The first option is to increase the radius of the rods in the linear defect. This pulls down modes from the upper slab modes, resulting in non-degenerate modes inside the bandgap. The waveguide can be designed to be singlemode by choosing the radius so that the defect modes do not overlap. However, increasing the radius also results in modes that are below the bandgap, inside the slab band continuum. The modes are lost into radiation because they do not fulfill the third requirement for creating a photonic crystal waveguide [119].

In the second approach, the radius of the rods in the linear defect is reduced. There is a limit to the size reduction, because the mode needs to be confined in the rods. The high-index guiding layer of each rod has a low-index cap and stilt, hence confining the mode in the vertical direction. However, the effective index of the linear defect waveguide is smaller than that of the surrounding photonic crystal. Thus, bandgap guiding is utilized to constrain the light in the planar direction. The modes localized in the defects decay exponentially, because they fall into neither the light cone nor the slab modes. The waveguide fulfills the three requirements. First, the design gives a single mode waveguide, because there is only one dispersion line for a given reduced radius. Second, it preserves symmetry in the $\Gamma$-X direction to ensure truly guided modes. Finally, projecting the slab mode on the reduced Brillouin zone shows that the defect bands are well in the bandgap to induce bandgap guiding.

Fig. 2-3 (a) shows the schematic of a photonic crystal waveguide that utilizes the second approach. Each rod consists of a GaAs guiding layer, with low-index $\text{Al}_x\text{O}_y$ stilt
and spacer layer above the GaAs substrate. Fig. 2-3 (b) shows a scanning electron micrograph (SEM) of the waveguide patterned in electron beam resist.

(a)  
(b)  

![Image](image.png)

Fig. 2-3: a) Schematic of the simulated structure consisting of 0.83μm GaAs guiding layer, 0.6μm AlₓOᵧ stilts, 0.9μm AlₓOᵧ spacer layer, and GaAs substrate. While the photonic crystal rods have diameter of 300nm, the defect rods have diameter of 250nm. b) Scanning electron micrograph (SEM) image of the pattern after the electron beam lithography (e-beam) step shows the defects inside the photonic crystal.

Simulations were performed for three different defect-rod radii and the results are given in Fig. 2-4 (a). The optimal defect rod diameter is 0.5a, which has a defect mode with a center frequency of 0.305 (c/a). As the radius is decreased, the mode shifts up in frequency and becomes more delocalized. The E-field of the localized mode is shown in Fig. 2-4 (b). The mode profile is simulated for a symmetric structure wherein the 0.83μm guiding GaAs layer is sandwiched between infinitely thick low-index AlₓOᵧ.
Fig. 2-4: a) The projected band structure shows that as the radius of the defect rods is decreased, the defect band moves up in the bandgap. Simulation shows the mode profile is well localized in the defect rods. b) a horizontal cut through the photonic crystal c) a vertical cut through the photonic crystal [118].
2.4 Efficient Waveguide Coupling

As mentioned in the previous section, most published experimental research has focused on coupling into photonic crystals consisting of air holes in dielectric slabs. However, the suggested mechanisms do not provide efficient coupling for photonic crystals consisting of dielectric pillars wherein light is coupled between a high-index conventional dielectric-waveguide and a photonic-crystal waveguide with a reduced radius, which has a lower effective-index than its surrounding. Thus, the coupling between the two systems presents a challenge.

2.4.1 Simulation Techniques

2D simulations were been performed to qualitatively identify many of the challenges in the coupler design at lower computational cost than the 3D simulations. The simulations employed a frequency domain model based on vectorial eigenmode expansion, and a staircase approximation of the index profile with a resolution of 20 pixels per lattice [124]. The modeling tool used was the Cavity Modeling Framework (CAMFR) [125].

In 2D, the bandgap extends from 0.235 to 0.300 c/a. If a defect radius of 0.20a (instead of the r=0.25a used in 3D) is selected, the defect mode extends in frequency from the lower band-edge to 0.270 (c/a).
2.4.2 Butt-Coupled Dielectric Waveguide

The first approach investigated was a butt-coupling of the input dielectric waveguide and the photonic crystal waveguide. The dielectric waveguide was placed 100nm away from the photonic crystal waveguide. Fig. 2-5 (a) shows a top-down scanning electron microscope (SEM) image of the structure, while Fig. 2-5 (b) shows the 2D calculated transmission through the entire structure. The simulation was performed for two different lengths (L) of the photonic crystal waveguide. The result shows that there are Fabry-Perot peaks in the transmission, hence making the transmission amplitude dependent on frequency. Moreover, the transmission is dependent on the length of the photonic crystal, and varies when the number of defect rods (waveguide length) is changed from 8 to 10.

![SEM image of the butt-coupling approach patterned in PMMA. b) Power transmission simulation result of the structure in (a).](image-url)
2.4.3 Tapered Dielectric Waveguide

In the next approach, the dielectric waveguide was tapered to the size of the defect waveguide and inserted into the photonic crystal in order to minimize radiation loss. Fig. 2-6 (a) shows an SEM image of the taper structure wherein the dielectric waveguide is tapered to the size of the defect waveguide over a length scale of several lattice constants. This approach tries, but does not succeed, to adiabatically transform the conventional waveguide mode to the photonic crystal waveguide mode by decreasing the modal confinement and by matching the mode profile to that of the photonic crystal waveguide. The simulation shows that the required high and broadband transmission from the tapered dielectric waveguide into the photonic-crystal defect waveguide is not achieved. These calculations indicate that tapering the conventional waveguide does not yield high coupling efficiency, because the approach suffers from Fabry-Perot reflections (because it is not a perfect taper) from the edges of the photonic crystal, which make the transmission dependent on frequency and the length of the photonic crystal waveguide. Also, the insertion of the waveguide into the photonic crystal, which breaks the translational symmetry, could have cause mini-bandgaps that reduced the transmission.
2.4.4 Adiabatic Coupling Scheme

To improve the poor coupling efficiency, two problems had to be solved. First, the propagation mechanism of the two waveguides had to be matched in order to obtain a good field profile. Second, the guiding mechanism had to be matched adiabatically to avoid reflections [126]. The two concerns in the previous design are illustrated in Fig. 2-7 (a). A new design that addresses the concerns is shown in Fig. 2-7 (b). The design
implements the adiabatic theory, which requires that the operating mode must not be evanescent at any intermediate point of the taper, and must be guided for every intermediate point of the taper [127].

In the input dielectric waveguide, the mode consists entirely of forward propagating field components. The waveguide mode in the photonic crystal is a forward propagating Bloch mode, but because of the strong scattering inside the crystal, this Bloch mode (with a net forward energy flux) consists of both forward and backward propagating field contributions (Fourier components). Stated differently, the ratio between the electric and magnetic field (related to effective 'impedance') will be very different for these two waveguides.

![Image](a) SEM image of the tapered waveguide inserted into the photonic crystal showing the coupling input region and the photonic crystal region. The arrows indicate that the dielectric waveguide has a mode with completely forward propagating field component, while the photonic-crystal waveguide has both forward and backward propagating field components. Also, the guiding is high-index guiding in the 'coupling input' region, while the guiding in the photonic-crystal 'guiding region' is low-index guiding due to the reduced radius of the rods. b) The new coupling approach solves the problems in (a) by dividing the 'coupling input' into two adiabatically tapered stages.
To achieve efficient coupling, it is necessary to adiabatically convert a forward propagating component in a conventional index contrast waveguide, into a combination of forward and backward propagating components prior to coupling into a photonic crystal defect waveguide. Likewise, in order to couple out of a photonic crystal waveguide, the forward and backward propagating components need to be adiabatically converted into a forward propagating component that propagates within the conventional waveguide. In the first stage of Fig 2-7 (b), a smooth transition is made from a traditional single mode waveguide to a waveguide consisting of a sequence of rods with a fixed period and with the same radius as the defect rods. By gradually increasing the spacing between the resonators from zero to the lattice constant of the photonic crystal waveguide, a coupled cavity waveguide emerges. In doing so, a transition is achieved from a mode profile that consists entirely of forward propagating components in the dielectric waveguide, to a mode profile that consists of both forward and backward propagating components in the coupled cavity waveguide.

All of the guiding in this first stage resides in high dielectric index material relative to its surrounding. As shown in Fig. 2-8 (a), the highly confined, index guided mode gradually becomes broader but is still mostly confined in the individual rods. The 2D simulation result of the first stage [Fig. 2-8 (b)] shows that an efficient mode profile transition occurs between the high-index dielectric and the 1D-periodic sequence of rods.
In the second stage, the 1D-periodic sequence of rods is transformed into a photonic crystal waveguide by introducing the cladding photonic crystal. The elimination of the presence of an abrupt photonic crystal interface is desired in order to avoid reflections. The challenge is to overcome the difference in guiding mechanisms. In the sequence of rods, light is guided in a region with a relatively higher effective-index since the surrounding medium is air. The mode is guided by total internal reflection, whereby the field is concentrated in a region having a higher refractive-index than the surroundings. In the photonic-crystal waveguide, the effective-index of the line-defect is lower than that of its surroundings, because the radius of the defect rods is smaller than the radius of the bulk rods. Hence, the light in the defects is surrounded by two ‘perfect mirrors’ formed by the adjacent bulk photonic crystal.
The transition between these two waveguides is accomplished by gradually reducing the angle at which the cladding bulk photonic crystal of larger radius rods approaches the coupled cavity waveguide, which transforms the coupled cavities into a photonic crystal waveguide as shown in stage II of Fig. 2-7 (b). The adiabatic introduction of the photonic crystal reduces reflections at the edges, which, as a result, minimize Fabry-Perot resonance fringes in the transmission spectrum. The mode localized in the photonic crystal waveguide is broad as it exponentially decays into the bulk photonic crystal. However, since the mode size has already been increased in the coupled cavity waveguide, it nearly matches the mode profile within the photonic crystal waveguide.

The cladding photonic crystal needs to be designed very carefully. For example, Fig. 2-9 (a) shows a photonic crystal wherein the rods are gradually introduced, i.e. the radius is changed from zero to the final value over many lattice periods. However, the transmission [Fig. 2-9 (b)] is not efficient because the taper goes through an intermediate state where the core and cladding rods have the same diameter that produces a bandgap that reflects the incoming radiation. By slowly inserting the photonic crystal, the radiative continuum is pulled down until it lies below the guided mode; hence, there is always an intermediate stage where the waveguide mode crosses the continuum and is no longer guided. As stated above by the adiabatic theorem, each intermediate stage of the waveguide should not couple to the radiative continuum [127].

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Fig. 2-9: a) The schematic shows slowly insertion of the photonic-crystal rods. b) The simulated power transmission through the structure shows inefficient coupling [127].

The field profile through the complete structure with the two-stage input and output coupling designs, combined with the photonic-crystal waveguide, is shown in Fig. 2-10 (a). The mode is very well localized in the linear-defect waveguide. The transmission simulation result in Fig. 2-10 (b) is close to 100% with a significant bandwidth. Moreover, it can be observed that the transmission does not vary significantly as the length of the photonic crystal waveguide is changed. Hence, the simulation shows that Stage II has succeeded in achieving transition from guiding in high effective-index to gap guiding in low effective index defect waveguide. By time reversal, the output coupling is identical to the input coupling.
Fig. 2-10: a) Simulated mode profile through the new adiabatic coupling approach. b) Simulated transmission through the structure shows efficient and high transmission that is only weakly dependent on the length of the photonic crystal waveguide.

Finally, 3D simulations were performed with FDTD resolution of 20 pixels per lattice. As the bandgap is smaller for the 3D structures, the defect mode has a very small bandwidth. The transmission is reduced because of the difficulty in matching the narrow pass-band of the first-stage and the line-defect waveguide mode. By changing the rod radius in the first stage from $0.25a$ to $0.23a$, better transmission is obtained through the
photonic-crystal waveguide as shown in Fig. 2-11. The taper transmission is 75%, significantly higher than the 30% obtained for the butt-coupling approach. To achieve better transmission, the taper needs to be significantly gradual.

Fig. 2-11: Power transmission result (3D simulation) comparing three different coupling approaches. The defect rod radius of Taper 1 is $0.25a$ while that of Taper 2 is $0.23a$. 
3.1 Overview

The fabrication of photonic crystals consisting of holes etched into dielectric slabs has been extensively studied. This wealth of knowledge, however, is not directly transferable towards the fabrication of photonic crystals composed of dielectric rods. This chapter provides a process flow for making the rod-based structures.

