Subwavelength-scale Light Localization in Complete Photonic Bandgap Materials

by

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Dr. Benjamin B. Yellen

Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the Department of Electrical and Computer Engineering in the Graduate School of Duke University

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ABSTRACT

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Abstract

The objective of this dissertation work is to examine light localization in semiconductors provided by a complete photonic bandgap via three-dimensional (3D) woodpile photonic crystals. A 3D photonic crystal is a periodic nanostructure that demonstrates omnidirectional Bragg reflection. These materials are anticipated to become a powerful tool for engineering light propagation and localization within subwavelength scales due to their complete photonic bandgap and the distinctive dispersion relation.

The approach of realizing microcavities in this dissertation is to combine multidirectional etching fabrication methods with mode gap design. Modulation of unit cell size along a line-defect 3D waveguide could bring a guiding mode into the mode gap region of the waveguide and form a microcavity with a resonance inside the complete photonic bandgap. The designed microcavities could be fabricated by multi-directional etching methods because they can structurally be decomposed into two sets of connected and straight dielectric rods.

Ultra-high-quality factor microcavities and sub-wavelength-scale waveguides are designed without introduction of local disorders. Monopole, dipole, and quadrupole resonant modes are demonstrated with a small modal volume. The smallest modal volumes obtained are 0.36 cubic half-wavelengths for a resonance field in vacuum, and 2.88 cubic half-wavelengths for a resonance field in a dielectric. Direct metal contacts with the microcavities do not significantly deteriorate the quality factors because the resonant fields are located inside the microcavities. Single-mode woodpile waveguides are also designed in both lateral and vertical propagation directions.

The multi-directional etching method is a simple approach to the fabrication of woodpile photonic crystals and designed optical components with a variety of crystal orientations and surfaces, including (110), (001), (100), and (010) planes. An arbitrary
surface plane \((mn0)\) is obtained with this method, where \(m\) and \(n\) are integers. Moreover, it can also produce large area woodpile photonic crystals with high precision in silicon and GaAs materials.

These optical components in woodpile photonic crystals would be building blocks of high-density, low-loss 3D integrated optics, cavity quantum electrodynamics (QED), nonlinear optics, and enable the realization of current-injection optical devices.
To my grandparents, my parents,

Huawei, Wenwen, and Jianjian.
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Chapter 1
Fundamentals of Light Localization in Photonic Crystals

1.1 Introduction
Subwavelength-scale localization of photons is a fundamental subject in optical physics and has technological impact on optical devices, such as low-threshold nanolasers, waveguides, switches, and integrated optical circuits. It is important to understand the minimal structural volume, in which light can be trapped, and the smallest dielectric optical resonator that determines the footprint of the integrated optical components. Meanwhile, photons have some advantages as information carriers over electrons because of their broad bandwidth and thus would carry a large amount of information. Research on photonic devices is growing rapidly, aiming to replace their electronic counterparts with photonic ones. In order to miniaturize the device and reduce power losses, light needs to be confined into a small space with minimal energy dissipation. These technological demands also motivate the study of strong light localization.

Conventional light localization technology is established with a simple refractive index change, for example total internal reflection at the interface of dissimilar materials, which enables light localization in fiber optics and whispering gallery optical resonators. However, total internal reflection begins to fail as the device size is reduced. Light localization is lost at sharp bends and curves when the incident angle exceeds the critical angle. Thus, the radiation loss in whispering gallery resonators—ring resonators, microspheres, etc.—grows as the radius decreases. When using the resonators in certain applications, one may have to compromise structural size in order to reduce loss, or vice versa.
Photonic crystals—new types of optical materials in which photons are manipulated in analogy to electrons in crystals—provide a new platform for strong localization of light. Similar to impurity states of electrons in solids, photons can be localized in photonic crystals where disorders are introduced. Microcavities, which have a much smaller modal volume than simple whispering gallery mode resonators, have been demonstrated via the hybridization of photonic crystals and index guiding as a method for 3D light localization.

Three-dimensional photonic crystals differ from other types of photonic crystals because they can possess a complete photonic bandgap. With this uniqueness, we expect to minimize both the mode volume and the radiation power loss in an effort to understand the limit of light localization. Three-dimensional photonic crystals are also the basic components for building optical devices, such as lasers, optical switches, and modulators.

In this dissertation, we design, fabricate, and characterize microcavities and waveguides based on 3D woodpile photonic crystals. An overview of the dissertation is as follows:

In Chapter 1, we introduce the 3D woodpile photonic crystal and discuss the uniqueness of its complete photonic bandgap in terms of light localization. We compare the characteristics of microcavities based on a 2D photonic crystal slab and 3D photonic crystal and discuss the applications of a 3D photonic crystal.

In Chapter 2, we describe woodpile photonic crystals with different crystal orientations that are fabricated using two types of multi-directional etching methods. GaAs-based woodpiles with (110) and (001) surfaces are fabricated with the two-top etching method, while silicon- and GaAs-based woodpiles with (100) and (010) planes are built with the one-top, one-side etching method. The fabricated woodpile structures are characterized by the reflectance spectrum measurements.

In Chapter 3, we show 3D woodpile photonic crystal microcavities that are designed by modulation of the unit cell size along a low-loss line-defect waveguide. The compact resonant modes are unique in terms of symmetry (monopole, dipole, and
quadrupole modes), and the location of electric fields. These unique microcavities consist of straight dielectric rods only; therefore, they can be fabricated for different orientations with the methods discussed in Chapter 2. Woodpile microcavities with direct metal contacts are also considered for the purpose of current injection nanolasers. Moreover, a hybrid microcavity that combines woodpile photonic crystals with a photonic crystal slab microcavity in order that we recycle simple 2D slab microcavity designs and improve the radiation loss from lossy photonic crystal slab components.

In Chapter 4, designs of single-mode waveguides in both planar and vertical directions are proposed by unit cell size modulation in the directions perpendicular to the guiding direction. With these designs, light can be directed into different levels of the circuits, which are the first step toward 3D light guiding and 3D integrated optics.

Finally, the work is summarized and the future prospects are discussed in Chapter 5.

In addition, I collaborated with Ms. Pantana Tor-ngern in fabricating indium tin oxide (ITO) clad 2D photonic crystal slab microcavities, aiming to realize current injection photonic crystal nanolasers, and with Mr. Samuel M. Drezdzon in designing a single-mode waveguide optical isolator that can be integrated into an optics chip. These works are summarized in Appendices A and B.

1.2 Photonic Crystals

The concept of photonic crystals was first proposed by E. Yablonovitch [1] for controlling the spontaneous emission and by S. John [2] for light localization in a randomly fluctuating lattice in 1987. Similar to atomic crystals in which the potential energy is periodically varied, photonic crystals are structures in which the permittivity is periodically modulated with a period comparable to the wavelength of light.

Two important characteristics of photonic crystals distinguish them from isotropic dielectric materials: (i) their dispersion, the relation of angular frequency and wavevectors, can be engineered, and (ii) they can have a photonic bandgap—an energy
range in which light propagation is prohibited in the photonic crystals. These two features make photonic crystals a powerful tool for molding light propagation and confining light. For instance, by introducing a point or line defect into an otherwise periodic photonic crystal, we create defect state(s) inside the bandgap so that a light wave with a frequency inside the bandgap cannot propagate anywhere but in the defect. This way, we can form a microcavity or waveguide. A photonic crystal waveguide has at least two advantages compared to waveguides formed by index guiding. First, thanks to the photonic bandgap, light can be guided in either high-index or low-index materials depending on the defect formed by adding or removing dielectric materials. Guiding light in low-index materials, such as air, is difficult for index-guiding type waveguides because the condition for total internal reflection is not satisfied. Second, slow light or small group velocity \([3, 4]\) realized at band edges enhances light-matter interaction. The enhanced optical nonlinear effects created by this interaction are useful for improving optical switching and storage \([5]\). More detailed applications of photonic crystals will be discussed in Section 1.5.

The order of dimensions of photonic crystals (N) can be one, two, or three, i.e. the refractive index is periodic in one, two, or three dimensions. For example, a Bragg mirror is a 1D photonic crystal, while a photonic crystal fiber utilizes a 2D photonic crystal. For N = 1 and 2, light propagation can be influenced by photonic bands and bandgaps along 1D and 2D periodic dimensions, but not along the other directions with the dimensions of the order 3-N. For N = 3, we can engineer light propagation three-dimensionally via 3D photonic bands and bandgaps, and 3D photonic crystals provide a means of molding light in a 3D space. A planar photonic crystal slab structure, shown in Figure 1-1(a), combines a 2D bandgap in a plane and index confinement in the third direction for 3D (2+1D) confinement of light.
Figure 1-1: A 2D photonic crystal slab microcavity and its escape light cone. (a) A cross-section view of a 2D photonic crystal slab with triangle lattice in the planar directions. The red line indicates active materials, such as a quantum well or quantum dot layer. (b) The escaping light cone of the 2D slab structure. Inside the cone, the mode is not confined, while outside the cone, the mode is confined inside the dielectric slab.

Figure 1-2: Diamond-like geometries with dielectric rods. (a) Rod-connected diamond structure. (b) Woodpile structure. (c) and (d) Modified woodpile structures with more layers to closely mimic a diamond lattice. (Ref. 6)
The 2D photonic crystal slab has advanced light localization technology. For example, regarding 2D photonic crystal slab lasers, Painter et al. first reported optically pumped, pulsed lasing in an InGaAsP quantum well (QW) wafer operating at 1.5 µm at low temperature [7]. Developments following the first photonic crystal laser demonstration include lasing in a quantum dot (QD) wafer [8], room-temperature, continuous-wave lasing operation [9], and electrically-pumped lasing [10]. Other functional optical components, including optical switches [11, 12], filters [13], and waveguides [14] were also constructed in photonic crystal slab platform. Albeit this progress in photonic crystal slab devices, the radiation loss through the escaping light cone remains a limiting factor of their performance, and it is difficult to further minimize the device footprint and power loss simultaneously.

Only 3D photonic crystals can possess a complete photonic bandgap. For the planar photonic crystal, the bandgap is incomplete because of the failure of total internal reflection within an escaping light cone. When light propagates from a dielectric slab with refractive index \( n \) to air, the relations \((n\omega/c)^2 = k^2 = k_{//}^2 + k_{\perp}^2\) and \((\omega/c)^2 = k_{//_{air}}^2 + k_{\perp_{air}}^2\) hold in the slab and air respectively, where \( k_{//} \) and \( k_{//_{air}} \) are the \( k \)-components parallel to the air-slab interface, and \( k_{\perp} \) and \( k_{\perp_{air}} \) are the components in the vertical direction to the interface. Due to momentum conservation in the direction parallel to the interface, \( k_{//} = k_{//_{air}} < \omega/c \) creates a real \( k_{\perp_{air}} \), i.e. light propagation is allowed in air, whereas light is confined in the dielectric slab if \( k_{//} \geq \omega/c \). Therefore, \( k_{//} = \omega/c \) defines a light line or the escaping light cone, and total internal reflection fails for \( k_{//} \) inside the cone [Figure 1-1(b)]. On the other hand, a 3D photonic crystal utilizes Bragg reflection in all directions, and it is the only geometry that possesses a complete photonic bandgap, prohibiting the propagation of light with any polarization in all directions.
1.3 Three-dimensional Photonic Crystals and Band Diagram

The band structures of photonic crystals can be solved with a wave equation and Bloch’s theorem. The position-dependent permittivity in 3D photonic crystals satisfies \( \varepsilon(\mathbf{r} + \mathbf{a}_i) = \varepsilon(\mathbf{r}) \), where \( \mathbf{a}_i \) are primitive lattice vectors \((i = 1,2,3)\). The smallest geometric unit being repeated is a unit cell. The photonic bands in the periodic structure are found via the time-independent wave equation derived from Maxwell’s equations:

\[
\left\{ -\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \nabla \times \right\} \mathbf{E}(\mathbf{r}) = \frac{\omega^2}{c^2} \mathbf{E}(\mathbf{r}), \tag{1.1}
\]

where \( \mathbf{E}(\mathbf{r}) \) is the electric field and \( c \) is the speed of light. According to Bloch’s theorem, the solution of equation (1.1) in a periodic structure satisfies:

\[
\mathbf{E}(\mathbf{r}) = e^{i \mathbf{k}_G \cdot \mathbf{r}} \mathbf{u}_{n,k}(\mathbf{r}), \tag{1.2}
\]

where the Bloch mode \( \mathbf{u}_{n,k}(\mathbf{r}) \) has the same translation symmetry as the permittivity:

\( \mathbf{u}_{n,k}(\mathbf{r} + \mathbf{a}_i) = \mathbf{u}_{n,k}(\mathbf{r}) \). With Fourier expansion, an inverse of the permittivity and Bloch function are written as:

\[
\varepsilon^{-1}(\mathbf{r}) = \sum_{\mathbf{G}} \kappa(\mathbf{G}) e^{i \mathbf{G} \cdot \mathbf{r}}, \tag{1.3}
\]

\[
\mathbf{u}_{n,k}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{u}_{n,k}(\mathbf{G}) e^{i \mathbf{G} \cdot \mathbf{r}}, \tag{1.4}
\]

where \( \mathbf{G} = \sum_i l_i \mathbf{b}_i \) is the reciprocal lattice vector, and \( l_i \) is an integer. The primitive reciprocal lattice vectors \( \mathbf{b}_j \) satisfy \( \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij} \). Substituting equations (1.2), (1.3) and (1.4) into (1.1), we obtain the eigen-equation for the periodic structure:

\[
-\sum_{\mathbf{G}} \kappa(\mathbf{G} - \mathbf{G}') (\mathbf{k} + \mathbf{G}') \times (\mathbf{k} + \mathbf{G}') \times \mathbf{u}_{n,k}(\mathbf{G}) = \frac{\omega_{n,k}^2}{c^2} \mathbf{u}_{n,k}(\mathbf{G}). \tag{1.5}
\]

By solving equation (1.5), we obtain the eigen-frequency \( \omega_{n,k} \) for the \( n \)th Bloch modes at \( \mathbf{k} \). This relation between angular frequency \( \omega \) and wavevector \( \mathbf{k} \) defines the photonic band diagram. A complete photonic bandgap is a spectral range without any solution for equation (1.5) for all wavevectors, i.e., the propagation of light within the frequency
range is prohibited. This happens for photonic crystals with certain lattices when the permittivity modulation contrast is large.