After the epitaxial growth (explained in the next section), the wafer is cleaved into ~7mm by ~7mm pieces which were processed individually [Fig. 3-1 (a)]. Each sample contains many sets of devices separated by 300μm and labeled with line markers for identification purposes [Fig. 3-1 (b)]. Each set has five photonic crystal devices and two straight dielectric waveguides. The devices include waveguides of varying length, different coupling structures, and waveguide bends. The vertical lines in Fig. 3-1 (b) and (c) indicate where each sample is cleaved to produce smooth and flat waveguide facets suitable for optical testing.
The process sequence required to fabricate the photonic crystal devices is schematically illustrated in Fig. 3-2. First, SiO$_2$ is sputter-deposited on the epitaxially-grown heterostructure. Then, PMMA resist is spun on each sample in preparation for scanning electron beam lithography (SEBL). After the e-beam exposure and development, a nickel evaporation and liftoff process leaves behind the desired patterns in nickel. Using the nickel as an etch mask, the patterns are etched into the SiO$_2$ layer. Then, the nickel is wet-etched and the patterned SiO$_2$ layer is used as a mask had to etch into the GaAs/AlGaAs layers. Finally, the SiO$_2$ is removed and the sample is oxidized in order to convert the AlGaAs into low index Al$_x$O$_y$. A detailed study of each step is given in the following sections.
Fig 3-2: Schematics of the process sequence involved in making the photonic crystals: 
a) SiO$_2$ sputter-deposition and PMMA spinning  
b) e-beam exposure and development  
c) nickel evaporation  
d) nickel liftoff  
e) SiO$_2$ etch  
f) nickel wet etch and GaAs etch  
g) AlGaAs etch  
h) SiO$_2$ etch and AlGaAs oxidation into Al$_2$O$_3$. 
3.2 Epitaxial Material Growth

The initial step in building photonic crystal waveguides involves the use of Gas Source Molecular Beam Epitaxy (GSMBE). This growth technique, which can deposit layers with atomic resolution [128], is done in an ultra high vacuum (UHV) environment (10^{-10} Torr base vacuum). The basic requirements of a MBE system are in situ sample heating and cleaning, and independently controlled sources for all constituent materials and dopants. High vacuum is achieved by baking and pumping the system at temperature ranging from 150 to 250°C, which will increase the vapor pressure of gases and water adsorbed on the inside walls of the chamber [128].

Sample growth is performed in Professor Kolodziejski’s Integrated Photonic Devices and Materials Group laboratory using the Riber 32P system. First, the sample is loaded into the Intro chamber, which is the load lock for the system and has a base pressure of 10^{-8} Torr. Then, the sample is moved into the Transfer chamber, which has a base pressure of 2x10^{-9} Torr, and degassed at 210°C for one hour to remove the absorbed moisture on the sample and the sample holder. The sample is then moved into a Buffer chamber that lies between the Transfer chamber and growth reactor. The base pressure of the Buffer chamber is at 10^{-9} Torr. Finally, the sample is moved into the Riber 32P growth chamber, which has a base pressure of 2x10^{-10} Torr. The chamber contains elemental Ga, In, Al, Si and Be effusion cells and an AsH₃/PH₃ cracker. During growth, the pressure increases to 2x10^{-5} Torr due to the presence of cracked or thermally decomposed (at 900°C) AsH₃ and PH₃. Also, the Riber system is equipped with an i-
situ spectroscopic ellipsometer and a Reflection High Energy Electron Diffraction (RHEED) system to characterize deposition rates and surface morphology [129].

After the 2-inch GaAs wafer is baked and transferred into the growth chamber, a 1.5 μm thick Al$_{0.9}$Ga$_{0.1}$As layer is epitaxially grown. GaAs and Al$_{0.9}$Ga$_{0.1}$As are closely lattice matched, which means that they have approximately the same lattice constant. As a result, stress/strain is not a problem in the growth. The composition can be varied by changing the temperature of the Ga and Al cells, which changes the flux ratio of the different types of atoms that arrive at the surface. By varying composition of Al and Ga, properties such as the index, electronic bandgap, and some chemical properties are varied. Next, a 0.5 μm thick GaAs layer is grown epitaxially on the Al$_{0.9}$Ga$_{0.1}$As.

During the growth, the wafer is continuously rotated to ensure uniform growth of material. Also, RHEED oscillations are used to measure the growth rate of the layers. Besides lattice matching, the use of MBE has the advantage of monolayer control and compositional control to 3% accuracy [130]. When the growth is finished, the sample is transferred to the Intro chamber which is then vented. A piece of the sample is cleaved and the thickness of the epitaxial growth is verified using x-ray diffraction.
Fig 3-3: SEM of epitaxially grown heterostructure. The structure consists of 0.86μm GaAs layer and 1.5μm Al_{0.5}Ga_{0.1}As layer on a GaAs substrate.

Fig 3-4: Schematic representation of the integrated MBE system.
Then, a 100 nm thick layer of SiO$_2$ is evaporated on the sample using an e-beam evaporator. The advantage of using an e-beam evaporator over inductive or resistive evaporators is that it avoids contamination from the high temperature of the crucible and the outgassing of coupling wires [128]. Ellipsometry on the evaporated sample piece gave a thickness of 96.7nm. However, the evaporated oxide is too thin to etch deep into the GaAs-based heterostructure (explained in Section 3). Sputter-deposition provides a thick oxide layer; however, the thickness has the potential to be irregular after depositing 350nm, varying over 5% across a 2-inch wafer.

3.3 Scanning Electron-Beam Lithography (SEBL)

3.3.1 Overview

Scanning electron-beam lithography is utilized to define the square lattice of dielectric rods. In electron beam lithography systems, electrons are emitted from the cathode of an electron gun through thermionic emission, field-aided emission, thermal field-aided emission, or photoemission. The electrons are focused into a narrow beam through the use of lens, deflection plates, and aperture arrangements. The direct-write e-beam lithography are classified as either vector-scan or raster-scan system. In a vector-scan system, the digital location of each area to be exposed is fed to the $x$ and $y$ digital-to-analog converters causing the beam to be directed to those pixels that must be exposed. In raster-scan systems, every pixel is scanned serially and a pattern is exposed by opening and closing a shutter [132].
Limitations on the smallest feature written by an e-beam lithography system arises from the size of the focused beam as well as proximity effects. When a pattern is being written, forward and backscattered electrons can expose nearby areas that are not intended for exposure. The beam becomes broadened because of forward scattering, which occurs over a small range of angles with respect to the incident velocity. Backscattering results in a large area background ("fog") exposure [131]. When compared to contact or proximity lithography systems, a disadvantage of e-beam systems is their small throughput due to the significantly longer write-time.

E-beam lithography was preferred for creating the photonic-crystal structures in this thesis, because the designs consisted of various aligned features which continually evolved based on device performance.

3.3.2 VS26 Scanning Electron-Beam Lithography (SEBL) System

The e-beam lithography is performed with the IBM VS26A Scanning Electron-Beam Lithography (SEBL) system, which has 50 kV external potential applied to accelerate electrons from the source (Fig. 3-5). The VS26 vector-scan system is capable of generating a beam spot-size smaller than 40nm. To perform a write, the system breaks the pattern into fields as small as 100 µm, which are exposed individually and stitched together. In order to write patterns within a field, electric and magnetic fields deflect the beam to the pixels that need to be exposed. To move from one field to another, the stage is physically moved using a laser-interferometer control.
Note: There is a molybdenum "heat shield" above each of the apertures on the VS-6 column.

Fig 3-5: Schematic representation of the VS26 system [132].
3.3.3 Preparation for e-beam exposure

In preparation for the e-beam lithography exposure, each sample (6mm by 6mm) is coated with a 200nm thick layer of polymethylmethacrylate (PMMA). The coating is performed by placing a droplet of PMMA (solution of 3% by weight in chlorobenzene) on the sample, spinning it at 3600 RPM for one minute, and baking it for one hour at 180°C. The design parameters are calibrated as accurately as possible through dose experiments, which include varying beam current, field size, and clock frequency. Proximity effect and write time are carefully taken into consideration to efficiently create the photonic-crystal structures close to the simulated device parameters. The device patterns are generated with Matlab and a Computer Aided Design (CAD) software called NanoWriter. A field size of 245.76 µm is used, which results a pixel size of 15 nm.

3.3.4 Development

The exposed PMMA is developed by rinsing the sample for 90 seconds in 1:2 mixture of methyl-isobutyl-ketone (MIBK) and isopropanol (IPA), which dissolves the exposed part of the PMMA layer and leave behind patterned holes; this is followed by a 30 second rinse in IPA. Finally, the sample is inspected using a Scanning Electron Microscope (SEM) to determine the size of the holes. The development is illustrated by the schematic in Fig. 3-6.
3.3.5 E-beam Experiment

The photonic crystal structures have many design constraints, such as accuracy in periodicity, input waveguide width, diameter, and shape. Various experiments are carried out to obtain the correct parameters and to understand proximity effect. The PBG patterns were designed in the CAD file as periodic squares boxes in a square lattice. The e-beam tool partitions the design into 15nm pixels [Fig. 3-7 (a)] and exposes each pixel. Hence, each box has a dose that is a superposition of the pixel exposures. Even though the patterns are designed as squares, they become circular when the applied dose is high enough. As the dose is increased, the features become more circular while the diameter becomes larger [Fig. 3-7 (b)]. The goal is to create holes that have a diameter of 300nm. Fig. 3-8 (c) shows the design (inset boxes) overlaid on the SEM depicting PMMA that has been exposed and developed. The figure shows that the square patterns have formed circles after development.
Fig. 3-7: a) Schematic illustration of a square divided into pixels. The beam diameter is bigger than each pixel. b) The superposition of the exposure of pixels results in a circular feature at a higher dose. c) SEM of circular hole patterns, which are initially designed as squares (inset) in a CAD file.

The input/output waveguides are written in a similar fashion as the photonic-crystal devices. As shown in the schematic in Fig. 3-8 (a), the waveguide is partitioned into pixels and exposed. The shaded region in Fig. 3-8 (b) demonstrates proximity effect, which makes the waveguide wider than the design in the CAD layout.

Fig. 3-8: a) Schematic illustration of a waveguide divided into pixels. The beam diameter is larger than the pixel. b) The superposition of the exposed single pixels results in a waveguide that is wider than the design.

Furthermore, proximity correction is required to alleviate the effect of writing the large waveguides adjacent to the photonic crystal devices. Fig. 3-9 (a) shows an SEM image of holes without the adjacent waveguides. Fig. 3-9 (b) shows a schematic of an input waveguide next to the photonic crystal. The result of the e-beam exposure is shown by the SEM image in Fig. 3-9 (c). Hence, the design required experiments wherein the exposure dose, spacing between the waveguide and photonic crystal, and waveguide width are varied to compensate for the proximity effect.
3.3.6 Results

Various dose experiments were performed in order to obtain the correct hole diameter (300nm) and to control the proximity effect. The SEM in Fig 3-10 (b) shows that the desired parameters have been achieved.
3.3.7 Stitching Errors

The errors that occur during e-beam exposure can be classified as interfield or intrafield errors. Intrafield errors cause pattern distortion within a field. These errors arise from aberrations in the lens and deflection fields, miscalibration of the digital-to-analog converters (DAC), electrostatic charging of sample and e-beam column, and thermal expansion of system parts [133].

Interfield errors (stitching errors) occur when adjacent fields are not aligned correctly with respect to each other. These errors are due to the miscalibration between the field size on the SEBL system and the actual field size measured by the laser interferometer, the presence of pitch or yaw in the sample stage, errors in stage position detection, thermal expansion of system parts, and drifts in the electrical sources [133]. In this thesis, interfield errors are relevant because the long input and output waveguides are created by stitching many fields together. Figures 3-11 (a) to (d) show the schematic of the possible stitching errors.

![Fig. 3-11](image)

Fig. 3-11: Schematic illustrations of stitching errors. a) The scan field length is shorter than stage field length (field scaling error). b) The scan field length larger than the stage field length (scaling error). c) The deflection axis is misaligned with the stage axis (field rotation error). d) The correct calibration gives well aligned waveguides [133].
An e-beam system with the record smallest stitching error, the spatial-phase-locked electron beam lithography (SPLEBL), has been demonstrated in MIT’s Nanostructures Laboratory (NSL) [134]. Unlike the VS26 system which relies on the accuracy of the laser interferometer controlled stage movement, SPLEBL implements a closed-loop feedback system that allows correction for calibration between the system’s field size definition and the actual field measured by the laser interferometer.

The first step in the field calibration and alignment scheme is to locate the gold droplet that is placed at the corner of the sample, and image it onto a frame-grabber using a back-scattered electron detector. The gold particle serves as a reference, and the stage is shifted a specific distance in the horizontal and vertical direction by the laser interferometer; at the same time, the pattern generator is deflected by the same distance [135, 136]. The presence of signal conversion errors in the DAC often results in a mismatch between the two movements. Hence, the particle usually does not reside at the same location within the same image frame when the stage and the e-beam are shifted back. The system’s autocorrelation program uses the back-scattered electron images to calculate the error correction signal that is necessary to rectify the mismatch and feed it back to the pattern generator unit to enable the deflection of the e-beam. This alignment process is repeated many times to minimize the errors. The SEM in Fig. 3-12 shows the stitching error in the VS26 system, after a good field calibration, is less than 15nm.
Fig. 3-12: SEM image illustrating the stitching of 500nm wide waveguides at the interface of 256μm fields. The field interface is indicated by the dashed vertical line. Good calibration results in 25nm stitching error.

3.4 Liftoff Process

E-beam lithography process leaves behind holes since PMMA is a positive resist. A liftoff process is required in order to reverse the image and leave behind a hard mask that can be used as a protective layer while etching into the oxide layer.

To achieve the required liftoff, the resist sidewall profile needs to be straight or undercut. These profiles allow the formation of a clear discontinuity between the metal film evaporated on the grating and in the trench since the sidewall is not coated. The ideal metal evaporation for a liftoff process is a normal incidence angle of deposition and would require a small area source. Undercut is desirable in planetary evaporation systems that use ion beam sputtering for higher throughput [131]. Liftoff is very useful for patterning materials that are difficult to pattern and can easily be used to make multilayer patterned films.

After the PMMA is developed, a 35 nm thick nickel layer is evaporated on the samples. The liftoff process strips off the PMMA with the nickel that is on top it. To
perform the liftoff, 1-methyl-2-Pyrrolidinone (NMP) solution is heated up to 90°C in a beaker. Two methods are tried to optimize the liftoff process. The first sample is heated in 1-Methyl-2-Propylidinone (NMP) solution for 25 minutes and then the beaker is transferred into an ultrasonic bath for 10 seconds. The second sample is simply left in the heated NMP solution for 45 minutes. At the end of the process, both samples are rinsed with acetone and methanol, and dried with a nitrogen blow-off gun.

The liftoff process was followed by an SEM inspection. Fig. 3-13 (a) shows an SEM of a device that had been in an ultrasonic bath; the circular nickel pillars have been partially destroyed and displaced. The liftoff process on samples that were left in the heated NMP for 45 minutes worked very well as shown in Fig. 3-13 (b). This process leaves behind a 2D array of 40 nm thick nickel posts, with input and output waveguides.

![Fig 3-13: SEM images of PBG patterns after liftoff.](image)

(a) The ultrasonic agitation partially strips of the photonic crystal and the adjacent waveguides. b) Leaving the sample in NMP solution for longer period results in a good liftoff.
3.5 Reactive Ion Etching

3.5.1 Overview

Material systems are patterned and etched by using wet or dry etch mechanisms. Wet etch is a purely chemical reaction that usually consists of three processes. First, the etchant species diffuse and adsorb to the surface of the sample. Second, a chemical reaction with the area of the sample that is not covered with an etch mask produces soluble byproducts. Third, these products desorb and diffuse away from the surface of the sample. To facilitate etching, the solution is usually heated and stirred. Reaction-limited etches are generally insensitive to agitation, but have a temperature dependence of the form [137]

\[ R = Ke^{\frac{-E_a}{kT}} \]  

\[ \text{(EQ 3-1)} \]

\( R \) is the etch rate, \( K \) is a temperature dependent constant, \( E_a \) is the activation energy, \( k \) is Boltzmann’s constant and \( T \) is the absolute temperature of the mixture. Wet etch results in isotropic sidewalls. Fig. 3-14 illustrates isotropic and anisotropic etches.

![Fig. 3-14: Grating patterns on a film. a) Pattern before etch. b) Pattern has isotropic sidewalls after wet etch. c) Pattern has anisotropic sidewall after a dry etch.](image-url)
Dry etches, which provide anisotropy and high selectivity, are carried out in a reactive ion etcher (RIE) or a high density plasma etcher. A plasma has an equal density of negatively and positively charged particles. RIEs are capable of generating ion density of $10^9 \text{ cm}^{-3}$. In a conventional parallel plate RIE systems, radio frequency (RF) power is capacitive-coupled into a thin sheath region around the electrode. The plasma starts as the RF power accelerates electrons in the vertical direction. The electrons collide with gas molecules and cause electron-impact dissociation, ionization, and excitation which sustain the plasma. Dissociation breaks molecules into free radicals, which are neutral atoms with incomplete bonding. Ionization induces the loss or gain of electrons, thus forming positive or negative ions. Excitation transfers enough energy to an orbital electron to displace it further away from the nucleus. As a result, the sustained plasma will have positive ions, negative ions, radicals, and neutral atoms [138]. For the plasma reaction to occur, the generated reactive species diffuse/bombard to the surface of the sample, adsorb to the surface, and penetrate the lattice. The reaction occurs if the process is not “thermodynamically uphill” ($\Delta G < 0$). Following the reaction, volatile by-products are desorbed from the surface and pumped out of the chamber. Pump speeds must be sufficient to remove volatile by-products to enable the replenishment of new reactive species in the sample [139]. This process is illustrated in Fig. 3-15.
RIEs and high density etchers produce anisotropic etches by utilizing a DC bias [Fig. 3-16 (a)]. Once the plasma is ignited, the electrons, which have lighter mass, are able to move a larger distance compared to the ions. During the process, the electrons collide with the electrode and induce a self-bias. As a result, an electric field is generated and the ions are accelerated directionally towards the sample. Free radicals, which are neutral, are not affected by the bias and hence diffuse to the sample in random directions, chemically reacting upon arrival. Even though ions are not directly responsible for the reaction, they play a major role on etch-rate and anisotropy by affecting adsorption, desorption, and removal of inert sidewall deposition [138].
As shown in Fig. 3-16 (b), very few electrons have enough energy to ionize gas molecules while many electrons have enough energy to dissociate the molecules. In an RIE, the ion density is coupled with the ion energy; high RF power is required to achieve a higher density of ions and more directionality [140]. However, the higher power may damage the sample due to extreme ion bombardment.

Advanced plasma etching techniques generate higher ion density by separating the power from the ion density. Electron cyclotron resonance (ECR) etchers use an external magnetic field and a resonance effect to confine the electrons. Resonance occurs in the systems when the applied microwave frequency is equivalent to the orbital frequency of electrons under an external magnetic field. The resonance accelerates the electrons and increases their mean free path prior to collision with the electrode. As the electrons travel a longer distance, they are able to dissociate and excite more molecules, producing higher density plasma ($\sim 10^{12}$ cm$^{-3}$) [140]. The ion energy is controlled separately by power applied to the electrode.

Another advanced technique is inductively coupled plasma (ICP) etching, in which a RF current circulating around the chamber in opposite directions causes an
alternating magnetic field in the vertical direction. The magnetic field induces a RF electric field which confines and accelerates electrons in a circular path. The circular motion gives the electrons a longer mean free path and minimizes their collision with the electrode and the sidewall. The energy of the ions is controlled separately by applying another RF source to the electrode, thus controlling the ion bombardment of the sample.

3.5.2 Oxide Etch Study

SiO$_2$ is etched by trifluoromethane (CHF$_3$), tetrafluoride (CF$_4$), or CF$_4$/O$_2$ plasma. When the plasma is sparked, the C combines with the O to form CO$_2$ while the F combines with the Si to form SiF$_4$ as a byproduct. CHF$_3$ is an excellent etchant for SiO$_2$ when using resist as a mask, since the process protects the resist by building carbon on the resist and reducing the resist removal [131, 138]. More detail on the use of CHF$_3$, CF$_4$, or CF$_4$/O$_2$ plasmas to selectively etch Si and SiO$_2$ is included in Chapter 6.

The nickel photonic crystal pattern is transferred to the SiO$_2$ by reactive-ion etching in CHF$_3$ plasma using the PlasmaTherm RIE in NSL. The RIE has helium (He), oxygen (O$_2$), CHF$_3$, and CF$_4$ gas lines. Before the etch proceeds, the chamber is cleaned using CF$_4$ and O$_2$ at 20mT. Adding CF$_4$ causes the dissociation of O$_2$ in order to form CO$_2$ [138]. The F atoms react with organic solids (H ligands) to form HF. After the cleaning step, the SiO$_2$ etching was calibrated using grating patterns as shown in Fig. 3-17 (a). As mentioned in Section 3.2, the stability of evaporated oxide and sputtered oxide is compared. The etch rate of the evaporated oxide was measured to be 28 nm/min. The etch rate of the oxide deposited by sputtering is ~40nm/min, as shown in Fig. 3-17 (b) and summarized in Table 3-2.
Fig. 3-17: a) SEM of a partially etched SiO₂ waveguide used for etch-rate calibration. b) Etch rate for the sputter-deposited SiO₂.

<table>
<thead>
<tr>
<th>Chemistry</th>
<th>Pressure (mT)</th>
<th>DC Bias (V)</th>
<th>Power (W)</th>
<th>Etch Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cleaning</td>
<td>4sccm: 20sccm</td>
<td>25</td>
<td>350</td>
<td>270</td>
</tr>
<tr>
<td>SiO₂ (sputtered)</td>
<td>15 sccm CHF₃</td>
<td>10</td>
<td>300</td>
<td>190</td>
</tr>
<tr>
<td>Oxide (evaporated)</td>
<td>15 sccm CHF₃</td>
<td>10</td>
<td>300</td>
<td>190</td>
</tr>
</tbody>
</table>

Table 3-2: Summary of SiO₂ etch parameters.

3.5.3 Nickel Wet Etch

After etching the oxide mask, the nickel mask is wet etched with Transene Thin Film Nickel Etchant (Nickel TFB). TFB is high-purity nitrate-based formulations for superior etching of evaporated or electroplated nickel films. The etch rate is 3nm/sec. Fig. 3-18 shows the resulting periodic oxide pillars after the nickel has been removed.
3.5.4 GaAs/AlGaAs Etch Study

The characterization for the GaAs/AlGaAs etches is examined using gratings that were patterned with photolithography. The etch experiment is challenging due to the need to achieve high aspect ratios, straight sidewalls, and minimized roughness. Hence, topics such as etch chemistry, directionality, etch mask sputtering, and selectivity have been investigated.

3.5.4.1 Boron Tri-Chloride (BCl₃) Etch Chemistry

BCl₃ is able to etch native oxide (Ga₂O₃, AlₓOᵧ) and sustain the reaction to produce smooth etched surfaces [6]. The plasma glow produces Cl radicals and BCl₃ fragments. The BCl₃ plasma reaction consists of sample etch by Cl radicals, bombardment by Cl and BCl₃ fragment ions, and desorption of the byproducts. The ionization and dissociation processes that are reported as follows [141]:

Fig. 3-18: SEM of periodic oxide pillars after the Ni has been wet etched.
$BCl_3 \rightarrow BCl_2 \cdot +Cl \cdot$

$BCl_3 \rightarrow BCl_2^- + Cl^+$

$BCl_3 \rightarrow BCl_2^- + Cl^-$

$2BCl_3 \rightarrow B_2Cl_4 + 2Cl\cdot$

$2B_2Cl_4 \rightarrow B_4Cl_4 + 2Cl\cdot$

The GaAs reacts with Cl radicals to form $Ga_2Cl_6$ and $As_4$:

$$GaAs + 3Cl^- \rightarrow \frac{1}{2} Ga_2Cl_6 + \frac{1}{4} As_4$$

Also, the AlGaAs reacts with Cl radicals to form $Al_2Cl_6$, $Ga_2Cl_6$ and $As_4$:

$$Al_x Ga_y As + 3(x + y)Cl^- \rightarrow \frac{x}{2} Al_2Cl_6 + \frac{y}{2} Ga_2Cl_6 + \frac{1}{4} As_4$$

The etching depends on the reaction enthalpy and on desorption from the surface. Study shows that the reaction enthalpy for $Al_2Cl_6$ and $Ga_2Cl_6$ are equal [141, 142], which implies that desorption determines the etch rate. The slower desorption rate of $Al_2Cl_6$ results in the slower AlGaAs compared to the GaAs etch rate. Desorption is heavily influenced by the pressure. At high pressure, the etching is desorption limited; a higher etch rate can be obtained by bombarding and removing byproducts with energetic ions at a higher power. At low pressure, the etching is adsorption or surface reaction limited; higher power results in lower etch rate, because the reactants are bombarded away before they react with the sample.
Furthermore, the reaction produces inert BCl$_x$ that coats and passivates the etched sidewall. The sidewall passivation is useful to obtain straight sidewalls (anisotropic etch) by preventing trenching, which occurs when horizontal ions and radicals impinge on the sidewall. Fig. 3-19 shows SEM of etch results wherein all parameters are kept the same and the pressure is varied. When the pressure is high, BCl$_3$ etches the GaAs; the AlGaAs is not etched since the byproduct (Al$_2$Cl$_x$) is desorbed quickly [Fig 3-19 (a)]. On the other hand, an anisotropic etch is obtained when the pressure is reduced [Fig 3-19 (b)].

![SEM of etch results](image)

**Fig. 3-19:** SEM of GaAs/AlGaAs etched in BCl$_3$ plasma at a) high pressure b) low pressure.

### 3.5.4.2 Directionality

In a RIE, ion bombardment controls anisotropy by promoting adsorption or desorption and by controlling the sidewall passivation throughout the etching. To maximize anisotropy, the ions bombarding the target should accelerate as close to the surface normal as possible, thus preventing ion-assisted chemistry at the sidewall. The strength of ion acceleration, and therefore the degree of directionality, is directly proportional to the DC bias.
The required chamber condition to achieve directionality is low pressure, low flow, and high dc bias. As the pressure is decreased, the mean free path of the ion is increased. The ions experience fewer collisions which might cause the ion to deviate from the preferred normal path created by the DC bias. At the masked surface, both ions and free radicals are present. The mask will not be affected since the radicals do not react chemically with the mask. In the region where ion-assisted chemistry takes place, the inhibitor is removed by the ions and etching proceeds rapidly. But on the sidewalls where there are few ions, the inhibitor acts as a mask and prevents chemical reaction from taking place [138]. This is schematically illustrated in Fig. 3-20.

Fig 3-20:  a) Ion and radical effect on the film and the mask during ion-enhanced anisotropic etching.  b) Enhancing anisotropy by intentionally forming a sidewall inhibitor [139].
3.5.4.3 Etch mask

To perform a high aspect ratio etch, a stable mask material is required. Photoresist, metal, and oxide masks were investigated. The etching requires low pressure and high DC bias, resulting in very energetic ions, which bombard and sputter off the mask material. The sputtering of the mask causes micromasking in the area that needs to be etched. Metal masks such as nickel and chrome are not etched in plasma; however, energetic ions can sputter off metal masks in a low pressure RIE. To summarize, anisotropic etches require low pressure and energetic ions, which can damage the mask material. Hence, a thicker and stable mask material is required.