Researchers have reported the existence of a complete photonic bandgap in diamond [15], diamond-like [16] and simple cubic symmetries [17]. A complete bandgap was first revealed in spherical structures with a diamond lattice. In later work, the isolated spheres were replaced with connected cylindrical dielectric rods because of their simple fabrication. The rod-connected diamond structure in Figure 1-2(a) is the structure that has demonstrated the highest bandgap of $\Delta \omega / \omega_{\text{mid}} \approx 30\%$ for $n = 3.6$, where $\Delta \omega$ represents the width of the bandgap, and $\omega_{\text{mid}}$ is the middle frequency of the bandgap. The ratio of bandgap width and middle frequency ($\Delta \omega / \omega_{\text{mid}}$) is often taken as a measure of the bandgap size. Figure 1-2(c) and (d) display a selection of layered photonic crystals that closely mimic the rod-connected diamond structure. However, these structures are still difficult to be realized experimentally. Another layer-by-layer diamond-like 3D photonic crystal is a woodpile structure proposed by Ho et al [18]. It simply repeats every four layers in the stacking directions as shown in Figure 1-2(b). In each layer, the woodpile photonic crystal consists of one-dimensional parallel rods along the x or y direction with equal spacing $a$, which is defined as the lattice constant in the xy plane. The rods in adjacent layers are vertically arranged and shifted by $0.5a$ from every other layer. For example, the nearest blue and green rods are separated by a distance of $0.5a$ along the x axis, and the same is true for the red and brown rods along the y direction in Figure 1-2(b).

We study woodpile photonic crystals with rectangular rods for designing optical components because their bandgap is larger than one that could be obtained in a woodpile structure using cylindrical rods [a]. This is explained by the large overlapping of dielectric materials at the lattice points in woodpile structures with rectangular rods. The

[a] One main reason that rectangular rods are commonly used in woodpile photonic crystals is that the fabrication is feasible with layer-by-layer techniques. With the directional etching method, we are not bound to this choice. In fact, a woodpile structure with any rod shape can be fabricated on the condition that the rods do not change in the etching direction.
simulation results comparing the bandgap range and size are shown in Figure 1-3. For dielectric rods with refractive index $n = 3.4$, the maximum $\Delta \omega / \omega_{\text{mid}}$ is only about 13.5% for cylindrical rods at radius $r/a = 0.3$ (filling factor $\sim 0.47$), while for rectangular rods, $\Delta \omega / \omega_{\text{mid}}$ reaches 18.4% for $h/a = 0.3$ and $w/a = 0.3$ (filling factor is 0.3).

Figure 1-3: Bandgap range and width for woodpile photonic crystals with rectangular rods and cylindrical rods. (a) and (b) Ranges of bandgap. (c) and (d) Ratio of bandgap width over the middle gap frequency.
Figure 1-4: Woodpile photonic crystal geometry and band structure. (a) and (b) Geometry of woodpile photonic crystal. (c) The first Brillouin zone for the woodpile photonic crystal in panel a. (d) Band diagram for a woodpile structure with refractive index $n = 3.4$, $w = 0.3a$, and $h = 0.3a$. A complete bandgap is in the range of $(0.3526, 0.4252)$ for the normalized frequency which is defined as $\omega a/(2\pi c)$ or $a/\lambda_0$. 
A woodpile photonic crystal has diamond-like lattice symmetry. A lattice point is represented by two vertically arranged rods that are indicated by the two red blocks in Figure 1-4(a), and the primitive unit cell [b] has a volume of \(2a^2h\) when \(4h = \sqrt{2}a\). The primitive lattice vectors of the woodpile photonic crystal are:

\[
\begin{align*}
\vec{a}_1 &= a\hat{y} \\
\vec{a}_2 &= \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + 2h\hat{z} \\
\vec{a}_3 &= -\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + 2h\hat{z}
\end{align*}
\]

The reciprocal lattice vectors are written as:

\[
\begin{align*}
\hat{b}_1 &= 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_i \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{4h} (\hat{y} - \frac{a}{4h}\hat{z}) \\
\hat{b}_2 &= 2\pi \frac{\vec{a}_1 \times \vec{a}_3}{\vec{a}_i \cdot (\vec{a}_1 \times \vec{a}_3)} = \frac{2\pi}{4h} (\hat{x} + \frac{a}{4h}\hat{z}) \\
\hat{b}_3 &= 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_i \cdot (\vec{a}_1 \times \vec{a}_2)} = \frac{2\pi}{4h} (-\hat{x} + \frac{a}{4h}\hat{z})
\end{align*}
\]

When \(4h = \sqrt{2}a\), the woodpile photonic crystal possesses a diamond lattice, otherwise, it is in a distorted diamond or diamond-like lattice. Therefore, for \(4h \neq \sqrt{2}a\), the first Brillouin zone has reduced symmetry. For example, in a diamond lattice (\(4h = \sqrt{2}a\)), the X and X’ points in momentum space are equivalent; it is the same for the K and K’, and W, W’ and W”” points. However, for a woodpile photonic crystal with \(4h \neq \sqrt{2}a\), these points are not equivalent, so that we need to calculate more k-points to correctly obtain the band diagram. The shape of the first Brillouin zone also depends on the relation

[b] Here, the primitive unit cell follows the definition of the smallest repeatable geometry to form a woodpile photonic crystal. However, one often refers a four-layer structure of size \(a \times a \times 4h\) as a unit cell such as the cyan blocks in Figure 1-4(b), because the woodpile photonic crystal can be built with this block repeated in x, y, and z directions of a Cartesian coordinate system. Thus, it is convenient and easy to count the number of unit cells. To distinguish these two, we name them primitive unit cell and unit cell respectively.
between $h$ and $a$. Figure 1-4(c) shows the first Brillouin zone of the woodpile in Figure 1-4(a) for $4h > a$. Some symmetric k-points are (in Cartesian coordinates) given by:

$$\Gamma = (0, 0, 0), \quad L = \frac{2\pi}{a} \left( \frac{1}{2}, 0, \frac{\xi}{2} \right),$$

$$X = \frac{2\pi}{a} \left( \frac{1}{2}, \frac{1}{2}, 0 \right), \quad X' = \frac{2\pi}{a} (0, 0, \xi),$$

$$K = \frac{2\pi}{a} \left( \frac{1}{2} \left(1 + \xi^2\right), 0, 0 \right), \quad K' = \frac{2\pi}{a} \left( \frac{1}{2} \left(1 - \xi^2\right), 0, \xi \right),$$

$$W = \frac{2\pi}{a} \left( \frac{1}{2} \left(1 + \xi^2\right), 0, \frac{1}{2} \left(1 - \xi^2\right) \right),$$

$$W' = \frac{2\pi}{a} \left( \frac{1}{2}, \frac{1}{2}, \frac{\xi}{2} \right),$$

and

$$W'' = \frac{2\pi}{a} \left( \frac{\sqrt{2}}{2} \left(1 - \xi^2\right), \frac{\sqrt{2}}{2} \left(1 - \xi^2\right), \xi \right),$$

where $\xi = a / 4h$.

In woodpile photonic crystals, the complete bandgap opens between the 2\textsuperscript{nd} and 3\textsuperscript{rd} bands with an appropriate filling factor and a refractive index contrast larger than 1.9 [18]. The woodpile band structure is illustrated in Figure 1-4(d), where the $k$-vectors along the x axis correspond to those labeled in Figure 1-4(c), and the y axis is a normalized frequency defined by $\omega a/(2\pi c)$ or $a/\lambda_0$ because Maxwell’s equations are scalable. The electric field distributions of the Bloch modes of the three lowest orders at the X and X’ points are displayed in Figure 1-5 and Figure 1-6, respectively, for the xy and xz planes. For the two modes below the bandgap, the majority of the field energy is concentrated in the high-index dielectric materials while the third mode has an increasing amount of energy in air.
Figure 1-5: The field distributions of the three lowest order Bloch modes at the X point. The structural parameters of the woodpile photonic crystal are: $w = h = 0.3a$, and $n = 3.4$. In the images, we show the field in $3\times3\times3$ unit cells.
Figure 1-6: The field distributions of the three lowest order Bloch modes at the $X'$ point. The structural parameters of the woodpile photonic crystal are: $w = h = 0.3a$, and $n = 3.4$. In the images, we show the field in $3\times3\times3$ unit cells.
A light wave exponentially decays in woodpile photonic crystals when its frequency is located inside the complete photonic bandgap. To visualize the bandgap effect, we observe the light propagation of a continuous source in air and inside a woodpile photonic crystal in Figure 1-7. The woodpile photonic crystal has the same structural parameters as the one in Figure 1-4(d), which has a complete bandgap in (0.3526, 0.4252). The normalized frequency of the light source is 0.385, which is located in the middle of the bandgap. As a consequence, the field evanescently decays quickly in the woodpile.

![Light propagation in air and the woodpile structure](image)

Figure 1-7: Light propagation in air and the woodpile structure. (a) Light propagation in air. (b) Light confinement in a woodpile photonic crystal by the complete photonic bandgap. The structural parameters of the woodpile photonic crystal are: \( w = h = 0.3a \), and \( n = 3.4 \). The light wave frequency is \( a/\lambda_0 = 0.385 \).

1.4 Photonic Crystal Microcavities

A microcavity is an important optical component for building many functional devices, such as nanolasers, filters, switches, and sensors. The characteristics of the microcavity directly influence the performance of these devices. In this section, we discuss photonic crystal microcavities based on a 2D photonic crystal slab and 3D photonic crystals and show the fundamental limits of light localization in a photonic crystal slab.

The quality factor \( (Q) \) and the mode volume \( (V) \) are the primary characteristic values of microcavities. The quality factor is linked with the photon lifetime \( (\tau) \) in the
resonator by $Q = \omega \tau / 2$, and the modal volume shows the size of the field distribution. The $Q$ factor is defined by:

$$Q = \omega \frac{U}{P}, \quad (1.6)$$

where $\omega$ is the angular frequency of the resonance, $U$ is the resonant field energy stored in the microcavity, and $P$ is the power dissipated away from the microcavity. In the photonic crystal community, a $Q$ factor exceeding one million is often recognized as an ultra-high-$Q$. The mode volume is defined by:

$$V = \iiint |E(\vec{r})|^2 d^3 \vec{r}, \max \left( \frac{|E(\vec{r})|^2}{|E(\vec{r})|^{\parallel}} \right), \quad (1.7)$$

where $E(\vec{r})$ is the electric field of the resonance mode.

For a photonic crystal slab microcavity, it is a challenge to achieve both high $Q$ and small volume due to partial optical confinement [19]. The power dissipation $P$ from a certain volume can be divided into two parts: the power loss in the planar directions of the slab ($P_{\parallel}$) and the loss into the vertical direction to the slab ($P_{\perp}$) due to the light wave radiation escaped through the light cone, i.e. $P = P_{\parallel} + P_{\perp}$. Thus, we obtain

$$\frac{1}{Q} = \frac{1}{Q_{\parallel}} + \frac{1}{Q_{\perp}}. \quad (1.8)$$

The total quality factor is limited by $Q_{\perp} = \omega U / P_{\perp}$ because the out-of-plane power loss $P_{\perp}$ is almost independent of the number of photonic crystal layers ($N$). The in-plane power loss $P_{\parallel}$ can be reduced by increasing the layers of photonic crystals used for confinement. When $P_{\parallel} \ll P_{\perp}$, the $Q$ factor becomes independent of the number of photonic crystal layers. This is clearly seen on the diagram of the $Q$ factor of a single defect microcavity as a function of $N$ in Figure 1-8. The $Q$ factor first increases and then saturates to $Q_{\perp}$ at a large $N$ value. To our knowledge, there is no theory to predict the maximum $Q$ factor and minimum mode volume that could be achieved in a photonic
crystal slab microcavity, even though many designs have developed from trial and error methods to more systematic approaches, such as momentum space design [19] and cancellation mechanism [20], which have the same principle to reduce the field components inside the escaping light cone. Figure 1-9 is a summary of $Q$ factor and mode volume for some reported 2D photonic crystal slab microcavities. The quality factor increases from several hundred in the simple defect structure [21] to tens of millions with sophisticated designs, such as double-heterostructure [22] or the local modulation of a line defect waveguide [23]. A $Q$ factor of $7 \times 10^7$ has been reported for a mode volume $V \sim 12 \left(\frac{\lambda_0}{2n}\right)^3$ in the modeling [23], while a $Q$ factor of nearly $10^6$ was experimentally demonstrated [24]. However, the $Q$ factor increases at the price of a large mode volume [19], and there is a fundamental or technological difficulty of building ultra-high-$Q$ resonators as the mode volume approaches $(\lambda_0/2n)^3$. Nozaki et al. [8] obtained the $Q$ factor of $10^5$ for $V \sim 1.2 \left(\frac{\lambda_0}{2n}\right)^3$, which is the smallest mode volume reported in 2D photonic crystal slab microcavities. In order to reduce the power loss, we often compromise the mode volume.