3.5.4.4 GaAs/AlGaAs Etch Characterization

Etch rate characterization was carried out after evaluating the above points and solving the relevant problems. The SEM image of a grating shown in Fig. 3-21 (a) demonstrates the result of the anisotropic and high aspect ratio etching that has been developed. Fig. 3-21 (b) shows the etch rate of GaAs and AlGaAs. The GaAs layer thickness was 850nm and the AlGaAs was 1500nm thick. After 10 minutes, 700nm of the GaAs is etched, with an etch rate of 70nm/min, implying that the GaAs layer gets completely etched after 12 minutes. From the plot, the etch depth after 15 minutes is 1000nm. 150nm of the AlGaAs has been etched in 3 minutes. Hence, the AlGaAs etch rate at the beginning is ~50nm/min. However, the plot indicates that the etch rate increases to ~60nm/min after a few minutes. The result is summarized in Table 3.3.
To conclude, the experiments have produced very stable, high aspect ratio, and anisotropic etches that are currently being used in many other projects at MIT. More detail specific to etching the photonic crystal pillar devices is given in Chapter 4.

<table>
<thead>
<tr>
<th>Material</th>
<th>Gas</th>
<th>Pressure (mT)</th>
<th>DC bias (V)</th>
<th>Etch rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs</td>
<td>BCl$_3$</td>
<td>5mT</td>
<td>100</td>
<td>~70nm/min</td>
</tr>
<tr>
<td>AlGaAs</td>
<td>BCl$_3$</td>
<td>5mT</td>
<td>100</td>
<td>~55nm/min</td>
</tr>
</tbody>
</table>

Table 3-3: Comparison of GaAs and AlGaAs etching chemistry and etch rate
3.5.4.5 Roughness Investigation

In order to investigate sidewall roughness of the above etch, "stair" patterns were designed and processed on a few samples. Each sample consisted of sets of 50μm long waveguides (Fig. 3-22). The sets were vertically offset from each other by two microns. The patterns were written by e-beam lithography with high current and large fields in order to minimize the exposure time. The samples then underwent the fabrication sequence including the BCl₃ etch.

Fig. 3-22: a) Schematic illustration of staggered stair design. Arrows indicate where sample was cleaved  
b) SEM image of the structure after etching in BCl₃ plasma.

To perform the roughness measurement, first the sample was cleaved as indicated by the arrows in Fig. 3-22 (a). The staggered stair design ensures the propagation of the cleaved facet very close to, but not touching, a few of the etched waveguides. The SEM images in Fig. 3-22 (b) and Fig. 3-23 show progressive close-up of the cleaved facet.
After the cleaving procedure, the samples are mounted as shown in Fig. 3-24. The waveguides are located by using the optical microscope inside the setup. Then, the AFM tip is brought down to the cleaved facet. A clear distinction is observed as the...
AFM scans the cleaved facet, and the etched waveguide. The RMS roughness of the GaAs layer is measured as 4.86nm, while that of the AlGaAs is 5.71nm.

3.6 Cleaving

As mentioned in Section 3.1, the samples are cleaved so that all the input and output waveguides have smooth facets for optical testing. To cleave each sample, the sample is nicked using a diamond scribe. Then, the crack is propagated by mounting the sample on a glass slide and applying pressure with another glass slide. Though primitive, the cleaving method works extremely well, resulting in flat waveguide facets as shown in Fig. 3-25. The cleaving procedure is performed before oxidation which transforms the AlGaAs into amorphous AlₓOᵧ.

Fig. 3-25: SEM images of cleaved waveguides. a) Cleaving the sample after oxidation results in a broken waveguide. b) Cleaving the sample before oxidation results in a smooth facet.
3.7 Wet Oxidation

When the etching and cleaving of the devices is completed, the Al$_{0.9}$Ga$_{0.1}$As layer is transformed into low-index Al$_x$O$_y$ using a wet thermal oxidation process. As explained in Chapter 2, light in the waveguides is localized in the vertical direction by index confinement.

3.7.1 Overview

One of the reasons that Si has been the mainstay in microelectronic device fabrication is the ability to form a robust native oxide. In 1978, a study was carried out to investigate the possibility of forming a native oxide on III-V compounds by oxidizing epitaxial AlAs at 100°C [143]. However, the quality of the resultant oxide did not fulfill the required standards for metal-insulator-semiconductor applications. A decade later, Al$_x$Ga$_{1-x}$As was found to form a stable oxide through steam oxidation at high temperature [144, 145]. While research effort still continues for a better understanding of the resulting properties, the oxide is being used in many optoelectronic devices such as vertical cavity surface emitting lasers (VCSEL) [146], distributed Bragg reflector (DBR) mirrors [147], microlenses [148], and low-loss bends [149] as a few examples.

For the oxidation process to occur, first the reactants are transported from the steam bubbler to the sample. Next, the reaction between the steam and the Al$_x$Ga$_{1-x}$As forms Al$_x$O$_y$ and some by-products. Finally, the volatile by-products are transported away from the oxide.

The oxidation initially proceeds as follows [150].

\[
2\text{AlAs} + 3\text{H}_2\text{O} (g) = \text{Al}_2\text{O}_3 + 2\text{AsH}_3 \quad \Delta G = -451 \text{ kJ/mole} \quad (\text{EQ 3-5})
\]

\[
2\text{AlAs} + 4\text{H}_2\text{O} (g) = 2\text{AlO(OH)} + 2\text{AsH}_3 \quad \Delta G = -404 \text{ kJ/mole} \quad (\text{EQ 3-6})
\]
The formation of arsine (AsH₃) through reaction of As and atomic H is energetically favorable with ΔG=-471 kJ/mole at 425°C; AsH₃ does not form through the reaction of As and H₂, because it is not favorable with ΔG=77 kJ/mole [151, 152]. Though AsH₃ can desorb as byproduct above 200K, not much of it is detected [152]. Furthermore, As₂O₃ is detected with Raman spectroscopy, implying that another reaction has taken place to decompose the arsine:

\[ 2\text{AsH}_3 + 3\text{H}_2\text{O} = \text{As}_2\text{O}_3 (\delta) + 6\text{H}_2 \quad \Delta G = -22 \text{ kJ/mole} \quad (\text{EQ 3-7}) \]

Constant Raman intensity for As was also observed throughout the reaction, indicating the following two processes, both of them energetically favorable:

\[ \text{As}_2\text{O}_3 (\delta) + 6\text{H}_2 = 2\text{As} + 3\text{H}_2 + 3\text{H}_2\text{O} \quad \Delta G = -131 \text{ kJ/mole} \quad (\text{EQ 3-8}) \]
\[ 2\text{AsH}_3 = 2\text{As} + 3\text{H}_2 \quad \Delta G = -153 \text{ kJ/mole} \quad (\text{EQ 3-9}) \]

Hence, both As and As₂O₃ acts as intermediate products of the reaction, with As₂O₃ being reduced to As in the end [153]. The resulting arsenic either diffuses from the film, resides in interstitial sites, or segregates to nearby interfaces [151].

Atomic H plays a crucial role in the reaction. When samples that are partially oxidized are then annealed in H₂-Ar, the Raman spectra show no change. However, when the samples are annealed in atomic H, the As₂O₃ intensity signal in the spectra decreases by 10% and the As signal increases by the same amount [153]. Furthermore, if O₂ is used as a carrier gas for the steam, the O₂ depletes the H and forms H₂O (ΔG=-1148J/mol) and fully suppresses the oxidation [154]. Thus, the two studies have conclusively demonstrated that atomic H reduces As₂O₃ into As, as stated in EQ 3-8. The above equations can be summarized as follows:
The equations show the possibility of forming AlO(OH). Elastic recoil detection (ERD) shows that the hydrogen concentration is too small to support hydroxide phases in the oxidized layer [155].

Transmission electron microscopy (TEM) images show granular, amorphous contrast in the oxide layer. Prolonged exposure to the imaging electron beam as well as high temperature is seen to crystallize some portion of the amorphous oxide into polycrystalline AlₙOₙ. Also, if the exposures are long, contraction of the oxide layer causes void formation at the GaAs/Al₂O₃ interface. Transition from AlAs to crystalline AlₙOₙ corresponds to a 20% linear contraction [156].

Energy dispersive X-ray spectra (EDXS) analysis of an oxidized Al₀.₉₂Ga₀.₀₈As sample indicates that the oxide is composed of the solid solution (AlₙGa₁₋ₙ)₂O₃. An Al to H ratio of 20:1 was discovered when using ERD, which proved that the film was mainly composed of AlₙOₙ as stated in EQ 3-5, rather than AlO(OH) as suggested by EQ 3-6. Transition from Al₀.₉Ga₀.₁As to AlₙOₙ corresponds to a 6.7% linear contraction [155].

In both AlAs and AlₙGa₁₋ₙAs oxidations, a formation of a thin dense amorphous layer at the oxidation front has been reported [157]. The layer contains As₂O₃, and the thickness increases as the oxidation temperature and the Al content increases [158]. To summarize, AlₙGa₁₋ₙAs is converted into low-index oxide through steam oxidation. The process forms As₂O₃ and AsH₃ as intermediate products. Most of the As₂O₃ and AsH₃ get reduced to form As, diffuse from the film, reside in interstitial sites, or segregates to a nearby interface. Very small amount of the AsH₃ is released as by-product, and some of

\[
2\text{AlAs} + 3\text{H}_2\text{O} = \text{Al}_2\text{O}_3 + 2\text{As} + 3\text{H}_2 + 3\text{H}_2\text{O} \quad \text{(EQ 3-10)}
\]

\[
2\text{AlAs} + 4\text{H}_2\text{O} = 2\text{AlO(OH)} + 2\text{As} + 3\text{H}_2 + 3\text{H}_2\text{O} \quad \text{(EQ 3-11)}
\]
the As$_2$O$_3$ escapes reduction to stay inside at the oxidation front. Oxidation of AlAs results in low-index Al$_x$O$_y$, while oxidation of Al$_x$Ga$_{1-x}$As results in (Al$_x$Ga$_{1-x}$)$_2$O$_3$. Finally, over-oxidation can induce roughness and delamination by converting the GaAs at the GaAs/AlGaAs interface into Ga$_2$O$_3$ at the interface.

As mentioned above, the oxidation can be classified into two regimes as reaction-limited (linear regime) and diffusion-limited (parabolic regime). If the process is reaction-limited, the oxidant is being supplied (diffused) to the Al$_x$O$_y$/AlAs interface at a rate which is faster compared to the rate required to sustain the chemical reaction occurring there. If it is diffusion-limited, the oxidant reacts at the interface as fast as it arrives, which implies that the rate of diffusion becomes the reaction limiting factor. The two limiting cases are shown by the diagram in Fig. 3-35.

![Diagram showing two limiting cases in Al$_x$Ga$_{1-x}$As oxidation process.](image)

(a) Reaction-limited.  
(b) Diffusion-limited.  

$C_G$, $C_S$, $C^*$, and $C_I$ are reactant concentration in steam, inside the oxide/steam interface, outside the oxide/steam interface, and at oxide/Al$_x$Ga$_{1-x}$As interface.  

Fig. 3-26: Schematic illustration of two limiting cases in Al$_x$Ga$_{1-x}$As oxidation process  
(a) Reaction-limited.  
(b) Diffusion-limited.  
$C_G$, $C_S$, $C^*$, and $C_I$ are reactant concentration in steam, inside the oxide/steam interface, outside the oxide/steam interface, and at oxide/Al$_x$Ga$_{1-x}$As interface.
The oxide thickness can be modeled by using the Deal-Grove model given as follows [159]:

\[
\frac{x_{ox}^2}{B} + \frac{x_{ox}}{B/A} = t \quad (EQ 3-12)
\]

In the equation, \(x_{ox}\) is the oxide thickness, \(B\) is the parabolic rate constant, and \(B/A\) is the linear rate constant. The equations can be reduced into a parabolic and linear limit as in EQ 3-13 and 3-14, respectively:

\[
\frac{x_{ox}^2}{B} = t \quad (EQ 3-13)
\]

\[
\frac{x_{ox}}{B/A} = t \quad (EQ 3-14)
\]

3.7.2 Setup

A schematic of the oxidation system is shown in Fig. 3-27. Steam is generated from de-ionized (DI) water in a flask, which is heated indirectly using a hot water bath that is set at 90°C. The temperature of the water is monitored using a thermometer emerged in the flask and another emerged into the bath. Steam is carried into the oxidation furnace by flowing dry nitrogen into the flask through a flow meter.

The temperature of the oxidation furnace is regulated by a digital temperature controller. Two thermocouples, one connected to the temperature controller and another manually placed at the center of the furnace, monitor the temperature at the center of the furnace. The quartz section between the outlet of the flask and the inlet of the quartz tube
is heated to prevent steam condensation. Excess steam and gaseous byproducts of the oxidation process are vented at the exhaust outlet of the furnace.

![Steam oxidation furnace setup](image)

Fig. 3-27: Steam oxidation furnace setup [160].

When the sample is ready for oxidation, it is placed in the center of a quartz boat, which is inserted to the middle of a quartz tube. Parameters such as nitrogen flow rate, water temperature, furnace temperature, quartz tube placement in the furnace, sample and boat placement are carefully monitored in order to achieve a successful oxidation.

The oxidation process starts by ramping the furnace temperature to 435°C while the boat is inside the chamber. Then, the boat is removed and inserted back into the furnace after placing the sample inside the boat. The sample is oxidized by bubbling nitrogen into the flask, which forces the steam into the quartz tube, until the end of the desired oxidation time. At the end of the process, the sample is removed from the chamber and the temperature of the furnace is reduced.
3.7.3 Experimental Results

The samples for the oxidation experiment were prepared by patterning a grating into epitaxially-grown GaAs/Al\textsubscript{x}Ga\textsubscript{1-x}As layers. The gratings are defined by photolithography and etched into the SiO\textsubscript{2} layer, which serves as a mask for subsequent low pressure BCl\textsubscript{3} reactive ion etch. The photoresist is removed by rinsing the sample with acetone before the BCl\textsubscript{3} etch. The SiO\textsubscript{2} layer is not removed from the GaAs. In Fig 3-28, the gratings are not completely oxidized.