The complete photonic bandgap in a 3D photonic crystal may resolve this challenge because the power loss decays exponentially in all directions if the resonant frequency is located inside the complete bandgap. Therefore, the $Q$ factor is expected to increase as the number of unit cells used for confinement increases without experiencing saturation unless other loss mechanisms, such as material absorption, become dominant. If a microcavity with small mode volume could be designed in a 3D photonic crystal, the $Q$ factor can be improved with increasing layers of confinement for a passive microcavity; ultra-high quality factor and small mode volume might be obtained simultaneously. In addition, the investigation of light localization in the complete photonic bandgap would be insightful for understanding the fundamental limits in light localization.
Figure 1-8: The quality factor of a single defect L1 cavity as a function of number of photonic crystal layers. The inset shows the structure of a photonic crystal slab L1 microcavity.

Figure 1-9: Summary of the $Q$ factor as a function of mode volume for pervious 2D photonic crystal slab resonator designs.
1.5 Applications of 3D Photonic Crystals

Three-dimensional photonic crystals are anticipated to overcome the boundary condition in 2D photonic crystal slab thanks to omni-directional Bragg reflection. This could improve the functionality of various applications. Moreover, a 3D photonic crystal may provide test beds for some fundamental physics experiments. A few examples are listed as follows.

- 3D integrated optics

  Three-dimensional placement of optical confinement structures in a 3D photonic crystal allow us to study high-density integrated optics. The number of connections in the devices may be increased with 3D photonic crystals. This could enhance the functionality of the integrated circuits. The footprint could also be greatly reduced.

- Low-threshold nanolasers

  With a photonic crystal microcavity, the density of states inside the bandgap is modified, resulting in suppression or enhancement of spontaneous emission by Purcell effect [25]. In order to reduce the laser threshold, the coupling of spontaneous emission to non-lasing modes should be suppressed, and at the same time, the coupling to the lasing mode(s) should be enhanced. Spontaneous emission is suppressed in the photonic bandgap due to the reduction of optical density of states. It has been demonstrated experimentally that the spontaneous emission rate can be reduced by a factor of 5 for both quantum dot (QD) [26] and quantum well (QW) [27] devices. On the other hand, the spontaneous emission rate of an emitter inside a cavity can be enhanced, compared to that without a cavity (in free space) because of the Purcell effect [25]. The enhancement rate is found via the Purcell factor:

\[
F = \frac{\Gamma_{\text{cavity}}}{\Gamma_{\text{freespace}}} \propto F_p = \frac{3Q(\lambda_0 / n)^3}{4\pi^2 V} \propto \frac{Q}{V},
\]

(1.9)

where \(\Gamma_{\text{cavity}}\) and \(\Gamma_{\text{freespace}}\) are the spontaneous emission rate in a cavity and in free space, respectively, and \(F_p\) is the Purcell factor when the exciton-light coupling is unchanged in
a cavity. The Purcell factor is maximized when an emitter is on resonance with the cavity mode and is physically placed at the field maximum. Hence, a large value of $Q/V$, i.e. ultra-high $Q$ factor and small mode volume, is desired.

- **Current-injection photonic crystal nanolasers**

  It has been a challenge to build current-injection photonic crystal lasers with a 2D photonic crystal slab because metal contacts significantly reduce the optical confinement due to the absorption loss. We expect to solve this problem with 3D photonic crystal microcavities, because the small overlapping of resonance field with metal contacts even when the metal directly contacts the microcavity.

- **Cavity quantum electrodynamics (cavity-QED)**

  In a strong-coupling cavity-QED system [28, 29], large ratios $g/k \propto Q/\sqrt{V}$ and $g/\gamma \propto 1/\sqrt{V}$ are desired for improving the quantum coherence, where $g$ is the emitter-cavity field coupling rate, and $k$ and $\gamma$ are decay rates of cavity and emitter. Vacuum Rabi splitting was observed between a single quantum dot and a compact resonator [30-32]. For example, in Ref. 31, the observed $g$ was as high as 20.6 GHz for strong coupling experiments.

- **Nonlinear optics**

  Nonlinear optical devices, such as switches, logic gates and memory, are indispensable for optical circuits [33]. Unfortunately, weak nonlinearity requires either high input power or a long interaction path. High $Q$ and small $V$ microcavities are expected to enhance nonlinear effects and reduce the energy by a factor of $V/Q^2$. Photonic crystal microcavities can have a much smaller mode volume than other optical microcavities, such as microring and microsphere resonators; thus, $V/Q^2$ is reduced by several orders in photonic crystal microcavities, resulting in a great reduction in the switching energy. For example, optical bistability is observed in silicon photonic crystals with less than a milliwatt of power: Tanabe et al. demonstrated a 400 µW using a high $Q$
microcavity coupled with a waveguide [34] and Barclay et al. reported input powers of 250 µW with fiber taper coupling to a microcavity [35]. Three-dimensional photonic crystal microcavities are anticipated to further enhance the nonlinearity.
Chapter 2
Fabrication of Woodpile Photonic Crystals

In this chapter, we describe the fabrication of 3D photonic crystals with various crystal orientations and surfaces in the optical wavelength range via multi-directional etching methods. The directional etching approaches produce silicon and GaAs woodpile structures in a two-patterning and two-etching process with high-resolution electron-beam lithography and high-aspect-ratio dry etching. The optical properties of the fabricated woodpile photonic crystals are characterized with reflectance spectra measurement.

2.1 Review of Fabrication Methods

The reported approaches for fabricating 3D photonic crystal in semiconductors with control of the disorder locations include multiple directional etching and layer-by-layer methods. Other fabrication techniques, such as 3D holographic lithography [36], and natural assembly of opals [37], are not discussed here because they do not produce the complete bandgap in high-quality semiconductors. We are interested in semiconductor materials with a high refractive index, at least 1.9, in order to open the bandgap in woodpile photonic crystals [18]; whereas the techniques requiring polymer materials with low refractive indices do not produce the complete bandgap. Moreover, the optical components based on 3D photonic crystals require precise placement of intentional defects via accurate control of fabrication process, but the natural assembly method lacks precise control of the defect locations. Therefore, this method is not considered even though a bandgap may open in the inverse opals of the silicon structure [37].
Figure 2-1: Yablonovite structure. (a) The schematic figure shows method of drilling three sets of holes proposed by E. Yablonovitch. (Ref. 38) (b) The Yablonovite structure fabricated by C. C. Cheng. (Ref. 39)

Figure 2-2: Electron micrographs of woodpile photonic crystals fabricated with layer-by-layer methods. (a) Cross-section image of woodpile made by Lin’s group. Rod spacing is 4.2 μm, width 1.2 μm, and height 1.6 μm. Scale bar is 5 μm. (Ref. 40) (b) Image of woodpile structure made by wafer fusion technique. The period is 0.7μm. (Ref. 41)

Figure 2-3: Micromanipulation method. (a) Micromanipulation of each woodpile layer. (Ref. 42) (b) SEM image of the woodpile photonic crystals fabricated by micromanipulation technique. The scale bar is 5 μm. (Ref. 43)
The multi-directional etching method was proposed for fabrication of the Yablonovite structure [38], which is the first demonstrated 3D photonic crystal with a complete bandgap. The Yablonovite structure was originally fabricated in the microwave frequency by drilling three sets of cylindrical holes [Figure 2-1(a)]. The structure fabricated by this method was scaled down to optical wavelengths with high-resolution lithography and dry etching techniques. In 1995, Cheng et al. fabricated a Yablonovite structure in GaAs by means of electron beam lithography and the angled chemically assisted ion beam etching (CAIBE) technique [44]. Figure 2-1(b) shows the fabricated Yablonovite photonic crystal with a bandgap at a wavelength of 1.3 µm [39]. For the last decade, the multi-directional etching method has not been actively investigated due to the lack of component designs based on the Yablonovite structure.

The layer-by-layer fabrication methods were developed after the existence of the complete bandgap was revealed in the layered 3D photonic crystal geometries, such as the woodpile structure. Three approaches are summarized as follows.

One approach reported by Johnson et al. is a repetitive deposition and etching method based on the conventional planar micro-fabrication technology. This method could construct 3D photonic crystals with intentional disorders [45]. Figure 2-2(a) displays the woodpile photonic crystals fabricated with the same method using polycrystalline silicon. It demonstrated a bandgap at 10-14.5 µm range [46, 40]. The materials used in this method are not single crystalline. Thus, it is difficult to include high-quality III-V materials and a gain medium in the structure for lasers. As a result, this method was not chosen for this research.

Noda et al. reported the layer-by-layer method combined with wafer bonding that allowed them to include III-V materials in 3D photonic crystals [41, 47, 48]. A pair of sample chips with 2D rod patterns are aligned face-to-face and bonded by means of wafer fusion, and then one substrate is removed by selectively etching a sacrificial layer between the substrate and patterned layer. This procedure is repeated to add more layers [Figure 2-3(b)]. The fabricated eight-layered (two unit cells in stacking direction)
woodpile photonic crystals demonstrated 99.99% reflection near a wavelength of 1.3 μm [47]. Active materials, such as quantum wells (QWs), and intentional defects are introduced to the structures made by this method [48]; however, lasing action is not demonstrated due to insufficient \( Q \) factor that is caused by insufficient number of unit cells, misalignment between layers, and rod shape decay produced in multiple wet etching processes.

Another layer-by-layer approach is micromanipulation technique, in which layers with rod patterns are stacked to build a woodpile microcavity [49]; see Figure 2-3(a). The fabricated woodpile photonic crystal is shown in Figure 2-3(b). The quality factor as high as 8600 was experimentally demonstrated in the microcavity fabricated with this method [43].

One common disadvantage for all these three layer-by-layer methods is that they could only produce a woodpile photonic crystal with a single crystal orientation. The fabricated woodpile has only (001) and (100) surfaces available. In 3D integrated optics and photonic crystal surface mode, it would be important to have 3D photonic crystals with arbitrary orientations and surfaces. Multi-directional etching method becomes a promising solution to this because woodpile photonic crystals could also be fabricated with this method. Takahashi et al. made silicon woodpile photonic crystals with (110) surface by the 45° off-angle etching [50]. Woodpile photonic crystals in III-V materials have not been fabricated with this method due to the limited etching selectivity.

2.2 Crystal Orientations in Woodpile Photonic Crystals

To understand the Miller indices for the crystal orientations, we first clarify the notations of the reference directions because the reference directions are not always the same between the woodpile photonic crystals and the electronic crystal wafers in fabrication. We denote \( xyz \) for woodpile photonic crystals as displayed in Figure 1-4(b): the parallel rods are in the \( xy \) plane, and the stacking direction is along the \( z \) axis. The wafer orientation is represented by \( x'y'z' \), where the vertical direction to the wafer surface is
defined as the z’ axis and, thus, the x’y’ plane is the wafer surface. In order to distinguish these two coordinate systems, the prime symbol is added to the Miller indices in wafer crystal coordinates. For example, (100) means the x direction regarding the woodpile structure, while (100)’ is the x’ direction in the wafer.

Woodpile photonic crystals with different crystal orientations and planes can be fabricated with the multi-directional etching method because they can structurally be decomposed into two sets of straight dielectric rods. In each set, the rods are parallel, so that they can be defined in one dry etching process. The etching directions determine the directions of these rods relative to the wafer. The second etching is in the vertical direction relative to the first etching such that the second set of rods is vertical to the first one. Therefore, the orientations of woodpile photonic crystals could be altered by the dry etching directions, and various crystal planes are also generated at the intersection of woodpile structures and the wafer surface during this process.

The procedure of the multi-direction etching methods can be summarized as a two-patterning and two-etching process. The etching masks for the two directional etchings could be defined via the high-resolution electron-beam lithography (EBL) for sub-micron woodpile photonic crystals. These two patterns can be in the same wafer plane or in two different planes. We will demonstrate one fabrication technique for each case: two-top etching method which has both patterns on the wafer surface [Figure 2-4(a)], and one-top, one-side etching method which has one pattern on the wafer surface, and the other on the wafer side facet [Figure 2-4(b)]. The two-top etching method is used to fabricate a GaAs woodpile structure with (110) and (001) surfaces with etching along ⟨101⟩’ and ⟨101⟩’ directions. In general, this method could be expanded to fabricate a woodpile structure with an arbitrary surface in the (mn0) plane, where m and n are integers, by etching in ⟨mn⟩’ and ⟨mn⟩’ directions. The one-top, one-side etching method produces silicon and GaAs woodpile structures with (100) and (010) surface planes. In the fabrication processes, a chemically assisted ion beam etcher (CAIBE) and a
deep reactive ion etcher (DRIE) provides high-aspect-ratio GaAs and silicon etching, respectively.

Figure 2-4: Woodpile photonic crystals with different crystal orientations. (a) Woodpile with (110) and (001) surfaces. (b) Woodpile with (100) and (010) surfaces.

Figure 2-5: Schematics of two-top etching method. (a) 2D patterns on the surface of wafer in two-top directional etching method. (b) The fabrication procedures. 1. The first EBL. 2. The first Cr RIE. 3. The first CAIBE. 4. The second EBL. 5. The second Cr RIE. 6. The second CAIBE.
Figure 2-6: Electron micrographs of the samples in process. (a) Cross-sectional image after Cr RIE. (b) Planar image after Cr RIE. (c) Cross-sectional image after the first 45° (101) direction) CAIBE. The etching depth shown in the figure is 1.8 µm, but larger etching depth (~3 µm) can be achieved. (d) Planar image after the first 45° CAIBE.

Figure 2-7: Cross-sectional electron micrographs of the fabricated GaAs woodpile photonic crystals. (a) A zoomed-out image. (b) A zoomed-in image. The two etching directions are indicated by arrows. The damage of the fabricated woodpile photonic crystal is due to the cleavage in order to observe the cross-section.
2.3 GaAs Woodpile Structures with (110) Surface

2.3.1 Fabrication Method

In order to fabricate woodpile photonic crystals with a (110) surface plane, we etch along the (101)’ and (101)’ directions that are 45° off the wafer surface. When the (110) plane of the woodpile is aligned with the wafer surface, i.e. the (001)’ plane, the structure is shown in Figure 2-4(a). On the wafer surface, the cross-sections of the dielectric rods form 2D patterns as displayed in Figure 2-5(a). These 2D patterns are divided into two groups: the one indicated by the blue color corresponds to the rods along (101)’ direction, and the orange one forms the rods along (101)’ direction. Therefore, we use these 2D patterns to define etching masks and etch along the (101)’ and (101)’ directions to produce a woodpile geometry with (110) surface.

Angled GaAs deep etching is achieved with the chemically assisted ion beam etching (CAIBE) process, which utilizes an argon (Ar) ion beam and chlorine reactive gas. The balance between physical and chemical etching ensures the vertical etching sidewalls. The CAIBE also provides a high etching selectivity of more than 20:1 for GaAs over chromium (Cr), so that deep GaAs etching is possible with a thin Cr mask.

We first describe the procedures for defining the first set of parallel dielectric rods. As sketched in Figure 2-5(b), a layer of 150 nm chromium is evaporated on a GaAs wafer, and high-resolution electron beam lithography (EBL) is performed on Zeon Chemicals ZEP520A resist, which is spin-coated on the sample, with a 50 kV Elionix ELS 7500EX instrument. The blue dashed rectangles in Figure 2-5(a) indicate the open areas after this first EBL. The open pattern size is $\sqrt{2}(a-w) \times h$ with a period of $\sqrt{2}a$ and $4h$ in the x’ and y’ directions. For the mid-bandgap wavelength at $\lambda_0 = 1550$ nm, where $a/\lambda_0 \approx 0.38$ for $w = h = 0.3a$ and $n = 3.4$, the lattice spacing is $a = 590$ nm. The Cr layer is etched through in an inductively-coupled plasma reactive ion etcher (ICP-RIE) with chlorine and oxygen gases. Anisotropic Cr etching is confirmed from the cross-sectional scanning electron micrograph in Figure 2-6(a). Figure 2-6(b) shows the planar
SEM image of the patterned Cr layer that functions as an etching mask during the following CAIBE process, in which the Ar gas pressure is maintained at $3 \times 10^{-4}$ Torr, and Ar ion acceleration voltage is 600 V. The sample is precisely aligned and fixed on a 45° tilt stage before being loaded into the reaction chamber so that GaAs is etched along the $(101)'$ direction. After CAIBE etching, the remaining Cr is removed by hydrochloric acid (HCl). The quality of GaAs etching is inspected by cross-sectional and surface SEM imaging as shown in Figure 2-6(c) and (d). High aspect-ratio deep etching is obtained in spite of a thin etching mask. The etching is 1.8 µm deep in Figure 2-6(c), and this could be increased to about 3 µm with a 150 nm Cr mask. One set of rods in woodpile is fabricated from this patterning and etching process.

The procedures described above are repeated to define the second set of dielectric rods. After chromium deposition and resist coating, we define 2D EBL patterns that are identical to the first ones but shifted by $h$ in the $y'$ direction. This is the only high-resolution pattern alignment step required in our woodpile fabrication procedure. Accurate alignment is achieved thanks to the high resolution (smaller than 30 nm) overlaying ability in the EBL instrument. After Cr RIE etching, the sample is rotated by 180° and fixed on the 45° stage again so that we can etch the chip along the $(\bar{1}01)'$ direction, which is perpendicular to the first angled etching along the $(101)'$ direction. Finally, the chromium etching mask is removed with HCl acid. Woodpile photonic crystals with a (110) surface and $150 \times 150 \times 2.25$ unit cells are fabricated with this two-patterning process. Figure 2-7 displays the cross-sectional SEM images of the fabricated woodpile photonic crystals in GaAs. The damage on the sample is caused by intentional cleaving operation.

### 2.3.2 Optical Characterization

In order to characterize the quality and optical properties of the fabricated woodpile structures, we measure the reflection spectra in the $z'$ direction. The measurement setup is shown in Figure 2-8. A tungsten lamp used in this study is a broad-band light source from 600 nm to more than 2400 nm. The light is illuminated on the sample surface via a
50× objective lens (NA = 0.55), which also collects the reflected beam. The reflected beam is directed into a spectrometer with a LN₂-cooled InGaAs single chip detector. A mirror on a flip is placed on the reflected beam path to redirect light toward a CCD camera for observation of the sample. The iris controls the size of the measurement area. We obtain the reflection spectra by normalizing the reflected light from the sample by the reflection curve from a metal-coated mirror.

For woodpile photonic crystals with the same structural parameters and number of unit cells in the z’ direction, the measured reflectance spectra match the calculation results with some deviations as shown in Figure 2-9. In measurement, unpolarized light is illuminated, whereas, in calculation, we consider both the x’- and y’-polarized incident light. High reflectance is observed from 1200 nm to 1550 nm in measurement. This indicates the existence of the photonic bandgap, and the position of the bandgap agrees well with calculation results. At 1300 nm, the reflectance is as high as 90%. The relatively high reflectance in measurement is observed at short wavelength ($\lambda_0 < 1200$ nm). This is probably due to the scattering caused by surface roughness. Inside the bandgap, the measured reflectivity is slightly lower than the calculated reflectivity because: (i) the fabrication is imperfect, and (ii) the incident light includes a large range of angles (inside a cone with 33° half angle) due to high numerical aperture (NA = 0.55). In calculation setting, the incident light is exactly vertical to the surface. Reflectance at $\lambda_0 > 1550$ nm is not measured as we use the InGaAs detector.
Figure 2-8: Reflectance spectrum measurement system. Incident light beam is focused on a sample through the IR objective lens (50×). Reflected light is collected and analyzed by the spectrometer with InGaAs detectors.

Figure 2-9: Reflectance measurement for unpolarized light (the black solid line) and calculation for x’-polarized (the red dashed line) and y’-polarized (the blue dashed line) light.
2.3.3 Discussions

A major advantage of the two-top directional etching technique is to produce woodpile photonic crystals with a variety of crystal orientations. We fabricate GaAs woodpile photonic crystals with a (110) surface plane with deep anisotropic GaAs etching provided by CAIBE. To our knowledge, this is the first demonstration of a GaAs woodpile with a (110) plane. In fact, a woodpile structure with an arbitrary surface in the $(mn0)$ plane can be produced in an appropriately modified two-top etching method with etching along the $<m0n>′$ and $<n0m>′$ directions. Applications, such as 3D integrated optics and novel research on surface modes, would greatly benefit from the development of the diverse crystal orientations and surface planes.

The two-top directional etching method is also a simple approach of fabricating large-area, high-quality GaAs-based woodpile photonic crystals. In principle, the area would cover up to a 6 inch wafer, which is the maximum wafer size allowed in our EBL system. Only one pattern alignment is required for fabricating multiple layers of woodpile photonic crystals; however, the layer-by-layer method requires one alignment step for every wafer fusion process.

One challenge of the two-top directional etching method is that the structure size in the $z′$ direction is restricted by the etching depth. Even with highly selective dry etching and hard etching mask such as chromium, it is still difficult to exceed a 4 µm etching depth especially for short wavelengths structures. A thick etch mask produces a long shadow along the $x′$ direction during the angled etching, and the holes become smaller or even closed when the mask thickness is $t = \sqrt{2}(a - w)$ or larger. For structures at short wavelengths, the lattice constant $a$ is small, so that the thickness $t$ is also small, resulting in short etching. For this reason, the woodpile photonic crystals have only 2.25 unit cells using this method. However, this method would be useful for studies on surface modes, which do not require a large structure in the $z′$ direction.
2.4 Silicon and GaAs Woodpile Structures with (100) and (010) Surfaces

Woodpile photonic crystals with (100) and (010) surface planes are fabricated in the one-top, one-side etching method. The axes of the woodpile and the semiconductor wafer are related by \( \langle 100 \rangle = \langle 100 \rangle' \), \( \langle 010 \rangle = \langle 001 \rangle' \) and \( \langle 001 \rangle = \langle 010 \rangle' \) in this method. Two-dimensional patterns formed on the wafer surface (the \( x'y' \) plane) and side facet (the \( y'z' \) plane) are displayed in Figure 2-10(a). We define these two patterns on the wafer top and side with EBL and etch in the directions vertical to the plane with the patterns, i.e. the \( z' \) and \( x' \) directions, to produce woodpiles with (100) and (010) surfaces. Figure 2-10(b) illustrates the structure after the first etching in the \( z' \) direction. Vertical etching outperforms the angled etching in terms of sidewall quality and etching depth because: (i) straight sidewalls are easily obtained thanks to physically symmetrical etching, and (ii) deep etching is feasible with a thick etch mask.

With a bond and polish process, we obtain a flat and smooth wafer side facet that is critical for uniform spin-coating of electron-beam resist. The cleaved facet is rough for non-ionic materials such as silicon, and even with a flat side, the abrupt height change causes non-uniformity of spin-coated resist near the edge, resulting in the poor quality of the EBL patterns. This problem is solved in the bond and polish method. In this process, two chips are bonded surface-to-surface with spin-on-glass (FG65, Filmtronics) as a filling material so that the bonded wafer side does not have any gap in the interface of the two chips. Moreover, spin-on-glass helps one to achieve low-temperature (below 250°C) wafer bonding, and the bonded chips are easily separated by etching the filling material with hydrogen fluoride acid. The side of the boned chips is finely polished so that the facet becomes flat without sudden changes near the area of interest.
Figure 2-10: Schematics of the one-top, one-side etching method. (a) 2D patterns on the x’y’ and y’z’ planes. (b) The structure formed after one directional etching in the z’ direction.

Figure 2-11: The samples under the processes on the edge of bonded chips. (a) Optical profiler of the polished side. Roughness average is 7 nm. (b) Optical microscope image of the polished side after evaporating 50nm chromium and spin-coating electron-beam resist (ZEP). Uniform coating is obtained. (c) Scanning electron micrograph of the Cr patterns on the side. (d) A zoomed-in image of panel c.
The fabrication procedures for silicon woodpile photonic crystals with (100) and (010) planes are described as follows. We first define patterns on the wafer side. Two cleaved Si chips of similar size, e.g. 15 mm long by 5mm wide, are cleaned and coated with FG65. The two chips are brought face-to-face with the edges aligned and placed on a hot plate ramping from 120°C to 250°C for 10 minutes. A pair of the sides of the bonded chips is polished with alumina-coated polish papers. One side needs only rough polish so that the bonded chips would stand stably on this roughly polished side during EBL and dry etchings; while the other side is carefully leveled and polished so that a mirror-like surface is obtained. The flatness of the finely polished side is measured via surface topography (Zygo NewView 5000) as depicted in Figure 2-11(a). The roughness average (Ra) is as small as 7 nm. Scanning electron micrographs confirm that a gap between two chips is a few micrometers and filled well with silica. As a result, electron beam resist is uniformly spin-coated on the side after a 50 nm thick Cr layer is evaporated [Figure 2-11(b)]. Next, 2D patterns are written on the area near the interface of two chips with the rods stacking direction (the z direction in woodpile) aligned along the interface (the y’ direction). The patterns are transformed into the Cr layer with RIE etching. Figure 2-11(c) and (d) depict the SEM images of the patterns on the side after Cr RIE. This completes the first 2D patterns on the wafer side. To prepare visible alignment markers for the second EBL on the top of the chip, we etch the markers about 2 µm deep. Then, the two bonded chips are separated with HF acid to remove the silica layer between them.

Next, we pattern the wafer surface. A dummy chip, the edge of which is also finely polished, is placed besides the patterned chip with minimal gap between them such that we could improve spin-coating quality near the edge of the surface. After evaporating a chromium layer on the surface, the second EBL patterns are written and shifted by a distance of \( h \) in the y’ direction relative to the first patterns with the help of the alignment markers and high-resolution registration capability in the lithography system. The chromium layer is then etched through with RIE. Figure 2-12(a) and (b) display the scanning electron micrographs imaging the Cr patterns on both top and side of a wafer, which are similar with those shown in Figure 2-10(a).
Figure 2-12: Scanning electron micrographs showing the second patterning process on silicon surface. (a) Chromium patterns on both top and side after second Cr RIE. (b) A zoomed-in image of panel a.