![SEM image of grating structures after partial oxidation.](image)

Fig. 3-28: SEM image of grating structures after partial oxidation. The resist has not been totally removed from the oxide mask. The GaAs layer is 850nm thick and the Al\textsubscript{0.5}Ga\textsubscript{0.5}As is 1500nm thick.

In another experiment, waveguides with widths that vary from 1.5\mu m to 200nm are fabricated on the same sample and etched to a depth of 1.8\mu m. Figure 3-29 shows the progression of the oxidation front for two waveguides of different width. In 3-29 (a), neither the waveguide nor the slab is completely oxidized. However, the thin waveguide in 3-29 (b) is completely oxidized even though the underlying AlGaAs slab is not.
Fig. 3-29: a) The SEM image of a 1.5μm wide waveguide shows partial lateral and vertical oxidation. b) SEM image of a 0.45μm waveguide shows complete lateral oxidation and partial vertical oxidation. Both waveguides were oxidized for 11 minutes at 415°C.

By oxidizing the samples containing waveguides of different width, the vertical and horizontal oxidation thickness is measured. The waveguides are oxidized for duration ranging from 2.5 minutes to 18 minutes at 415°C [Fig 3-30]. The oxidation rate, which is the same as the B/A coefficient in the linear limit, is ~38nm/min.

Fig. 3-30: Lateral and vertical oxidation rate characterization.
Chapter 4

Square Lattice of Dielectric Rods:

Devices

4.1 Overview

Various photonic crystal waveguide devices were fabricated after studying the required process steps as explained in Chapter 3. Several iterations ("generations") were required to tailor the processes developed in the previous chapter towards the sub-500nm photonic crystal feature sizes. With a successful process sequence, linear defects are introduced to create photonic-crystal waveguides. Various coupling approaches were explored, including designs such as butt-coupling, tapered dielectric input waveguides, and a novel adiabatic scheme. The epitaxial growth is performed using the Riber32 gas source molecular beam epitaxy (GSMBE) system in Prof. Leslie Kolodziejski’s Integrated Photonic Devices and Materials Group. The processing was accomplished in Prof. Henry Smith’s Nanostructures Laboratory (NSL), which is equipped with the tools that are needed to carry out the fabrication as well as process characterization.
4.2 Photonic Crystals: Generation-I through Generation-V

The fabrication of the photonic crystals is first investigated without introducing defects for waveguiding. Mask materials such as evaporated oxide, sputtered oxide, nickel, and titanium were investigated. Furthermore, RIE parameters such as gas flow, pressure, and DC bias were studied to create high-aspect ratio, anisotropic rod structures.

4.2.1 Generation-I: Using Evaporated Oxide Mask

Generation-I devices were fabricated on GaAs wafers without the epitaxially grown layers in order to conserve time and material. The devices consisted of $1.5 \mu$m wide conventional waveguides. The process flow is shown in Fig. 4-1. A 100nm thick SiO$_2$ layer was evaporated by e-beam on the GaAs before spinning PMMA for e-beam exposure. Then, a liftoff procedure was performed using nickel, after which the nickel was used as a mask for the oxide etch. Finally, the nickel was removed with a wet etch and the oxide layer was used as a mask to etch into the GaAs.

![Process flow for Generation I devices.](image)

Fig. 4-1: Process flow for Generation I devices.
Results from the different steps in the process flow are illustrated by the SEM micrographs shown in Fig. 4-2. The figure shows that the process sequence was successful up to the GaAs etch step [Fig. 4-2 (d)]. The GaAs etch was carried out using BCl\textsubscript{3} plasma at 5mT and 120 volts DC bias. As from the SEM image in Fig. 4-2 (d), the oxide mask was sputtered away as the etching progressed due to the bombardment from the energetic ions. The top edge of the GaAs rods was also etched since the oxide mask was sputtered away. In order to reduce the effect of the energetic ions on the mask, the applied DC bias was reduced to 100 volts; however, the oxide mask was still sputtered away. Increasing the evaporated mask thickness (~300nm) was not possible because of the lack of uniform thickness across the samples. Hence, various metal masks were investigated to replace the evaporated SiO\textsubscript{2} mask.

![SEM images of Generation-I devices](image)

Fig. 4-2: SEM images of Generation-I devices. a) After e-beam exposure and development of PMMA. b) After nickel evaporation and liftoff. c) After RIE of oxide and wet etch of nickel. d) After etching into the GaAs layer.
4.2.2 Generation-II: Use of Metal Mask

Utilizing metal masks reduces the number of steps in the fabrication sequence. To enable liftoff, the thickness of the evaporated metal was limited to 50nm since the thickness of the PMMA was 200nm. The process flow is indicated in Fig. 4-3.

Fig. 4-3: Process flow for Generation II devices.

To avoid sputtering away the metal, the etching was performed at a pressure of 10mT and at a DC bias of 100 volt. The SEM image in Fig. 4-4 (a) shows the photonic-crystal pattern transferred into GaAs/AlGaAs using nickel etch mask in BCl₃ RIE. The nickel mask was sputtered away by the energetic ions. Titanium metal mask was also explored; however, the mask did not withstand the low pressure etch as illustrated by the SEM image in Fig. 4-4 (b).
Fig. 4-4: SEM image of Generation-II devices. a) After the BCl3 RIE, the nickel mask is sputtered away. b) The titanium mask does not withstand the etch conditions.

4.2.3 Generation-III: Using Sputter-Deposited Oxide Mask

The Generation-II samples consisted of an epitaxially grown heterostructure on a GaAs substrate. The thicknesses of the epitaxial GaAs and AlGaAs layers were 850nm and 1.5μm respectively. A 400nm thick SiO$_2$ mask was deposited on the wafer using the NSL sputter deposition machine. The deposition properties are explained in Chapter 3.1.

![Diagram](image_url)

Fig. 4-5: Process flow for Generation-III devices.
The process sequence is shown in Fig. 4-5. The SEM images in Fig. 4-6 show the photonic crystal patterned in the oxide layer, and then transferred to the GaAs/AlGaAs layer. The BC$_3$ etching was performed at 10mT and 120 volt DC bias. The etch rate was 125nm/min. Though a high aspect ratio etch was achieved without damaging the thick mask, the sidewall of the rods was sloped. The devices were oxidized after the etch, in order to convert the AlGaAs into low index Al$_x$O$_y$. The sidewall slope of the rods is attributed to the sloped oxide mask and the etch chemistry.

Fig. 4-6: SEM images of Generation-III devices. a) Photonic crystal patterns in sputter-deposited SiO$_2$. b) Patterns etched into GaAs/AlGaAs and oxidized. c) Close-up of (b). d) A set including two photonic crystal devices and a straight dielectric waveguide.
4.2.4 Generation-IV: Sculpting Rods

The etch parameters were altered in order to improve the sidewall profile. The pressure was reduced to 5mT and the DC bias was increased to 120 volts. Fig. 4-7 (a) and (b) show SEM micrographs of samples which had a 200nm SiO₂ mask. The etch depth was 1.7 µm and the overall etch rate was 140nm/min. Increasing the DC bias, which increases the ions’ directionality, enabled a straight sidewall profile even though it sputtered away the oxide mask. In (c) and (d), the oxide mask thickness was increased to 300nm. The SEMs show that the oxide caps of the PBG region have been partially sputtered away during the etching; however, the 1.5µm wide oxide cap on the input/output waveguides were not as severely affected.

(a) ![SEM micrograph](image1)
(b) ![SEM micrograph](image2)
(c) ![SEM micrograph](image3)
(d) ![SEM micrograph](image4)

Fig. 4-7: SEM images of Generation-IV devices. In (a) and (b), the oxide mask was completely sputtered away. In (c) and (d), the oxide mask was partially sputtered away.
To improve the etching results, the oxide mask thickness was increased to 300nm and the DC bias was reduced to 100 volts. The result in Fig. 4-8 shows that a straight sidewall profiles have been achieved. The oxide mask was removed and the samples were ashed in an oxygen/helium plasma to reduce the sidewall roughness (due to sidewall deposition) that was observed after the BCl₃ etch. To obtain the desired diameter for the pillars at the end of the process, the patterns were adjusted at the e-beam design stage. The final result is given in Fig. 4-8 (b). The Al₀.₉Ga₀.₁As was oxidized into Al₂O₃.

Fig. 4-8: SEM of Generation-IV devices after etching improvement  
(a) straight sidewall profile 
(b) size of rods is reduced by adjusting at the e-beam exposure step
4.2.5 Generation-V: Final Devices for Optical Testing

In order to create single mode input/output dielectric waveguides, the thickness of the epitaxially grown GaAs layer was reduced. The final optimized process sequence is given in Fig. 4-9.

![Diagram of the process sequence](image)

**Fig. 4-9: Final optimized process flow**

After the nickel liftoff, the oxide mask is etched and the nickel is removed using a wet etch process. Once the patterns were transferred into the GaAs/AlGaAs heterostructure, the oxide caps were completely removed with CHF₃ plasma and plasma ash. Finally, the samples were cleaved and oxidized. The result is given in Fig. 4-10. The optical characterization of the samples is explained in Chapter 5. The various “generation” devices are summarized in Table 4.1.
Fig. 4-10: The SEM images show photonic crystals that have been successfully fabricated and optically characterized. The number of columns was varied in order to observe the development of the bandgap as the coherent scattering increases. SEMs (a), (b), and (c) show the patterns after e-beam exposure and development in PMMA. SEMs (d) and (e) show a top-down view of the patterns at the end of the process while (f), (g), and (h) show side-view of the structures. The height of the GaAs layer is 500nm and the Al$_2$O$_3$ is 1.2μm.
<table>
<thead>
<tr>
<th>Generation</th>
<th>Mask</th>
<th>Pressure, DC Bias</th>
<th>Etch Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>100nm evaporated SiO₂</td>
<td>5mT, 100 volts</td>
<td>75nm/min</td>
</tr>
<tr>
<td>II</td>
<td>50nm evaporated Ni, Cr</td>
<td>10mT, 100 volts</td>
<td>67nm/min</td>
</tr>
<tr>
<td>III</td>
<td>500nm sputter dep. SiO₂</td>
<td>10mT, 120 volts</td>
<td>125nm/min</td>
</tr>
<tr>
<td>IV</td>
<td>200nm sputter dep. SiO₂</td>
<td>5mT, 120 volts</td>
<td>140nm/min</td>
</tr>
<tr>
<td></td>
<td>300nm sputter dep. SiO₂</td>
<td>5mT, 120 volts</td>
<td>140nm/min</td>
</tr>
<tr>
<td>V</td>
<td>300nm sputter dep. SiO₂</td>
<td>5mT, 100 volts</td>
<td>80nm/min</td>
</tr>
</tbody>
</table>

Table 4-1: Summary of fabrication parameters and results.

### 4.3 Photonic Crystals Waveguides: Introducing Line-Defects

Line-defects were introduced during the e-beam lithography exposure by reducing the diameter of the desired row of defect holes. A careful e-beam dose experiment is required to obtain the correct diameter for the defects and the photonic crystal. An SEM image of a photonic crystal defect is shown in Fig. 4-11. The defect holes have diameter of 245nm while the surrounding photonic crystal has diameter of 297nm. In order to investigate the loss of the photonic crystal waveguides, the number of columns was varied as shown in Fig. 4-12.
Fig. 4-11: SEM image of the photonic-crystal waveguide in PMMA after e-beam exposure and development. The diameter of the defect hole is 245nm while that of the diameter of the photonic crystal is 297nm.

Fig. 4-12: SEM of photonic crystal waveguides after e-beam exposure and development in PMMA. The number of columns is varied from 2 to 8 in order to investigate the loss incurred as a function of length. The input and output waveguides are 230nm wide. The diameter of the defects is 245nm while that of the photonic crystal is 290nm.
4.4 Photonic Crystals Waveguide Coupling Structures

As discussed in Chapter 2, coupling into photonic crystals required many simulations. As the simulations were being performed, various coupling designs were being fabricated in parallel. The initial designs that were fabricated [Fig. 4-13] were based on the coupling scheme reported by Mekis et al [161]. The input waveguide was tapered to the size of the defect waveguide, and the output waveguide was the inverse-taper. Fabrication of these devices was terminated because the multimode nature of the input and output waveguides was not be suitable for optical testing.

![Fig. 4-13: SEM images of coupling structures. a, b) The structure patterned in SiO₂. c) The structure etched into GaAs/AlGaAs. d) A set of devices wherein the length (number of columns) of the photonic crystal waveguide is varied.](image-url)
In the next set of coupling structures, both the input and output waveguides were tapered from a width of 550nm to the size of defect rods (250nm) and inserted into the photonic crystal. Simulations showed about 65% efficiency in coupling from the dielectric waveguide to the line-defect waveguide. However, the structure suffered from Fabry-Perot reflections, which made the transmission dependent on the length and frequency. The fabricated structures are shown in Fig. 4-14.

![Fig. 4-14: SEM of photonic crystal waveguides with tapered input and output coupling waveguides](image)

(a) after PMMA e-beam exposure and development  
(b) at the end of the fabrication process with BCl₃ etch and oxidation.