Figure 2-13: Scanning electron micrographs of the fabricated silicon samples. (a) The cross-section view showing deep and straight silicon etching. (b) and (c) Structures after two silicon DRIE etching.
Finally, the sample is etched twice in the directions vertical to the wafer side and surface with a deep reactive ion etcher (DRIE), which provides deep anisotropic silicon etching by the alternative etching (SF₆ gas) and sidewall passivation (C₄F₈ gas) processes. The passivation process yields an inert layer on the sample to protect the sidewalls from being attacked during the etching process. This produces nearly vertical sidewalls, about 89.7° in our experiments, as displayed in Figure 2-13(a). Deep RIE also has high selectivity, larger than 100:1 for silicon over Cr etching. Hence, only a thin Cr layer is needed as an etching mask. The resulting structures after two silicon etchings, shown in Figure 2-13(b) and (c), are woodpile photonic crystals with (100) and (010) surfaces. It is difficult to observe the internal structures because silicon is hard to be cleaved, especially through the patterns without damaging the samples. The damages on Figure 2-13(c) are caused during the attempts to cleave through the patterns.

With a similar fabrication method, GaAs woodpile photonic crystals with (100) and (010) crystal planes are built. This time, the CAIBE process provides deep and anisotropic GaAs etching [Figure 2-14(a)]. The SEM image of the sample after the second EBL on the wafer side facet is displayed in Figure 2-14(b), where the dark region is the first etched patterns.

Figure 2-14: Scanning electron micrographs of the fabricated GaAs samples. (a) The cross-section view showing deep and straight GaAs etching. (b) The sample after the second EBL on the wafer side facet.
2.5 Summary

Multi-directional etching methods are unique in terms of the variety of the crystal orientations and planes in the fabricated woodpile photonic crystals. By varying the dry etching direction, we could change the orientations in the fabricated woodpile structures. We demonstrate GaAs woodpile with (110) and (001) planes, and silicon and GaAs woodpile with (100) and (010) surfaces. The directional etching methods also provide a simple way to fabricate woodpile photonic crystals of multiple unit cells with high placement accuracy in one fabrication cycle. We hope this could provide a straightforward way to integrate 3D optical devices based on different crystal orientations on the chip.
Chapter 3
Woodpile Photonic Crystal Microcavities

In this chapter, we make use of the complete photonic bandgap to localize light in a subwavelength space. Two types of microcavities are studied: one is designed with a mode gap approach, whereas the other is a hybrid microcavity. The first type of microcavity can be built with available microfabrication technology because they only consist of straight dielectric rods. High quality factor is possible in these cavities even with direct metal contacts. The second type of microcavities provides some insight for reducing the radiation loss in 2D photonic crystal devices without complicated designs.

3.1 Review of Past 3D Photonic Crystal Microcavity Designs

In spite of the promising performance of 3D photonic crystals, the progress in 3D photonic crystal microcavity designs have been hindered, probably due to their structural complexity and a large requirement for computation resources. To date, only a few 3D photonic crystal microcavity designs [51-53] have been reported, and all use the introduction of three-dimensionally-localized disorders that represent point defects. No systematic analysis has been conducted in order to understand the properties of the designed resonant modes, such as symmetry, mode volume, and the $Q$ factor dependence on structure size. Examples of multi-mode and single-mode woodpile microcavities are shown in Figure 3-1(a) and (b), respectively. Even though an ultra-high $Q$ factor was demonstrated for the single-mode microcavity in simulation, it requires about 8700 (29×15×20) unit cells to reach a $Q$ factor of $3 \times 10^7$, and the modal volume information has not been discussed. These resonators are designed by locally adding dielectric materials and could only be fabricated by a layer-by-layer method, which also limits the available crystal orientations in the fabricated microcavities.
Figure 3-1: Schematics of point-defect 3D photonic crystal microcavities via the addition of local dielectric materials. (a) A multi-mode microcavity via the connection of two rods. (Ref. 53) (b) A single-mode microcavity via the addition of dielectric materials to one rod. (Ref. 51)

3.2 Woodpile Microcavities by Unit Cell Size Modulation

3.2.1 Computation Methods

Subwavelength-scale optical waveguides and microcavities are modeled by 3D plane-wave expansion (PWE) [54] and 3D finite-difference time-domain (FDTD) methods [55]. The dispersion relation of a waveguide with a supercell of 5×1×5 unit cells is calculated by the PWE method with 8.1×10⁵ plane waves. The calculation results provide the allowed propagation frequency as a function of the specific propagation vector \( \mathbf{k} \), and we can visualize the mode profile of the guiding modes. The results assist us in the selection of the appropriate waveguides for the desired microcavity mode symmetries and estimation of the resonant frequency. The propagation loss of the waveguide mode is calculated from results of the 3D FDTD method with the Bloch boundary condition in the propagation direction (the y axis) and the perfect matching layer (PML) boundary condition [56] in the other directions. The waveguide supercell has \( N\times1\times N \) unit cells, where \( N \) is a positive integer. The quality factors of the guiding modes are calculated for different \( N \) values. Three-dimensional FDTD is then employed to compute the microcavity modes, including the resonant frequencies, the \( Q \) factors, and the field distributions. The PML boundary condition is applied to all of the walls of a computational space. Unless otherwise stated, the resolution is set to 30 points per lattice.
constant \(a\), which corresponds to approximately 75 points per wavelength, for both PWE and FDTD simulations.

The geometric parameters of the calculation are described here. The dielectric rods that constitute the woodpile microcavity have a refractive index of 3.4, which correspond to that of GaAs or silicon at optical communication wavelengths. In woodpile photonic crystals, both \(w/a\) and \(h/a\) are set to 0.3, where \(w\) is the width of each rod in the xy plane, \(h\) is the height in the z direction, and \(a\) is the center-to-center distance of the rods in the same layer. The length \(a\) is also known as a unit cell length in x and y directions. The unit cell volume is \(a \times a \times a_z\), where \(a_z = 4h\) is the unit cell length in the z direction. The frequency in this work is represented by the normalized frequency \(a/\lambda_0\), where \(\lambda_0\) is the mode wavelength in vacuum. For a woodpile unit cell using the aforementioned parameters, the complete photonic bandgap ranges from 0.3526 to 0.4252. The microcavity is formed by sandwiching the waveguide II of \(N_x \times 1 \times N_z\) unit cells with two waveguides I of \(N_x \times m_y \times N_z\) unit cells on the sides along the y direction, where \(N_x\), \(m_y\), and \(N_z\) are integers that denote the sizes of the waveguide supercells. Therefore, the microcavity has \(N_x \times N_y \times N_z\) unit cells, where \(N_y = 2m_y + 1\).

Similar to the \(Q\) separation analysis in 2D photonic crystal slab\(^\text{19}\), the power loss \(P\) in a 3D photonic crystal microcavity is divided into power losses along three axes onto planes that enclose the microcavity, i.e. \(P = P_x + P_y + P_z\), so that

\[
\frac{1}{Q} = \frac{1}{Q_x} + \frac{1}{Q_y} + \frac{1}{Q_z}
\]

For a microcavity that consists of \(N_x \times N_y \times N_z\) unit cells, the direction with the smallest \(Q_i\) \((i = x, y, \text{ or } z)\) value (the largest power loss) primarily limits the total \(Q\) factor. In order to achieve a certain value of the \(Q\) factor in a microcavity with a small volume, it is desired to have similar \(Q_i\) in all directions, i.e. \(Q_x \approx Q_y \approx Q_z\). For this reason, we analyze the separated power losses of a microcavity mode to understand the strength of confinement in each direction, such that the designs can be improved by enhancing the confinement of light in the weak confinement direction identified in the analysis.
Figure 3-2: The woodpile microcavity geometry and the band diagram along the waveguide direction. (a) A woodpile microcavity that is constructed by connecting waveguide I and II, which have different lattice constants in the y direction. (b) Schematic of the band diagram along the waveguide direction (the y direction).
3.2.2 Design Concept

In order to construct 3D photonic crystal microcavities, we use the so-called mode gap method, wherein a mode is introduced into the mode gap by unit cell size modulation along a waveguide. This design method is also referred to as the unit cell size modulation method. This technique is first introduced into 2D photonic crystal slab system, and it is sometimes regarded as a double-hetero-structure microcavity. Figure 3-2(a) illustrates an example of the woodpile microcavity geometries. The waveguide consists of a line defect, which can be realized, for instance, by including a rod with different width, or by adding or removing a rod in a woodpile structure [57]. The addition of the waveguide produces two frequency ranges in terms of light propagation in the waveguide geometry: (i) guiding (or transmission) ranges, wherein light propagates along the waveguide, and (ii) mode gap ranges, wherein light transmission is forbidden in any direction. A slight variation in the lattice size along the waveguide propagation direction shifts the frequencies of the transmission and mode gap regions without changing other properties of the modes, which results in a frequency difference for light propagation similar to the potential barrier in double-hetero-junction in crystals [Figure 3-2(b)]. Thus, photons with specific energies can only exist in the modulated waveguide region so as to form a resonant mode.

A microcavity can be seen as waveguides that are connected with different lattices in the guiding direction. For example, in Figure 3-2(a), the waveguide with a lattice constant \( a \) in the y direction defines waveguide I, whereas the one with a lattice constant \( a' \) is waveguide II. The guiding modes of waveguide II, which has a large lattice constant \( a' \), shift to lower frequencies, such that a guiding mode in waveguide II falls into the unguided frequency range of waveguide I. Therefore, by sandwiching waveguide II with waveguide I on both sides along the propagation direction, the guiding mode in waveguide II evanescently decays in waveguide I, i.e. this mode is trapped into the waveguide II region and becomes a resonant mode when the waveguide II region is sufficiently short. Waveguide II is seen as a core region, whereas waveguide I is
considered to be a cladding region. The lattice matching condition is satisfied when the lattice size in these two waveguides is the same in the xz plane. With a careful choice of modulation size along the waveguide direction, a high $Q$ factor can be obtained in a small microcavity while maintaining a small mode volume.

An appropriate waveguide selection is an important step for constructing the microcavity and improving the figures of merit of the resonant modes, i.e. high $Q$ factor in small resonators and a small mode volume, from the following four aspects:

(i) A mode gap found in the waveguide band diagram is utilized for optical trapping.
(ii) The mode gap size represents the depth of the light propagation barrier in frequency and, thus, determines the amount of radiation loss through the coupling to the cladding waveguide.
(iii) The waveguide loss is a clear indicator of the microcavity loss in the xz plane, i.e. the power loss that is orthogonal to the waveguide and, thus, the resonator $Q$ factor.
(iv) The symmetry of the waveguide mode determines the symmetry of the resonator mode.

Based on this prior knowledge, we calculate the dispersion relations $\omega(k)$ for three types of waveguides and analyze the $Q$ factors and the symmetries of the waveguide modes that will be pulled into a mode gap for the formation of resonant modes. The parameters of the line defect are then systematically varied so that we can optimize the microcavity performance.

Next, a small modulation in the unit cell length is applied to the core region along the waveguide direction only. Large changes in the core region significantly degrade the $Q$ factor because (i) an abrupt structure change may cause a large amount of scattering loss; (ii) the distorted photonic crystal in the core region may lose the complete bandgap, resulting in power losses in the x and z directions; and (iii) the largely shifted resonant frequency may be in close proximity to other guiding modes in the cladding waveguide, resulting in a large coupling loss in the y direction. As a result, a small variation is preferred for the lattice in the core region; however, if the modulation is too small, the
light propagation potential barrier would be too shallow to reduce the coupling of the guiding mode in the core region to the cladding waveguide regions. Therefore, for a microcavity that is formed by a certain waveguide mode and with a given structural size, we calculate the dependence of the $Q$ factor and mode volume on the modulation size along the waveguide direction and choose the modulation that results in the largest $Q/V$ ratio.

Here, we describe three of the designed resonant modes, namely the quadrupole, dipole, and monopole modes that are induced in a woodpile photonic crystal. We demonstrate the selection of microcavity structural parameters in order to acquire a resonant mode with a certain symmetry, and the 3D FDTD simulation results are discussed for each mode.

### 3.2.3 Quadrupole Mode

We first analyze a woodpile waveguide containing a single line-defect formed by a rod of different width in order to build the microcavity. In woodpile photonic crystals with a rod width of $w$, we change the width of a single rod to $w_x$ to form a waveguide. This rod is referred to as the defect rod. For simplicity, the waveguides are named according to the defect rod width: WG0.5 for a waveguide with $w_x = 0.5a$, WG0.6 for $w_x = 0.6a$, and WG0.7 for $w_x = 0.7a$. The geometry and the dispersion relation of WG0.6 are illustrated in Figure 3-3(a) and (b), respectively.

This waveguide produces two mode gaps: mode gap $A$ below guiding mode-a and gap $B$ between mode-b and mode-c. The frequency range of each mode gap varies with the line defect width $w_x$, and the modeling results are summarized in Figure 3-3(c). Using these two mode gaps and the three guiding modes (mode-a, -b, or -c), there are three unique cases in which we can pull an optical waveguide mode into a mode gap: (i) pull the mode-a down into gap $A$, (ii) push mode-b up into the gap $B$, and (iii) pull mode-c down into gap $B$. Case (iii) is first examined. The lattice constant and the rod width in waveguide II is increased along the propagation direction so that mode-c is pulled into mode gap $B$. 