In order to increase the coupling efficiency, a novel adiabatic design was implemented. When the coupled cavity waveguides are fabricated, the holes were brought closer in the e-beam layout by reducing the period by 10% until they merged together into a conventional waveguide. The tapered cladding was designed by offsetting the holes by 10% every period. The process sequence that has been explained in Section 4-1 was used to fabricate the devices. The fabrication result SEM images are shown in Fig. 4-15.
Fig. 4-15: SEM of a novel coupling scheme for photonic crystal waveguides. a) and b) show the design after e-beam exposure and development in PMMA  c) shows the coupled cavity waveguide without the cladding photonic crystal  d) shows the complete photonic crystal waveguide with the coupling structure  e) and f) show a close up of the coupling scheme  g) shows a top-down view of the etched structure  h) shows a dielectric waveguide, coupled cavity structure, and coupling structure fabricated together on the same chip.
Chapter 5

Square Lattice of Dielectric Rods:

Optical Characterization

5.1 Characterization Setup

The optical characterization of the photonic crystal devices were carried out in Professor Ippen’s Optics Lab. The setup, shown in Fig. 5-1, consists of a high resolution tunable laser with the range of 1430 to 1610nm, a movable stage with 10nm resolution, and a high resolution confocal signal collection assembly. Furthermore, while one infrared camera is utilized to detect signals from the cleaved output waveguide facet, another monitor mounted vertically monitors the radiation due to damaged waveguides and the reflection/loss at the coupling junction of the photonic crystal.

A high numerical aperture lens assembly is used to couple the laser into the input waveguide, and the signal from the output waveguide is measured with photodiodes while the laser is tuned with a computer interface. At the output, a polarization splitter separates TE and TM polarized light in order to carry out full polarization analysis. Furthermore, stray light is spatially filtered by using a pinhole aperture. Fig. 5-2 (a) shows the IR image of the output facet after light is coupled into one of the waveguides. In Fig. 5-2 (b), the pinhole prevents substrate-guided background radiation from entering the detector.
Fig. 5-1: Optical characterization setup [162].

Fig. 5-2: a) IR image of the output facet of an array of waveguides. Light can be observed at the output facet of one of the waveguides. b) The output is spatially filtered to filter out background radiation modes.
5.2 Devices on Sample

As mentioned in Chapter 3, many sets of devices were fabricated on each sample. Each set contains four photonic crystal devices and two dielectric waveguides. The dielectric waveguides serve two purposes. First, the output is useful for normalizing the signal from the photonic crystal devices. Second, the waveguides insure consistent coupling between devices in a set. The light is launched into the dielectric waveguides, and the output is maximized by adjusting the high resolution stage. Some of the sets on the sample consist of photonic crystals (no defects) wherein the number of rows varied as shown in Fig 5-3 (a). Other sets include the adiabatic taper design and the coupled cavity waveguides together as shown in Fig. 5-3 (b). The sets are repeated on the sample to ensure repeatability of the measurement.

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Fig. 5-3: a) A set of devices consisting of a dielectric waveguide, and photonic crystal (no defect) of varying length.  b) A set of devices consisting of a dielectric waveguide, coupled cavity waveguide, and a photonic crystal waveguide with adiabatic coupling scheme.
5.3 Dielectric Waveguide Characterization Result

Most of the light is coupled into the dielectric waveguide is lost due to scattering at the input facet as shown by the IR image in Fig. 5-4 (a). The scattering is due to modal mismatch as well as waveguide facet imperfection. The IR image obtained from the sample surface is very useful to investigate waveguides that are damaged resulting in loss of light into radiation modes as shown in Fig. 5-4 (b). The fiber-to-waveguide coupling is maximized by adjusting the input lens assembly and the high resolution stage on which the sample is mounted. In Fig 5-4 (c), light is coupled into the waveguide and the output signal is maximized.

Fig. 5-4: IR image of  a) scattering loss as light is coupled from an input lens assembly into the input facet of the dielectric waveguide,  b) a damaged waveguide leaking out the coupled light  c) coupled light being guided by a high quality dielectric waveguide.
The input dielectric waveguide needs to be polarization preserving in order to ensure that the desired TM mode reaches the photonic crystal. Polarization mixing occurs in a multimode waveguide and results from scattering due to sidewall roughness and lack of anisotropy of waveguide sidewall. After TM polarized light is launched into the waveguide and the output power is maximized, a polarization splitter is employed at the output facet to select and direct TE and TM signals to two different detectors.

The optical characterization result in Fig. 5-5 shows the output light from the dielectric waveguide is mainly TM polarized. The difference between the detected TM and TE output light power is more than 20dB; the detected power of the TE polarized light is near the detector’s noise level. Similar measurements have been observed using other straight waveguides on the sample indicating that the waveguides are polarization preserving.

The oxidation time plays a major role in affecting the transmission through the dielectric waveguides. Fig. 5-6 compares the measured optical power transmission through a waveguide that has been oxidized for the desired oxidation time (8 minutes), and another waveguide that has been over-oxidized (22 minutes). The oxidation was carried out at 415°C. The transmitted power through the over-oxidized sample is drastically reduced possibly due to oxidation-induced contraction that causes delamination at the GaAs/AlGaAs interface. Furthermore, Ga and As may be diffusing towards the interface of the epitaxial layers and increasing the interfacial roughness (thus increasing loss).
Fig. 5-5: TM and TE polarized light transmission power detected at the output facet of a straight dielectric waveguide.

Fig. 5-6: Comparison of transmitted power through a waveguide oxidized for 8 minutes and a waveguide oxidized for 22 minutes at 415°C.
5.4 Bandgap Characterization Result

The optical performance of the photonic crystals were measured after verifying that the dielectric waveguides are mainly polarization preserving, and capable of delivering the desired TM polarized light to the photonic crystal. Some of the measured photonic crystals consist of two periods of rods while others consisted of four periods. The signal from the photonic crystals with six or more periods of rods was very low and hence difficult to quantify.

![Photonic Crystal Images](image)

**Fig. 5-7:** The top SEM images show photonic crystals with two and four rows. The graph plots the measured normalized transmission through the structures. The photonic crystal with two rows does not have a bandgap. However, the photonic crystal with four rows demonstrates a bandgap for the wavelength range of 1448 and 1482 nm.
Figure 5-7 shows the measured power transmission through the photonic crystals (no defect rows). The transmission through the photonic crystal with two periods of rods does not have a prominent gap. However, the photonic crystal with four periods or rods demonstrates the formation of a photonic bandgap from 1448 to 1482nm.

5.5 Photonic-Crystal Waveguide Coupling Characterization

After verifying the existence of a bandgap and measuring the wavelength range of the photonic bandgap, the subsequent set of measurements characterized the line-defect photonic-crystal waveguides which consisted of the two-stage, adiabatically-tapered coupling scheme. The SEM image in Fig. 5-8 shows the optically characterized device.

![SEM image of a photonic-crystal waveguide with two-stage adiabatically-tapered coupling scheme.](image)

Fig. 5-8: Top down SEM image of a photonic-crystal waveguide with two-stage adiabatically-tapered coupling scheme.

The optical power transmission through the waveguide is presented in Fig. 5-9. The result shows that the frequencies that were previously inhibited by the bulk photonic
crystal are now guided by the line-defect waveguide. To verify that the transmission is repeatable, various similar devices were tested on the sample. The figure shows the consistency of the transmission through two similar devices on the same chip.

Fig. 5-9: Transmission through the device shown in Fig. 5-9 shows enhanced transmission inside the bandgap. The characterization of two similar devices on the same chip demonstrated similar and consistent power transmission.

5.6 Coupling and Guiding Efficiency

Even though there is a clear increase in transmission inside the gap, the power through the photonic-crystal line-defect waveguides is much less than that obtained through the dielectric waveguides. The sample was analyzed by imaging with an IR camera mounted vertically in order to identify the sections of the waveguide that cause radiation loss. The four different wavelengths shown by the arrows in Fig. 5-10 (a), two at the band-edge and two more inside the bandgap, were selected and launched into the line-defect waveguide. The figure also shows the IR image for each wavelength.
When launching light through the line-defect waveguides at wavelengths of 1454nm and 1460nm (which have shown high transmission inside the gap), a bright stripe is observed across the photonic crystal waveguide. However, the stripe disappears when the launched wavelengths were changed to 1445nm and 1470nm, which are near the edges of the bandgap.

Furthermore, at 1445nm and 1470nm, significant scattering is detected roughly 10 μm before the photonic crystal. Similar scattering is detected at 1454nm and 1460nm. Thus, the radiation is independent of the wavelength. The adiabatic tapering of the dielectric waveguide into coupled cavity waveguides occurs roughly 10 μm before the photonic crystal, and coincides with the observed large radiation loss.

During the fabrication, the adiabatic transition from the dielectric waveguide to the 1D-sequence of rods does not occur over the same length scale as the simulated structure. This is because e-beam proximity effects determine how closely two rods are patterned; for example, the proximity effect can lead to unintended overlap of two rods. Also, the size of the rods in the taper region varies, again due to proximity effect. Finally, the transition region might have more roughness scattering loss due to the connectivity of the rods.
Fig. 5-10: a) The four arrows indicate the wavelengths of light launched into the photonic crystal. b) IR image of the transmission through the photonic crystal. At 1454nm and 1460nm, which are wavelengths that have high transmission in (a), a bright streak is observed across the photonic crystal. At 1445nm and 1470nm, which are at the band-edges, the streak disappears. In all of the images, the bright light indicates radiation loss. c) By comparing the radiation to an exact image of the photonic crystal (IR image taken under angular white light illumination), the radiation source is tracked to be the area of transition from the dielectric waveguide to the coupled cavity waveguides (roughly 10 μm away from the photonic crystal).
To verify that the junction is indeed causing the loss, light is launched into the coupled cavity waveguides that does not have the photonic crystal cladding layer, shown in Fig. 5-11 (a). The IR image, given in Fig 5-11 (b), shows large radiation loss similar to the previous structure. Thus, the conclusions are that the adiabatic transition from the dielectric waveguide into the coupled cavity waveguide induces the large loss.

![SEM showing the coupled cavity waveguide without the cladding layer](image1.png)

![IR image of the transmission through the CCW in (a) shows large radiation at the transition region.](image2.png)

Fig. 5-11: a) SEM showing the coupled cavity waveguide without the cladding layer  b) IR image of the transmission through the CCW in (a) shows large radiation at the transition region.

### 5.7 Optical Characterization Conclusion

In conclusion, photonic crystals composed of a square lattice of dielectric rods were optically characterized. A bandgap is observed for the wavelength range between 1448nm and 1482nm for a photonic crystal with four periods of dielectric rods.
Furthermore, bandgap guiding is achieved by introducing a line-defect inside the photonic crystal and by utilizing a novel two-stage coupling scheme.

IR images indicated that the first stage of the coupling scheme induced a significant amount of the loss through the device. Due to proximity effect, the fabrication of the first stage is not as adiabatic as the simulated structure. Another fabrication technique, described in the following chapter, will be useful in improving adiabatic transition at the first coupling stage. Furthermore, more e-beam dose experiments will help in compensating for proximity effects. Finally, a more sophisticated setup is being constructed to improve the measurement including measuring the observed scattered intensity from the top of the waveguides. This setup will be useful for characterizing the photonic crystals consisting of more periods of rods.
Chapter 6

Passive and Active Photonic Crystals: Novel Devices and Fabrication Techniques

6.1 Overview

The first half of the chapter describes a new process sequence which utilizes a novel negative e-beam resist called hydrogen silsesquioxane (HSQ). The HSQ simplifies the process sequence required to fabricate photonic-crystal waveguides. The process consists of three steps. First, the HSQ is spun on the sample and the photonic-crystal patterns are created by e-beam lithography. Second, developing the sample removes the unexposed area and leaves behind HSQ patterns. Finally, the HSQ patterns serve as an etch mask for etching into the substrate. By using the three-step method, also known as the ‘expose-develop-etch (EDE) method’, various photonic crystal devices have been created in GaAs/AlGaAs heterostructures and SOI substrates.

Compact light emitters are very important for the integration of optical devices on the same chip. The second half of the chapter proposes a novel electrically-activated linear-waveguide photonic-crystal microcavity laser. A compact microcavity is created by introducing a defect inside the photonic crystal. Furthermore, electrical-activation and edge-emission are achieved by overlapping waveguides that are patterned in different layers. The fabrication sequence and the preliminary fabrication results are presented.
6.2 *HSQ for Fabrication of Photonic-Crystal Devices*

6.2.1 Introduction to HSQ

Interconnect delay (RC delay) in ultra large scale integration (ULSI) is becoming a bottleneck in the improvement of the speed of microelectronic devices. In order to alleviate the RC delay, intensive research is underway to create low-k interlayer/intermetal (ILD/IMD) films that will replace the SiO$_2$ in ULSI multilevel interconnection [163]. Some of these novel materials are deposited by chemical vapor deposition (CVD), while others are spin-on-glass (SOG). Recently, Applied Materials Inc. has produced a low-k material called Black Diamond, which uses the CVD technique [164]. Some of the SOG materials are organic with Si-methyl groups which reduce the film density (thus lowering the index); however, the films exhibit poor adhesion [165]. Other SOG materials are inorganic with hydrophobic pores [166]. The SOG material that is used for this thesis is HSQ.