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Figure 3-3: The geometry and properties of a woodpile 3D photonic crystal waveguide with a defect rod of width $w_x$. (a) The geometry of a waveguide WG0.6, where the defect rod width is $w_x = 0.6a$. The supercell has $5 \times 1 \times 5$ unit cells. The Bloch boundary condition is applied in all directions in the calculation. (b) The dispersion relations for WG0.6. Note that there are two mode gaps: mode gap $A \in (0.3576, 0.3834)$ and mode gap $B \in (0.4028, 0.4089)$ in a dimensionless frequency unit ($a/\lambda_0$). (c) The mode gap frequency ranges as a function of the line-defect width. (d) The waveguide $Q$ factor as a function of the number of unit cells $N$. The supercell size is $N \times 1 \times N$. Black squares, red circles, and blue triangles show the $Q$ factor for mode-c in WG0.7 ($w_x = 0.7a$) and that for mode-a in WG0.6 ($w_x = 0.6a$) and WG0.5 ($w_x = 0.5a$), respectively.
Figure 3-4: The properties of the cavity modes constructed on a $w_x = 0.7a$ waveguide, and a comparison of loose and tight confinement. (a) The profile of the $E_x$ component in the central $xy$ plane of the waveguide. (b) The profile of the $E_x$ component in the central $xy$ plane of the cavity with $a' = 1.033a$. (c) The profile of the $E_x$ component in the same plane of the cavity with $a' = 1.067a$, and $w_y' = 0.333a$. The total number of unit cells of these structures is $7 \times 11 \times 7$. (d) The development of the $Q$ factor with the number of unit cells in the cavity with $a' = 1.067a$, and $w_y' = 0.333a$. 

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In order to obtain a large mode gap $B$, we choose a defect width $w_x = 0.7a$ based on the data in Figure 3-3(c). The profile of the $E_x$ field component of mode-c in the middle of the $xy$ plane in WG0.7 is mapped in Figure 3-4(a). The out-of-propagation loss of mode-c is evaluated by calculating the $Q$ factor of the waveguide, assuming an infinite number of unit cells along the propagation direction; see the data that is represented by black squares in Figure 3-3(d). The $Q$ factor exponentially increases as $N$ increases, where $N$ is the number of unit cells in the $x$ and $z$ directions of the waveguide supercells.

A small amount of modulation is first induced so as to preserve the waveguide mode and also observe the transition from the loose confinement to tight confinement of light. The smallest meaningful change in the parameter is $0.033a$ because the resolution is set to 30, i.e. 30 grids in one lattice constant $a$. Thus, the unit cell length $a'$ is increased to $1.033a$ while keeping the same rod width in the core region. One mode at $a/\lambda_0 = 0.3928$ is found to have a similar field distribution as in the waveguide [Figure 3-4(a)], but due to a small frequency difference, the field slowly decays in the cladding waveguide region; see Figure 3-4(b). The resonant frequency is so close to the upper edge of mode gap $B$ that this mode still couples to the guided mode in the cladding waveguide. The field distribution is elongated along the $y$ direction, resulting in a large mode volume, and the $Q$ factor does not rapidly increase as the number of unit cells increases.

In order to improve the light confinement for this mode, we increase the modulation in the core region so that the mode can be further pulled into the mode gap. The parameters in the core region are selected as: lattice constant $a' = 1.067a$ and rod width $w_y' = 0.333a$; hence, a resonator mode with a lower resonant frequency $a/\lambda_0 = 0.3898$, which is near the middle of the mode gap ($a/\lambda_0 = 0.3886$), is formed. Figure 3-4(c) depicts the $E_x$ field distribution, which becomes localized in the center region and appears to be unchanged as the number of unit cells increases in the cladding regions. The calculated $Q$ values for different microcavity sizes are shown in Figure 3-4(d). By measuring the power loss in each direction, it is discovered that the light confinement per one unit cell is weak along the waveguide direction, i.e. $Q_y < Q_z$ and $Q_y < Q_z$ for $N_x = N_y$. 

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= N_z. When the numbers of cladding layers in the x and z directions are fixed at N_x = N_z = 7, the $Q$ factor initially exponentially grows as $N_y$ increases and then becomes saturated when $N_y \geq 23$. This is because the light confinement in the y direction becomes strong at large $N_y$ values and, instead, power losses in the x and z directions become dominant. Therefore, in order to further improve the $Q$ factor, it is necessary to increase $N_x$ and $N_z$. This is confirmed in the modeling: the $Q$ factor saturates at around $8.5 \times 10^3$ at $N_y \geq 23$ for $N_x = N_z = 7$ but increases to about $3.2 \times 10^4$ after adding four more unit cells in the x direction and two more in the z direction ($N_x = 11$, $N_z = 9$) at $N_y = 23$. The modeling results also demonstrate that the saturated $Q$ factor, for constant $N_x$ and $N_y$ values, is close to the waveguide $Q$ factor for the same $N_x$ and $N_y$, i.e. the cavity $Q$ factor at a large $N_y$ approaches the waveguide $Q$ factor. This is because the waveguide $Q$ factors are calculated by neglecting power losses along the light propagation direction, and the losses are considered to remain unaffected in the microcavity due to the small perturbation. As a result, the maximum $Q$ factor for certain $N_x$ and $N_y$ values can easily be estimated by calculating the waveguide $Q$ factor, which only requires a small amount of computation recourses. This also proves that a low-loss waveguide is crucial for achieving a high $Q$ factor at small $N_x$ and $N_y$ values.

Inside the core region, the microcavity has a field profile that is similar to that of the waveguide, whereas the field quickly decays when penetrating into the cladding unit cells. Profiles of the electrical field amplitude are depicted in Figure 3-5(a) and (b). The quick decaying field proves that the mode frequency is indeed within a waveguide mode gap in the cladding region. Odd mirror symmetry is applied to both the central yz ($x = 0$) and xz ($y = 0$) planes to form this mode. We also check the 3D vector plots of the electric field and confirm that this is a quadrupole mode. The vector plots in the central xy and xz planes are shown in Figure 3-5(c) and (d), respectively. The calculated mode volume is $8.32 \left(\frac{\lambda_0}{2n}\right)^3$, which is similar or slightly smaller than what is typical for 2D photonic crystal slab double-hetero-structure microcavities.
Figure 3-5: The field distributions for mode-c in WG0.7 and the quadrupole mode. (a) The electric field amplitude of mode-c in WG0.7. The supercell size is $7 \times 1 \times 7$. (b) The electric field amplitude of the quadrupole mode in the middle of the xy plane. $a' = 1.067a$, $w_y' = 0.333a$, $N_x = N_z = 7$, and $N_r = 15$. (c) The vector plot of the electric field of the quadrupole mode on the xy plane. (d) Same as in panel c but on the xz plane.
3.2.4 Dipole Mode

We construct a dipole mode by pulling the guiding mode-a down into mode gap $A$. As previously discussed, appropriate line-defect parameters should be chosen to form a low-loss waveguide with a large mode gap. Based on the data depicted in Figure 3-3(c) and (d), the waveguide with $w_x = 0.5a$ has the largest mode gap $A$; however, the guiding mode-a is quite lossy in this case because the mode frequency is near the upper edge of the complete photonic bandgap. On the other hand, the mode-a in the waveguide with $w_x = 0.6a$ has an extremely high $Q$ factor thanks to the mode frequency that is located in the middle of the bandgap, and at the same time, WG0.6 also has a relatively large mode gap $A$. Considering both of these factors, the waveguide defect line width is chosen to be $w_x' = 0.6a$.

A resonant mode with a normalized frequency $a/\lambda_0 = 0.3800$, which is near the middle of the mode gap, is observed when the parameters in the core region are set to be: $a' = 1.2a$, and $w_y' = 0.4a$. Figure 3-7(a) presents the $E_x$ distribution on the $z = 0$ plane. The electrical field distributions of mode-a in the waveguide with $w_x = 0.6a$ and the microcavity mode are compared in Figure 3-6(a) and (b). As modulation increases in the core region, the field penetration into the cladding unit cells becomes small, and the mode is more confined within the core region. Odd and even mirror symmetry is applied to the central $yz$ ($x = 0$) and $xz$ ($y = 0$) planes in order to obtain this mode. The vector plots in the central $xy$ and $xz$ planes depicted in Figure 3-6(c) and (d) confirm it to be a dipole mode. This mode has an extremely small mode volume of $2.88 (\lambda_0/2n)^3$ due to the tight light localization.
Figure 3-6: The field distributions for mode-a in WG0.6 and the dipole mode. (a) The electric field amplitude of mode-a in the middle of the xy plane in WG0.6. The supercell size is $7 \times 1 \times 7$. (b) The amplitude of the electric field in the middle of the xy plane in the dipole mode. $a' = 1.2a$, $w_y' = 0.4a$, $N_x = N_z = 7$, and $N_y = 11$. (c) The vector plot of the electric field of the dipole mode on the xy plane. (d) Same as in panel c but on the xz plane.

Figure 3-7: The properties of the dipole mode based on the waveguide with $w_x = 0.6a$. In the core region, $a' = 1.2a$, and $w_y' = 0.4a$. (a) The $E_x$ distribution in the central xy plane of the cavity. $N_x = N_z = 7$, and $N_y = 11$. (b) The $Q$ factors for different unit cell numbers $N = N_x = N_y = N_z$. It increases exponentially with $N$, and no saturation is observed.
For this dipole mode, the quality factor exponentially increases with structure size. The confinement per one unit cell is estimated to be very similar for all directions, so we equally increase the unit cell numbers in all directions \((N_x = N_y = N_z = N)\). Figure 3-7(b) shows the calculated \(Q\) factor as a function of \(N\). The \(Q\) factor exponentially develops with \(N\) and reaches \(2.9 \times 10^8\) for \(N = 17\). No sign of saturation is observed thanks to the confinement provided by the complete photonic bandgap. In the modeled range, the \(Q\) factor can be approximated by the following equation: 

\[
Q = 10^{1.5214 - 0.4201N}
\]

We notice that the computational error grows for a microcavity with a large number of unit cells and becomes significant when \(N > 17\). The precise evaluation of an ultra-high \(Q\) factor requires large computational resources, and a long evolution time because of the slow decay of the resonant mode energy; however, in the range of analysis, we could confirm the exponential increase of the \(Q\) factor.

In comparison to the quadrupole mode, the dipole mode achieves the same \(Q\) factor in a much smaller microcavity. For example, in order to obtain the \(Q\) factor of one million, about \(11 \times 35 \times 9 = 3465\) unit cells are required for the quadrupole mode, whereas only \(11^3 = 1331\) unit cells are necessary for this new resonant mode. This is explained by two reasons. First, the mode gap \(A\) that is employed in this resonator design is wider than the mode gap \(B\) that is used to construct the quadrupole mode, and the resonant frequency is located deeply in the middle of the gap, resulting in a weak coupling of the microcavity mode into the cladding waveguide. Thus, the power loss in the \(y\) direction is reduced in comparison to the quadrupole mode for the same number of photonic crystal unit cells in the \(y\) direction. Second, the \(Q\) factor of mode-a in WG0.6 is approximately one order of magnitude higher than that of mode-c in WG0.7, indicating small radiation power losses in the \(x\) and \(z\) directions. As a result, a small photonic crystal microcavity is needed to obtain an ultra-high \(Q\) factor in this dipole mode microcavity. Note that the slope of the \(Q\) factor increase is steeper for mode-c in WG0.7 than that for mode-a in WG0.6 because mode-c is close to a midgap point.
Figure 3-8: Properties of the waveguides that are formed via the insertion of one rod of width $w_x$.
(a) The dispersion of the waveguide with $w_x = 0.2a$. (b) The frequency ranges of the mode gap as a function of the inserted rod width. (c) The $Q$ factor of the guiding mode-$d$ for the waveguides with $w_x = 0.1a$ and $w_x = 0.2a$. The waveguide supercell has $N \times 1 \times N$ unit cells.
3.2.5 Monopole Modes

The mode gap approach is applied to the design of monopole modes, which are expected to have the smallest mode volume among the studied modes. The investigation of monopole modes in the complete photonic bandgap would help us understand the fundamental limitation of the $Q$ factor and mode volume. Two types of ultra-high $Q$ monopole modes are designed here: (i) one with a field maximum that overlaps with dielectrics is useful for enhancing light-matter interaction, and (ii) one with a mode that is localized in air or vacuum and has the potential to function as an ultra-compact device to trap atoms, ions or particles by optical fields.

The waveguide that builds the monopole mode with a field maximum at the dielectrics is introduced by adding a rod of width $w_x$ along the $y$ axis. The dispersion for $w_x = 0.2a$ is shown in Figure 3-8(a). The guiding mode above the mode gap has even symmetry regarding the x direction, such that it is potentially suitable for the construction of a monopole mode in the cavity. The frequency range of the mode gap is varied as a function of $w_x$; see Figure 3-8(b). The waveguide with an inserted rod of width $w_x = 0.1a$ has a larger mode gap than that of the waveguide with $w_x = 0.2a$; however, mode-d in this waveguide is more lossy than that in the $w_x = 0.2a$ waveguide; see the $Q$ factor of mode-d in Figure 3-8(c). Therefore, microcavities based on both waveguides are studied. The microcavity geometry is shown in Figure 3-9, wherein $N = 5$, $w = 0.3a$, $h = 0.3a$, $w_x = 0.2a$, $a' = 1.2a$, and $w_y' = 0.5a$. In the 3D FDTD calculation, the mesh resolution is 20.