HSQ has a cage structure which contributes to its low-index property (Fig 6-1). However, the cage structure is converted into a network structure during thermal curing. Solvent loss is induced by heating the HSQ up to 250$^\circ$C. Curing at 435$^\circ$C causes network redistribution and thermal dissociation of Si-H bonds. Above 435$^\circ$C, the pore networks collapses [167]. Thermal curing cleaves the Si-H bonds, transforming of the cage structure into a dense Si-O-Si network [168].
The dissociation of Si-H bonds during thermal curing is facilitated by exposing the samples to an O₂ environment. The oxygen completes the dissociated Si-H bonds to form a structure similar to SiO₂ [169]. Si-H/Si-O ratio in the HSQ film increases with increasing film thickness, but decreases with increasing curing temperature [170], implying that it is easier to form Si-O-Si network structures from thinner HSQ films. Furthermore, it has been observed that the Si-H/Si-O ratio decreases at the HSQ/Si interface; the decreased ratio indicates the existence of a reaction that increases the Si-O content which improves the adhesion [170].

HSQ is not only a good interlayer dielectric, but also a good negative resist for e-beam exposure. The scission of Si-H bonds in HSQ by e-beam exposure induces cross-linking. After the exposure, development using Tetra-Methyl Ammonium Hydroxide (TMAH) remove the HSQ that has not been cross-linked. One advantage of HSQ over other negative resists is its small polymer size, which reduces the line-width fluctuation [171, 172].
6.2.2 Expose-Develop-Etch (EDE) method for photonic crystals

Chapter 3 explained the fabrication sequence that was developed to create the photonic-crystal structures. The process, however, involved numerous steps. Most of the difficult and time-consuming steps in the previous process are replaced by the expose-develop-etch (EDE) fabrication sequence which utilizes HSQ, as shown in Fig. 6-2.

![Diagram](image)

Fig. 6-2: The left side is the previous process sequence explained in Chapter 3. The shaded area of the process sequence is replaced by the three-step HSQ process indicated on the right side.

The HSQ used in this project was Dow Corning’s FOx-14. After placing a drop of HSQ on a sample (6mm by 6mm), the spinning speed was set to 3600 RPM to obtain a thickness of 300nm. The sample was then heated at 150°C for two minutes and at 220°C for two more minutes to drive off the solvent. In order to avoid the absorption of water and overexposure to O₂/N₂ (which would lead to the formation of Si-OH bonds), the sample was patterned by e-beam immediately after coating with HSQ.
In order to discover the appropriate dose for the photonic-crystal structures, various circular and rectangular shapes were initially patterned by e-beam over a range of doses; the optimal development time for the dose was found to be one hour. The SEM images in Fig. 6-3 demonstrate the effect of underdevelopment, overexposure, and optimal exposure/development.

![SEM images of photonic crystal structures in HSQ on Si substrate after e-beam exposure and development a) under-developed b) overexposed c) optimized exposure.](image)

Even though spin-coating HSQ on GaAs produces a planar layer, most of the patterns were stripped away, as shown in Fig. 6-4, after the e-beam exposure and development. The adhesion problem did not occur for Si or SiO₂ substrates. As mentioned above, the Si-H bonds dissociate when the HSQ is exposed by e-beam. The incomplete Si bond easily attaches to Si or to the SiO₂, due to the Si-O-Si cage/network structure of the HSQ. However, a similar reaction does not occur for the GaAs substrate, which usually has a thin layer of native Ga₂O₃.
Fig. 6-4: SEM image of photonic-crystal structures in HSQ on GaAs substrate after e-beam exposure and development. a) The input waveguides were delaminated due to lack of adhesion. b) The photonic-crystal patterns were also delaminated.

The problem was resolved by evaporating ~10nm of SiO$_2$ on the GaAs surface as an adhesion layer before spinning the HSQ on the sample. The samples were developed for an hour and stirred to test the adhesion, which was very stable and unaffected. Using the above process, various devices were created as shown in Fig. 6-5. Some of the devices were line-defect waveguides with the two-stage adiabatic taper coupling scheme. Furthermore, the patterns included novel devices such as add-drop filters (based on Ref. 173), waveguide bends, and dielectric waveguides passing through the photonic crystal.
Fig. 6-5: SEM of photonic crystal structures in HSQ on GaAs substrate (with 10nm SiO$_2$ adhesion layer) after e-beam exposure and development.  

- (a-c) Photonic crystal without defects where the number of rows is varied. 
- (d-f) Photonic crystal with defect rows. 
- (g) A dielectric waveguide passing through a photonic crystal. 
- (h, i) Tapered input coupling. 
- (j) Waveguide bend. 
- (k) Add-drop filter design (based on S. Fan’s design in Ref. 173).
6.2.3 Devices on GaAs/AlGaAs

The discussion in Section 6.2.1 indicated that HSQ is converted into Si-O-Si through thermal curing at high temperature in a N\textsubscript{2} or an O\textsubscript{2} environment. However, the curing step is not necessary after e-beam exposure, because the Si-H bond is already dissociated by the e-beam. The HSQ is converted into cross-linked Si-O-Si, serving as a hard mask for subsequent high-aspect-ratio etches. The results in this section indicate that HSQ has a mask quality that is comparable to sputter-deposited SiO\textsubscript{2}.

The e-beam exposed patterns are transferred into the GaAs/AlGaAs layers by reactive ion etching using a BCl\textsubscript{3} plasma. Because BCl\textsubscript{3} can penetrate thin native oxide layers, a CHF\textsubscript{3} plasma is not required to etch through the 10nm thick SiO\textsubscript{2} adhesion layer. Instead, the BCl\textsubscript{3} plasma etches through the SiO\textsubscript{2}, GaAs, and AlGaAs layers.

The sidewall roughness was characterized using the method explained in Chapter 3. Stair patterns were exposed in the HSQ. After developing for one hour, the patterns were etched into the GaAs/AlGaAs layers. Then, the samples were cleaved, and AFM measurements were carried out. The measurement indicated RMS sidewall roughness of 7.48nm.

The SEM images in Fig. 6-6 show the results of using the HSQ patterns [Fig. 6-5] as hard mask for the subsequent BCl\textsubscript{3} reactive ion etch into the GaAs/AlGaAs layers. The SEM image in 6-5 (a) shows the photonic crystal before the HSQ mask was removed. The rest of the SEM images illustrate various photonic-crystal devices after the HSQ mask had been removed using a CHF\textsubscript{3} plasma.
Fig. 6-6: SEM images of GaAs/AlGaAs structures etched using HSQ mask. a) Before the removal of the HSQ. b-d) Photonic crystals of varying number of rows after etching the HSQ mask. e) Adiabatically tapered two-stage coupling structure after the HSQ mask is removed.

6.2.4 Devices Constructed in Silicon-on-Insulator (SOI)

III-V material systems are very valuable for photonic integrated-circuits because of their ability to emit as well as guide light. III-V devices such as lasers, diodes, modulators, amplifiers, and detectors have been the driving force behind the telecommunication revolution. Furthermore, the ability of compound semiconductors to
emit light, combined with their high electron mobility enabling high speed circuits, suggests that III-V substrates are a top candidate for the development of photonic integrated-circuits (PIC).

However, the III-V fabrication technology lags behind the silicon industry. For example, 200mm diameter InP wafers do not exist and 200mm GaAs wafers are not commercially available, while the Si industry is successfully transitioning towards 300mm technology. The advance of Si fabrication technology has allowed the development of silicon microphotonicics for high density integration of photonic devices. Despite the inability of Si to emit light due to its indirect bandgap, various passive photonic devices are created by using state-of-the-art processing technologies that have been developed for CMOS fabrication. For example, Arrayed Waveguide Grating (AWG) made from silica plays a key role in wavelength division multiplexing (WDM). Furthermore, current fabrication tools are used to integrate the photonic devices and CMOS devices on the same chip, hence leading to mass production of photonic circuits. With this motivation, IBM has created photonic-crystal device by patterning a large area triangular lattice of holes in SOI, and investigated approaches to couple to the devices directly from fiber [174].

The fabrication of photonic-crystal devices consisting of periodic pillars, in the SOI material system, has been investigated by this thesis. The devices were created by using the EDE method discussed in section 6.2.2. First, HSQ was spun on the SOI samples. Unlike the GaAs samples, a thin SiO₂ adhesion layer is not required for the SOI samples. The patterns were written by e-beam lithography with the desired dose and the samples were developed for one hour.
Next, the HSQ patterns served as hard mask for etching into the Si layer of the SOI. Reactive ion etching was carried out in Cl₂ plasma at 8mT pressure, 15 sccm gas flow, and 120V DC bias. The etch rate was ~40nm/min. Over-etching with Cl₂ plasma affected neither the HSQ mask nor the SiO₂ layer under the Si, because the reaction is thermodynamically unfavorable.

While etching the oxide layer of the SOI, the etch chemistry removes the HSQ mask. Hence, the chemistry has to etch the HSQ/SiO₂ selectively from the unprotected Si. CF₄/O₂ etches both Si and SiO₂. If the thickness of the HSQ mask is smaller than the required etch depth into the SiO₂ layer, the Si pillars become partially etched after the removal of the HSQ. By using CHF₃, however, the SiO₂ layer can be selectively etched from the Si layer.

The SEM images in Fig. 6-7 illustrate the various photonic-crystal devices that were patterned in SOI material system with the aforementioned Cl₂ and CHF₃ plasma reactive ion etching.
Fig. 6-7: SEM images of photonic-crystal devices in SOI material system. a-c) Line-defect photonic-crystal waveguides.  d, e) Adiabatically tapered two-stage coupling structure. f, g) $90^\circ$ bends. h) Channel add-drop filter.  i) Dielectric waveguide passing through the photonic crystal (designed based on Ref. 118 and 175).
6.3 Electrically-Activated Linear-Waveguide Photonic-Crystal Microcavity Laser

6.3.1 Overview of Photonic-Crystal Lasers

Compact light emitters are important for the creation of photonic integrated circuits. The light emitters need to have low bias current and high efficiency to avoid the generation of excessive heat loads. Furthermore, the emission needs to be in-plane to allow for monolithic integration with other components on the same chip [176-178]. Edward Purcell first proposed that spontaneous emission can be manipulated by utilizing a small cavity that has dimensions on the order of the emission wavelength [179]. With the growth of semiconductor fabrication techniques, intense effort has been devoted towards the creation of compact microcavities capable of controlling the emission of light from a gain medium [180-182].

The vertical cavity surface emitting laser (VCSEL) is one of the first lasers with a microcavity on the order of the wavelength. In VCSELs, photons generated from an active layer are reflected between epitaxially-grown Bragg reflectors [183]. Another example of a microcavity laser is the microdisk laser, which utilizes total internal reflection (TIR) at the edge of a high refractive index disk to form low-loss whispering-gallery modes [184].

Significant research has taken place to control and modify the emission of optical radiation by using photonic-crystal microcavities [185-189]. Photonic crystals provide flexibility in geometry that allows fine-tuning of the defect-mode radiation pattern and the emission wavelength [190]. Furthermore, photonic crystals provide the potential to create compact, low-noise, and low-threshold lasers [191].
Most of the research reported in the literature has focused on 2D photonic-crystal microcavity lasers. While the high-index slab confines light in the vertical direction, the 2D photonic crystal localizes the light in the plane. The photonic crystal is created by patterning a triangular lattice of air holes in the dielectric. A resonant cavity can be created by removing a single hole from the photonic crystal as shown in Fig. 6-8 (a) [192]. In another report, a thin InGaAsP-containing slab (for emission near 1.55 μm) is first patterned with a 2D photonic crystal that consists of a 10 μm hexagonal cavity, after which the photonic-crystal slab is fused to a thicker low-index slab [193] [Fig 6-8 (b)]. Furthermore, a hexagonal ring waveguide resonator defined by 2D PCs, has been demonstrated as shown in Fig. 6-9 (a) [194].

![Fig. 6-8: a) The SEM image shows the photonic-crystal defect microcavity is created by eliminating one hole and increasing the radius of two nearby holes. The laser, pumped with 830nm wavelength, shows external threshold pump power of 6.75mW [192]. b) The SEM image of a slab photonic-crystal fused to a low index substrate. The laser showed threshold pump power of 9.2mW for incident 980nm light [193].](image-url)
VCSELs have also been enhanced by incorporating photonic crystals into their design. For example, by etching holes on the top 14-17 layers of an Al_{0.15}Ga_{0.85}As/Al_{0.95}Ga_{0.05}As VCSEL [Fig 6-9 (b)], a side-mode suppression ratio (SMSR) of 45dB has been reported for singlemode operation by controlling the radius and the period [195].

![SEM image of a ring laser](image1)

**Fig. 6-9:** a) SEM image of a ring laser. The laser showed threshold pump power of 3mW [194].

b) Schematic of a VCSEL patterned with 2D photonic crystal [195]

Despite all the effort dedicated towards designing surface emitting photonic-crystal lasers, edge-emitting lasers are necessary for monolithic integration with other devices on the same optical chip. It is difficult to cleave ridge waveguides below ~100µm in order to create short cavities; also, much higher edge reflectivity is required as the cavity length is reduced [196]. Experiments have been performed to integrate 2D PCs with ridge waveguide lasers [197], wherein a triangular array of air holes is etched through the waveguide of the laser at one end of the ridge as shown in Fig. 6-10 (a).
1D photonic crystals provide a more effective approach for creating edge-emitting lasers. Fig. 6-10 (b) shows a ridge waveguide, wherein the cavity length has been reduced to 20 μm by employing highly reflective, deeply-etched DBRs (1D photonic crystals) [198]. The structures demonstrated a threshold current of 1.2mA (and an output power of 1.1mW for 10mA input current).