Monopole modes can easily be identified because an even mirror symmetry condition is applied to the $x = 0$ and $y = 0$ planes. Figure 3-10 depicts some electric field energy profiles of the monopole mode, which has a maximum field in the central dielectric rod.
Figure 3-9: Design of woodpile photonic crystal monopole mode overlapping with dielectrics. The unit cells size is $5 \times 5 \times 5$.

Figure 3-10: Electric field energy distribution of the monopole mode overlapping with dielectrics on the xy, yz, and zx planes that intersect the middle point of the structure with $N = 5$. 
Figure 3-11 depicts the analysis results of the monopole mode. As seen in Figure 3-11(a), there is an optimum $w_y/a$ range for the monopole mode with $w_x = 0.1a$, $a' = 1.2a$, and $N = 15$. At $w_y' = 0.6a$, the $Q$ factor is maximized, and the mode volume is as small as $0.36 (\lambda_0/n)^3 = 2.88 (\lambda_0/2n)^3$. The corresponding normalized resonance frequency is 0.372. The quality factor dependence on the microcavity size $N$ is presented in Figure 3-11(b). For $N = 23$ and $w_x = 0.2a$, the $Q$ factor is 900 million. This design outperforms any 2D photonic crystal resonator design, and would enhance the interaction rate in a solid-state cavity QED system.

Next, a monopole mode overlapping with air or vacuum is studied. The calculated dispersion relation for a waveguide constructed by the removal of one rod from a woodpile photonic crystal is depicted in Figure 3-12. A mode gap exists below a guiding mode with even symmetry. The lattice constant and rod width in the core region are widened such that the guiding mode is lowered into the mode gap region so as to form a cavity mode. The same monopole mode is found for different modulations of unit cells along the $y$ direction. Here, we only show the analysis results for one modulation: $a' = 1.1a$ and $w_y' = 0.35a$; see Figure 3-13 for some views of the resonator structure. The mode with normalized frequency of 0.361 is confirmed to have an electric field maximum that overlaps with vacuum. The electric field energy distributions are displayed in Figure 3-14(a), and the $Q$ factor dependence on the microcavity size $N$ is presented in Figure 3-14(b). For $N = 27$, the $Q$ factor is 65 million. The mode volume is as small as $0.36 (\lambda_0/2)^3$, which is indeed extremely tiny.
Figure 3-11: Modeling results for the monopole mode, in which the field maximum overlaps with dielectrics. (a) The $Q$ factor, mode volume, and normalized frequency as a function of $w_y/\alpha$ for $w_x = 0.1\alpha$ and $N = 15$. (b) The quality factor vs. the unit cell number $N$ for some different size variables with the monopole mode overlapping with dielectrics. The inset depicts the $E_z$ component on the central $xy$ plane.

Figure 3-12: The dispersion of a woodpile waveguide formed by the removal of one rod.
Figure 3-13: Design of a woodpile photonic crystal monopole mode that has field maximum overlapping with air or vacuum. The unit cells size is 5×5×5. The parameters in the core region are: \( a' = 1.1a \) and \( w_y' = 0.35a \).

Figure 3-14: The properties of the monopole mode overlapping with vacuum. (a) The electric field energy distributions on the xy, yz, and zx planes that intersect the middle point of the structure with \( N = 7 \). (b) The \( Q \) factor vs. the microcavity size \( N \). The inset depicts the \( E_z \) component on the central xy plane.
This monopole mode microcavity is potentially useful for the optical trapping of particles because the majority of the fields reside in the $n = 1$ medium, and all of the dielectric rods that form the cavity are straight. Particles may be dropped from a rod opening on the side of the microcavity toward its center. In order to evaluate the optical trapping capability of this structure, we calculate the forces that are induced by the monopole mode field. Using a monochromatic field and dipole approximations, the cycle-averaged force [58] is represented by

$$\langle \vec{F} \rangle = \sum_{i=x,y,z} \langle \mu \nabla E_i \rangle$$

(3.1)

where the dipole moment $\mu_i$, and electric field $E_i$ are

$$\mu_i = \text{Re}\left[ \alpha \hat{E}_i(\vec{r}) e^{-i\omega t} \right]$$

(3.2)

$$E_i = \text{Re}\left[ \hat{E}_i(\vec{r}) e^{-i\omega t} \right].$$

(3.3)

The modal field is assumed to be unchanged due to the existence of a particle. The time-independent electric field $\hat{E}(\vec{r})$ can be expressed as a product of the amplitude $E_0(\vec{r}) \in \mathbb{R}$ and a unit polarization vector $\vec{n}(\vec{r}) \in \mathbb{C}$; hence, the force can be written as

$$\langle \vec{F} \rangle = \frac{1}{2} \sum \text{Re}\left[ \alpha \hat{E}_i(\vec{r}) \nabla \hat{E}_i^*(\vec{r}) \right]$$

$$\quad = \frac{1}{2} \alpha_\kappa E_0(\vec{r}) \nabla E_0(\vec{r})$$

(3.4)

$$\quad + \frac{1}{2} \alpha E_0^2(\vec{r}) \sum \left[ \text{Re}\left\{ \vec{n}_i(\vec{r}) \right\} \nabla \text{Im}\left\{ \vec{n}_i(\vec{r}) \right\} - \text{Im}\left\{ \vec{n}_i(\vec{r}) \right\} \nabla \text{Re}\left\{ \vec{n}_i(\vec{r}) \right\} \right]$$

where the polarizability $\alpha = \alpha_\kappa + i\alpha_\epsilon$ ($\alpha_\kappa, \alpha_\epsilon \in \mathbb{R}$). The first and second terms in the right hand side represent the dipole and scattering forces, respectively. In the analyzed mode, the dipole force is dominant, so only the dipole force is considered in the following discussion. There are two electric field amplitude maxima for this mode. The dipole force is directing to these two points, and a passive particle nearby can be trapped around one point; see Figure 3-15 as an example of the optical force near one maximum electric field point. We confirmed this force direction three-dimensionally.
3.2.6 Discussion

Our study demonstrates that the properties of waveguide modes and the mode gap value appear to be determinant factors for characteristics of the proposed woodpile microcavity designs. It is essential to study low-loss 3D photonic crystal waveguides with a large mode gap inside the complete photonic bandgap for the tight 3D confinement of light. The modeling results confirm that the $Q$ factor exponentially increases with the number of unit cells in the range of analysis for all types of mode designs. As expected, the 3D photonic crystal microcavities that are formed in the complete band gap are extremely low-loss, even for a small mode-volume mode. We may not need to compromise the mode volume to increase the figure of merit.
Figure 3-16: The resonator $Q$ factor and mode volume for a different amount of unit cell size modulation. The waveguide has a line defect $w_x = 0.5a$, and the parameters ($a'$, $w_y'$) in the core region are shown on the top axis. The unit cell size of these structures is $9 \times 9 \times 9$.

Table 3-1: Comparison of the properties of woodpile microcavities. The point-defect mode microcavity is formed via the addition of dielectric materials of size $0.85a \times 0.425a$ at one rod as shown in Figure 3-1(b) (Ref. 52).

<table>
<thead>
<tr>
<th></th>
<th>Quadrupole</th>
<th>Dipole</th>
<th>Monopole in dielectric</th>
<th>Monopole in air</th>
<th>Point-defect mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of unit cells for $Q \sim 1 \times 10^5$</td>
<td>$11 \times 35 \times 9$ (3,465)</td>
<td>$11^3$ (1,331)</td>
<td>$&lt; 17^3$ (&lt;4,913)</td>
<td>$20^3$ (8,000)</td>
<td>$29 \times 11 \times 20$ (6,380)</td>
</tr>
<tr>
<td>Mode volume $((\lambda_0/2n)^3)$</td>
<td>8.32</td>
<td>2.88</td>
<td>2.88</td>
<td>0.36</td>
<td>-</td>
</tr>
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</table>
Here, we discuss the impact of modulation size on the cavity $Q$ factor and mode volume by analyzing a dipole mode in a waveguide with $w_x = 0.5a$. The waveguide with a defect rod width of $w_x = 0.5a$ is selected because it has the largest mode gap $A$, which ranges from 0.3576 to 0.4035, in the analyzed defect width range. A large mode gap allows one to widely swing the modulation; thus, it helps one observe the full development of the performance of the cavity mode. As the unit cell modulation is gradually strengthened, the resonant frequency is lowered, as expected (Figure 3-16). The $Q$ factor is high for the modes that are located deep inside the mode gap, and it decreases quickly as the mode frequency become close to one of mode gap edges. Modes formed by a small modulation, as explained in Section 3.2.2, are still coupled to the cladding waveguide due to a small potential barrier, so the loss along the waveguide direction is dominant. The mode is elongated, and the mode volume is large as in the case for the mode with a resonant frequency of 0.4028 in Figure 3-16. As the mode frequency decreases, the coupling to the cladding waveguide also decreases, and the mode becomes well confined in a small mode volume. For large modulation, the photonic crystals in the core region are distorted, and the mode is near the lower edge of the mode gap such that the $Q$ factor decreases. Except for the highest frequency mode, all of the other modes have very similar mode volume, which is approximately $3.0 \left(\lambda_0/2n\right)^3$. The mode volumes of higher $Q$ factor modes are slightly larger than those of modes with lower $Q$ factors.

In order to understand the strength of optical confinement in the designed microcavities, we compare our resonant modes (quadrupole, dipole, and monopole modes) to the previous design with a single local defect (the single-mode in Ref. 52). Two factors are considered: the structure size at the same $Q$ factor ($Q \sim 10^6$ in the table) and the mode volume. The results are listed in Table 3-1. Except for the monopole mode in air, all of the other modes require fewer unit cells than the single-mode cavity in order to produce a $Q$ factor of one million. This could, for example, increase the device density of 3D integrated optics and also simplify fabrication requirement. The dipole mode requires the smallest microcavity size because it is pulled down into the middle of a wide mode gap, and the waveguide used therein has an extremely small out-of-propagation
loss. In term of mode volume, the monopole in air has the smallest volume, which is $0.36 (\lambda_0/2)^3$.

### 3.3 Woodpile Microcavity Fabrication

The ultra-high-$Q$ woodpile photonic crystal microcavities designed in Section 3.2 are unique in that all of the dielectric rods are straight in the microcavities. Identical to unmodified woodpile photonic crystals, these microcavities can be decomposed into two sets of dielectric rods. Therefore, these microcavities can be fabricated with the multi-directional etching methods discussed in Chapter 2. This way, we can fabricate woodpile microcavities of various crystal orientations.

The fabrication procedures for the designed microcavities are the same as those for periodic photonic crystals, except for some changes in the EBL 2D patterns. Here, we consider the fabrication of the dipole mode microcavity with a (110) surface in GaAs as an example. The microcavity is shown in Figure 3-17(a). If the microcavity is rotated such that the (110) crystal plane overlaps the wafer surface, the 2D patterns on the wafer surface depicted in Figure 3-17(b) result: the blue rod indicates a wide rod in the waveguide, whereas the orange rods indicate lattice size modulation along the $x'$ direction. All of the other procedures, including EBL, dry etching, and alignment, are the same for fabricating photonic crystals without intentional disorders. The optical microscopy image of a woodpile photonic crystal microcavity with $40 \times 55 \times 2.25$ unit cells is shown in Figure 3-18(a), wherein the modulation position is indicated by the arrow, and the interference color changes caused by modulation are clearly seen. The planar and cross-sectional SEM images of the microcavity are depicted in Figure 3-18(b) and (c). Active materials could be included inside the microcavity by fabricating the designed microcavity in a QW or QD wafer.
Figure 3-17: The schematics of the fabrication of the dipole mode microcavity using the two-top etching method. (a) A proposed GaAs-based woodpile photonic crystal microcavity defined in an epitaxially-grown wafer with an active material layer indicated by the green region. The blue rod is a wide rod that forms a waveguide, and the applied unit cell length modulation is indicated by the period of $\sqrt{2}a'$. At the intersection of the waveguide and the modulation, a microcavity is formed. (b) The 2D patterns that formed on the intersection of the woodpile microcavity in panel a with the wafer surface.
Figure 3-18: Fabricated dipole mode microcavity on a GaAs wafer. (a) An optical microscope image of the microcavity surface. The arrow indicates the position of the unit cell length modulation. (b) Electron micrograph of the microcavity surface. (c) Electron micrograph of the cross-section of the microcavity.

Figure 3-19: The quality factors of the dipole mode microcavity as a function of the number of unit cells in each direction.
As explained in Section 2.3.3, the number of unit cells in the $z'$ direction is constrained for woodpile structures that are fabricated by the two-top etching method. There are too few unit cells in $z'$ direction to form a high-$Q$ microcavity; hence, the resonance peak is not clearly observed inside the bandgap when we measure the reflectance spectra. The one-top, one-side etching method is anticipated to produce a microcavity with enough unit cells and form a high-$Q$ resonance. The fabrication of a GaAs microcavity with (100) and (010) surfaces is under investigation. For example, for a dipole mode at a 1.0 μm wavelength, the lattice constant is 380 nm, so that 3.42 μm deep etching generates a microcavity with nine unit cells in the two etching directions (the x and y axes). The number of unit cells in the $z$ direction would be large in this fabrication method. The calculated $Q$ values exceed $10^5$ for a dipole mode with $9 \times 9 \times N$, where $N$ is a large number that indicates the number of unit cells in the $z$ direction. The fabricated microcavity is expected to have a high quality factor.