This section proposes a microcavity laser design wherein the length of the cavity is less than 1 μm. Photonic-crystal microcavity filters have previously been experimentally demonstrated [130]. Moreover, quantum wells have been incorporated into the filter designs to create optically-pumped microcavity lasers; however, the design has not been successful due to fabrication challenges [32]. The following section proposes a novel, electrically-activated linear-waveguide photonic crystal microcavity laser.
6.3.2 Proposed Novel Laser Design

The new design uses waveguides patterned in two different layers in such a way that the waveguide of one layer is rotated from the waveguide of the other layer, hence crossing at an angle as shown in Fig. 6-11. As a result, the two waveguides overlap only in a small region. Outside of the overlap region, the two waveguides are patterned with one-dimensional (1D) photonic crystals composed of the appropriate number of holes that have the required diameter. The 1D photonic crystal forms a bandgap where certain frequencies are not allowed to propagate.

Fig. 6-11: Schematic showing a design for electrically-activated photonic crystal laser. Light is emitted from the top waveguide in (a) while it is emitted from the bottom waveguide in (b).
The presence of the unpatterned overlap region, which breaks the periodicity of the 1D photonic crystal waveguides, introduces a photonic crystal defect where one or more modes reside inside the photonic bandgap. The photonic crystals on each side act as perfect mirrors, and the defect serves as a high $Q$ optical microcavity resonator. By designing the defect length appropriately, the emission wavelength can be controlled.

One of the waveguides contains an active material useful for the generation of photons; the other waveguide is used as a guiding layer that directs the light out of the defect region. The active material can be quantum wells or quantum dots emitting at the desired wavelength. For example, Fig. 6-11 (a) shows the laser with the lasing waveguide below and the guiding waveguide on top crossing at an angle. The active material is near the top of the lower waveguide, hence close to the upper guiding waveguide to improve modal overlap. Conversely, Fig 6-11 (b) shows the laser with the top waveguide generating the light, and the lower waveguide emitting the light.

The two waveguides are coupled and the optical mode that emanates from the active material extends across both waveguides at their intersection. The hole number, size, and periodicity, as well as the waveguide width and height can be controlled as desired. As a result, the reflectivity of the photonic crystal mirrors can be controlled by constructing the photonic bandgap in the appropriate manner.

The waveguide layers are doped in a p-i-n fashion and connected to contact pads in order to apply a bias voltage and transport the carriers to the active material; though holes are etched in the waveguide, they still have material continuity to provide a continuous path for current when a bias is applied. Applying a bias voltage induces population inversion and the recombination of carriers in the active material in the
photonic crystal defect region. Hence, light is generated at the intersection of the two waveguides. The waveguide with the active material has a larger number of holes in order to highly confine the generated photons in the overlap region. The light leaks into the waveguide of the second layer, which has more holes on one side than the other side. By adjusting the number of holes and the placement of the active material, the light is directed in the desired direction.

6.3.3 Fabrication Process Sequence

Lithography of the top waveguide:

After the material system is epitaxially-grown, the wafer is cleaved into smaller pieces and coated with HSQ resist in preparation for scanning electron beam lithography. Then, the top waveguide and contact pad designs are patterned into the HSQ. The result of developing the HSQ is shown by the schematic in Fig. 6-12 (a).

Etch of the top waveguide:

The HSQ defined by e-beam in the previous step serves as an etch mask while etching into the InP-based first-layer of the heterostructure. After the reactive ion etching is completed, the HSQ is stripped off by using CHF_3 plasma as shown in Fig. 6-12 (b).
**Lithography of photonic crystal and the bottom waveguide:**

The etched sample is recoated with HSQ in preparation for a second e-beam exposure. The e-beam lithography is complicated because of the required alignment to the feature (InP waveguide) etched in the previous step. The layout is mapped to the alignment marks that exist on the sample, and the exposure is performed after a careful field calibration. To provide alignment tolerance, the waveguide in the second layer has smaller width than the waveguide etched in the first layer. Hence, complete overlap of the waveguides is achieved even if the alignment is offset by tens of nanometers. Fig. 6-12 (c) shows a schematic of well-aligned exposure and HSQ development.

**Etch sequences to define the photonic crystal waveguides:**

Using the HSQ as a hard mask, an etch step is performed to transfer the photonic crystals into the InP waveguide. Next, a different etch chemistry is utilized to define the waveguide, contact pad, and photonic crystal pattern into the GaAs-based second layer of the heterostructure. The AlGaAs-based third layer, which will be oxidized, is also etched. Fig. 6-12 (d) shows the pattern after the etch steps have been performed. Finally, the HSQ is removed from the sample and the laser structure remains [Fig. 6-12 (e)].
**Undercutting:**

The GaAs-based waveguide which is beneath the top InP passive waveguide is undercut in order to provide current confinement in the active region. To achieve the undercut, a photolithography exposure is performed as shown in Fig. 6-12 (f); then, a wet etch chemistry is utilized to selectively etch the section of the GaAs-based waveguide which is not covered with photoresist.

**Oxidation and metal deposition:**

After the wet etch, the sample is wet-oxidized to convert the underlying AlGaAs layer into a low-index oxide. Finally, a metal evaporation and liftoff step is performed to deposit a metal layer on the contact pads. The electrically-activated laser structure at the end of the above process steps is shown in Fig. 6-12 (g).
Fig. 6-12: Schematic of the fabrication sequence:  
a) e-beam lithography  
b) top waveguide etch followed by mask removal  
c) e-beam lithography of photonic crystal  
d) etch holes into the first layer, and then etch deeper into the second layer to define the waveguide and the holes  
e) remove HSQ mask  
f) photolithography to define undercut region  
g) final structure after undercutting, oxidation, and metal evaporation on contact pads.
6.3.4 Preliminary Fabrication Results

*Material System:*

The various layers are epitaxially-grown using a gas-source molecular-beam epitaxy system. The passive layer was grown as a 200nm thick In$_{0.5}$(Ga$_{0.7}$Al$_{0.3}$)$_{0.5}$P layer doped with Si to dope the layer n-type. The lasing layer consisted of a separate confinement heterostructure (SCH) containing In$_{0.15}$Ga$_{0.85}$As quantum dots (QD) with 25nm GaAs barrier layers. The SCH is clad with 35nm n-type Al$_{0.3}$Ga$_{0.7}$As:Si layer, and a 125nm p-type Al$_{0.3}$Ga$_{0.7}$As:Be layer. A schematic of the material system is given in Fig. 6-13. The photoluminescence data in Fig. 6-14 shows emission from the quantum dots at 1285nm.

![Fig. 6-13: Schematic of the epitaxially-grown material system.](image-url)
InGaAs QD PL

![InGaAs QD PL](image)

Fig. 6-14: Room temperature photoluminescence experiment shows emission from the In$_{0.15}$Ga$_{0.85}$As quantum dots at ~1280nm.

**Patterning the top layer:**

After the HSQ was patterned by e-beam lithography, the top InP-based layer was reactive-ion-etched with CH$_4$/H$_2$/O$_2$. The HSQ mask was then removed using a CHF$_3$ plasma. Fig. 6-15 shows optical images of the etched first layer after the HSQ was removed.

![Optical micrographs](image)

Fig. 6-15: Optical micrographs of the contact pad and waveguide etched into the first layer.
Aligning e-beam lithography:

Aligned e-beam lithography was performed after recoating the sample with HSQ. Utilization of global alignment marks alone did not produce the desired alignment accuracy. For example, the SEM image in Fig. 6-16 (a) shows that the exposed HSQ pattern was misaligned with respect to the first layer waveguide. Moreover, field rotation was observed at the edge of the field as shown by the SEM image in Fig. 6-16 (b). The SEM also shows that the HSQ from the previous step was not completely removed.

![Fig. 6-16: a) The top-down SEM image shows the second layer was shifted from the first layer. b) Side-view SEM image of the sample cleaved near a field boundary also shows field rotation error. Also, residual HSQ is observed on the etched waveguide of the first layer.](image)

In the second experiment, both global and field alignment marks were defined along the first waveguide. Then, the HSQ mask was completely removed before spinning a new layer of HSQ for the second exposure. The photonic crystal waveguides were exposed into the HSQ by utilizing the global alignment marks in combination with the field alignment marks. The SEM images in Fig. 6-17 show the improvement in
alignment. The second layer pattern was directly positioned on the etched waveguide of the first layer. As mentioned previously, the first layer waveguide was wider than the second waveguide by 50nm; hence, the edges of the first layer waveguide are visible beneath the top HSQ waveguide pattern [Fig. 6-17 (d)].

Fig. 6-17: a) SEM image of the HSQ after the e-beam exposure of the second layer shows the middle waveguide and the second contact pad. At greater magnification, the middle section demonstrates the second layer is extremely well aligned on the etched first layer waveguide as seen in the SEM images in (c) and (d).
Chapter 7

Conclusion

7.1 Accomplishments

In summary, photonic crystals are anticipated to have impact on large-scale photonic integrated-circuits by allowing the creation of compact and efficient devices such as waveguides, splitters, microcavity filters, channel add-drop filters, light emitting diodes, and lasers. Previous efforts have exclusively focused on photonic crystals composed of triangular lattice of air holes in dielectric slabs. This thesis has presented the successful design, simulation, fabrication, and optical characterization of photonic crystals composed of a periodic array of dielectric rods in a square lattice.

The cylindrical rods of the photonic crystal consist of a 500nm thick high-index epitaxial GaAs layer and 900nm thick low-index Al\textsubscript{x}O\textsubscript{y} layer. An additional 600nm thick Al\textsubscript{x}O\textsubscript{y} spacer layer is below the cylindrical rods isolating the GaAs guiding layer from the GaAs substrate. The heterostructure is grown using gas source molecular beam epitaxy on a (100) GaAs substrate. The Al\textsubscript{x}O\textsubscript{y} is initially grown epitaxially as Al\textsubscript{0.9}Ga\textsubscript{0.1}As. The fabrication sequence includes electron beam lithography, metal liftoff, reactive ion etching, and wet-oxidation. The process achieves the desired high-aspect-ratio and anisotropic sidewall profile.

To facilitate efficient coupling from a conventional high-index-contrast waveguide into the photonic-crystal line-defect waveguide, a two-stage coupling scheme was employed. In the first stage, the single-mode strip waveguide was transformed into a
waveguide consisting of a one-dimensional (1D)-periodic sequence of rods with a fixed period and having the same radius as the final line-defect. In the second stage, the 1D-rod waveguide was transformed into a 2D photonic-crystal line-defect waveguide by the inclusion of the surrounding 2D photonic crystal.

To optically characterize the devices, light was launched into the GaAs slab and the signal from the output facet was analyzed. The transmission measured through a 2D photonic-crystal device having four rows of rods demonstrated a bandgap over the wavelength range from 1448 to 1482 nm. Employing the two-stage coupling scheme, an increase in transmission was observed within the measured bandgap, demonstrating lateral guiding of light due to the bandgap rather than total internal reflection. The measurements were reproducible for many devices on the same chip. To our knowledge, the results are the first experimental demonstration of bandgap guiding for rod-based photonic-crystal devices for 1.5μm light.

Moreover, a novel expose-develop-etch (EDE) method was developed for the fabrication of photonic crystals. The EDE method utilizes a negative e-beam resist known as hydrogen silsesquioxane (HSQ). Upon e-beam exposure, cross-linking converts the HSQ into Si-O-Si structure. Thus, the exposed patterns become hard masks for subsequent reactive ion etch steps. The EDE method increased the efficiency and yield of the fabrication by eliminating the need for a thick SiO₂ mask deposition and nickel liftoff. Various photonic-crystal devices were created in GaAs and SOI material systems by using the EDE method.

Finally, the thesis has presented the invention of an electrically-activated linear-waveguide photonic-crystal microcavity laser. The design separates the light-generation
and light-guiding processes by creating overlapping waveguides that are patterned in different epitaxially grown layers of a heterostructure. The waveguide layers are doped in a p-i-n fashion and connected to contact pads in order to apply a bias voltage. The control over wavelength (color) and emission direction, as well as the compact size obtained by utilizing photonic crystals, will make the laser useful photonic integrated circuits. The first half of the fabrication sequence has been successfully completed.

\section*{7.2 Future Work}

The thesis has successfully demonstrated bandgap guiding for rod-based photonic-crystal devices, and provides room for further investigation based on the initial results. First, waveguide loss analysis for the line-defect photonic-crystal waveguides would be beneficial. To achieve waveguide loss measurements, line-defects of varying length have been fabricated and the optical characterization setup is being optimized. Second, comparing the various coupling designs would be very useful. Measurements need to be carried out to obtain a quantitative understanding of the coupling-loss of the two-stage coupling design. Finally, analyzing 90°-bend waveguides would be the next logical step. However, the bends require designing resonators at the corner in order to minimize coupling into radiation modes. The SEM images in Fig. 6-18 illustrate some of the devices that are being fabricated. The devices combine 90°-bend waveguides with various coupling schemes.
Fig. 7-1: The SEM images illustrate 90°-bend waveguides with various coupling approaches. (a), (c), (e), and (g) show bends with sharp corners. (b), (d), (f), and (h) show bends with resonators at the corners.
Furthermore, the EDE method provides an efficient way of fabricating rod-based photonic-crystal devices. Prototypes of various waveguides, coupling approaches, add-drop filters have been fabricated. However, the parameters (such as period and diameter) of the devices were based on simulated 2D structures that were reported in literature. To create devices that are suitable for testing, careful 3D simulations need to be carried out.

Finally, the fabrication sequence of the electrically activated laser needs to be completed. The RIE chemistries for GaAs-based and InP-based epitaxial materials have already been studied. The lithography steps required for undercutting the waveguides and for performing metal liftoff are being investigated. Also, simulations are required in order to design the photonic crystal with the proper parameters for a desired wavelength. Experimental demonstration of the laser would provide the first-ever electrically-activated edge-emitting photonic crystal laser.
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