### 3.4 Woodpile Microcavity with Metal Contacts

High-$Q$ microcavities with metal electrodes would benefit photonic devices, such as current injection microlasers; however, when the metallic materials overlap with the optical field, they deteriorate the resonance due to the absorption loss. The optical confinement provided by total internal reflection has non-negligible field components at the interface of a change in refractive index. Except for 3D photonic crystal microcavities, other types of microcavities use total internal reflection at all or some directions, so direct metal contacts at these microcavities would degrade the optical confinement. As a result, the past current-injection microcavities use indirect metal contacts to save the resonance [10], resulting in complex structures and a large resistance.
Figure 3-20: Metal clad woodpile dipole mode microcavity. (a) The geometry. (b) The $Q$ factor for different cladding materials and structure size.

Figure 3-21: Metal clad 2D photonic crystal L3 microcavity. (a) The geometry. (b) The $Q$ factors vs. number of layers for different cladding materials.
Our approach to form high-$Q$ photonic crystal microcavities with metal electrodes is to use 3D photonic crystal microcavities, wherein light is omni-directionally confined by Bragg reflection. The resonant modes are localized in the cavity center, and significantly decay in the cladding region of the microcavity. For a microcavity with a sufficient large number of unit cells, the field is negligible on the surface of the microcavity. Absorptive metallic materials can be directly placed on the surface without affecting the quality factor because of almost no overlapping between the metal and the resonant field; however, it is difficult to make such large 3D microcavities. We demonstrate that a high quality factor is feasible even in a relatively small 3D microcavity with metal cladding.

Two metallic materials are considered in our analysis: gold, which represents lossy metals, and indium tin oxide (ITO), which is a conductive material with a low absorption. The metallic materials have a complex-valued permittivity $\varepsilon_m = \varepsilon_{m1} + i\varepsilon_{m2}$ (complex-valued reflective index $n_{mc} = n_m + ik_m$). The complex permittivity of gold is $\varepsilon_m = -117 + 11.8i$ ($n_{mc} = 0.55 + 10.8i$) at around $\lambda_0 = 1550$ nm. For ITO at $\lambda_0 = 1200 - 1300$ nm, $\varepsilon_m$ is between $1 + 0.1i$ and $1 + 0.3i$.

We evaluate the practicability of metal clad woodpile microcavities by calculating the quality factor at different microcavity sizes. The dielectric resonator in this study is the woodpile dipole microcavity that is discussed in Section 3.2.4. Direct metal contacts are placed at both ends of the microcavity in the $x$ direction, as displayed in Figure 3-20(a). The calculated $Q$ factors for different metallic materials are shown in Figure 3-20(b), wherein a no metal contact case (air-cladding) is also listed for comparison. The $Q$ values do not appreciably decrease thanks to the small field that overlaps with the metallic materials. Even with the very lossy gold electrodes, the $Q$ factor achieves more than $8 \times 10^4$ in a resonator with nine unit cells in each direction.

For comparison, we analyze a 2D photonic crystal slab microcavity that is clad with the same metallic materials. The photonic crystal slab microcavity is formed by omitting three air holes—the so-called L3 microcavity. The structural parameters for the
L3 microcavity are: radius of the holes $r = 0.3a_{L3}$, slab thickness $d = 0.9a_{L3}$, and the adjacent holes shift $s = 0.2a_{L3}$, where $a_{L3}$ is the in-plane lattice constant. Metallic materials are placed at both the bottom and the top of the slab; see Figure 3-21(a). For gold electrodes, the $Q$ factor saturates at around 60. It is possible to slightly increase the $Q$ factors in the L3 microcavities with low-loss conductive contacts, such as ITO; see Figure 3-21(b). The $Q$ factor saturates quickly because of the absorption from the contact material. For $\varepsilon_m = 1 + 0.1i$, the maximum quality factor is about 800 so that lasing action would be possible with careful fabrication processes (Appendix A summarizes the fabrication of the 2D photonic crystal slab microcavities with ITO contacts on the bottom and the top of the slab); however, the quality factor decreases to only about 400 with a small increase in the imaginary part of the permittivity ($\varepsilon_m = 1 + 0.2i$).

For 2D photonic crystal slab microcavities with metal contacts, the choice of metallic materials is limited, whereas 3D photonic crystal microcavities do not have such limitations. We can choose any metals as electrodes, regardless of their absorption. This advantage makes 3D photonic crystal microcavities a promising candidate for building current injection devices, such as nanolasers and modulators, with simple configurations.

3.5 Hybrid 3D-2D slab-3D Microcavity

3.5.1 Introduction

In this section, we demonstrate another method to realize omni-directional light confinement with a hybrid 3D-2D slab-3D microcavity. In Section 3.2, we have designed ultra-high-$Q$ resonant modes inside a complete photonic bandgap by the modulation of a woodpile lattice. Complete bandgap materials act like a perfect mirror for light waves with frequencies that are inside their bandgap, i.e. light is reflected regardless of the incident direction. Optical components based on planar photonic crystal slab, including microcavities and waveguides, suffer from radiation loss through the escaping light cone. By placing a woodpile photonic crystal on the top and bottom of the slab, we expect to obtain omni-directional light confinement when the mode frequency is inside the
complete bandgap of the cladding woodpile structures. This may provide a simple way of improving the optical confinement of 2D photonic crystal devices without complicated designs.

The early development of planar photonic crystal microcavities requires a substantial amount of design resources due to trial and error approaches. Simple microcavity designs, such as single-defect microcavities, tend to show low $Q$ factors with a maximum value at about 2,000. The quality factor can be improved using sophisticated designs, for example, by introducing line defects [59], and using L3 (three holes missing) microcavities with two-hole shifting [60], etc. The increase in $Q$ factor is explained by the reduction of the field components inside the escaping light cone. A momentum space Fourier transform method is reported to quantitatively analyze the field components inside the light cone [19, 59-61], and some inverse methods are proposed so as to reduce the loss inside the light line without trial and error. These efforts further raise the $Q$ values; however, these can only decrease to some extent, but not eliminate the power radiation loss into the escaping light cone. As a result, even with sophisticated designs [22, 23, 60], the $Q$ factor of 2D slab microcavities can only be increased to some extent, and still saturate for finite photonic crystal unit cells. In addition, the mode volume is large for high-$Q$ microcavities [19, 22, 23, 60], i.e. one obtains a high quality factor at the expense of a large mode volume, resulting in a limited choice in the mode volume. Another approach is to clad the slab microcavity with distributed Bragg reflectors (DBR) [62, 63] on the top and bottom of the slab; however, this quasi-3D photonic crystal, which is 1D-2D slab-1D hybrid microcavity, does not have omni-directional optical confinement, and ultra-high quality factor has not been demonstrated.
Figure 3-22: The L1 cavity and the y-dipole mode. (a) Schematic of the L1 cavity without the woodpile cladding. There are five layers in both the x and y directions for optical confinement. (b) The $H_z$ distribution in the middle of the xy plane in the slab. (c) The amplitude of the electric field in the middle of the xz plane.

Figure 3-23: Hybrid microcavity and the y-dipole mode. (a) Schematic of the hybrid microcavity that is constructed by cladding the L1 cavity with woodpile photonic crystals on the top and bottom sides of the slab. The woodpiles are stacked along the x direction. There are five layers in the slab. Each woodpile photonic crystal has $6 \times 6 \times 5$ unit cells. The gap size g is $0.05a_2D$. (b) The $H_z$ distribution in the middle of the xy plane in the slab. (c) The amplitude of the electric field in the middle of the xz plane.
3.5.2 Approach

A 3D photonic crystal with a complete bandgap provides three-dimensional confinement. We expect to reduce the vertical radiation loss in the planar photonic crystal components by cladding the slab with 3D photonic crystals. Chutinan et al. [64] sandwiched an intermediate layer with 3D photonic crystals for lossless 3D integrated optics. Instead of this intermediate layer, we use the available microcavities [22, 23, 60], or straight or bended waveguides [65] based on a 2D photonic crystal slab. The objective is to recycle simple 2D slab designs and improve the vertical optical confinement without requiring substantial computational resources.

3.5.3 Hybrid Microcavity Design

The hybrid structures are constructed by cladding 2D slab nano-optical devices with 3D photonic crystals, which have complete photonic bandgaps that overlap with the mode frequency of the 2D slab optical components. Here, we demonstrate the enhancement of $Q$ factor by using some simple but low-$Q$ 2D microcavity design—a 2D slab triangular lattice photonic crystal missing a single hole, i.e. the so-called L1 cavity [21].

The L1 cavity exhibits a small mode volume with a low quality factor because a large portion of the Fourier-transformed field component resides inside the escape light cone in the momentum space. The L1 cavity analyzed in this work has a slab thickness of $d = 0.95a_{2D}$ and a hole radius of $r = 0.3a_{2D}$, where $a_{2D}$ is the lattice constant of the 2D slab photonic crystal. The refractive index of the slab is 3.4. Figure 3-22(a) illustrates the structure of the L1 cavity. In the 3D finite-difference time-domain analysis [55], we selectively excite the y-dipole mode with a mode frequency of $0.271(c/a_{2D})$, where $c$ is the velocity of light in vacuum. The field distributions are mapped in Figure 3-22(b) and (c). The saturated quality factor, which is determined by the radiation loss in the vertical direction to the slab, is as low as 205 [see the data indicated by blue diamonds in Figure 3-24(b)], but the mode volume is as small as $2.9 (\lambda_0/2n)^3$, where $\lambda_0$ is the mode wavelength in vacuum.

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We consider three design factors when placing woodpile photonic crystals on the top and bottom sides of the slab to form a hybrid microcavity. First, we match the mode frequency with the midgap of the woodpile with an appropriate choice of the lattice constant \( a_{wp} \) of the woodpile photonic crystal. For a woodpile with a dielectric material index \( n = 3.4 \), rod width \( w = 0.3a_{wp} \), and rod height \( h = 0.3a_{wp} \), the complete photonic bandgap ranges between \( 0.35(c/a_{wp}) \) and \( 0.43(c/a_{wp}) \). Assuming little change in the mode frequency induced by placing the woodpile on the top and bottom surfaces of the L1 cavity slab, we choose \( a_{wp} = 1.5a_{2D} \) such that the mode frequency, which is approximately \( 0.271(c/a_{2D}) \), is inside the band gap \([0.23(c/a_{2D}), 0.29(c/a_{2D})]\). Second, we may choose an arbitrary crystal orientation of the woodpile photonic crystal relative to the 2D slab thanks to the omni-directional band gap. Here, we choose the x axis as the woodpile stacking direction. Third, we choose the gap size \( g \) between the slab and its nearest surface of woodpile photonic crystal. We vary the gap size and study the effect of the value \( g \) on the performance of the 3D-2D slab-3D hybrid microcavity.

Figure 3-23(a) depicts the structure of the 3D-2D slab-3D hybrid microcavity. The structure size is defined by the number of 2D slab unit cells in the x and y directions \( (N_{x,2D} \text{ and } N_{y,2D}) \) and the number of woodpile unit cells on each side in the x, y, and z directions \( (N_{x,wp}, N_{y,wp}, \text{ and } N_{z,wp}) \). In the 3D FDTD calculation, the structure size \( N \) is chosen to be \( N = N_{x,2D} = N_{y,2D} = N_{z,wp} \). Because the lattice constant of the 2D slab can differ from that of woodpiles, the number of unit cells is not necessarily the same for the 2D slab and the woodpile in the x or y directions; instead we choose \( N_{x,wp} = \text{Round}\left[a_{2D} \cdot N_{x,2D} / (2h)\right] \) and \( N_{y,wp} = \text{Round}\left[\sqrt{3}a_{2D} \cdot N_{y,2D} / a_{wp}\right] \) such that the woodpile covers the 2D slab photonic crystal area.

We first analyze the effect of gap size between the slab and the woodpile on the quality factor of the y-dipole mode. The mode frequency is slightly lowered as the gap size is decreased, as shown in Figure 3-24(a); however, the mode symmetry is preserved. Figure 3-23(b) and (c) depict the \( H_z \) component in the middle of the xy plane and the amplitude of the electric field in the middle of the xz plane, respectively. Figure 3-24(b)
depicts the quality factor of the hybrid microcavity as a function of structure size $N$ for different gap sizes. Except for a small $N$ (e.g. $N = 3$), the confinement apparently improves more when using woodpile photonic crystal cladding in comparison to that without cladding (i.e. $g = \infty$). For $N = 3$, the quality factor is independent of the value of $g$ because the radiation loss dominates in the planar directions of the slab, and the quality factor is not significantly altered by the cladding woodpile. For the same $N$, as the value of $g$ decreases, the quality factor first increases due to the reduced power loss through the gap. The quality factor reaches a maximum value at $g = 0.05a_{2D}$ and decreases slightly as we further reduce the gap size to 0, i.e. the woodpile photonic crystals touch the slab. This is probably because the perturbation is stronger for $g = 0$ than for $g = 0.05a_{2D}$. For large values of $g$, the quality factor saturates as $N$ increases, such as in the case of $g = a_{2D}$ [see the green triangles in Figure 3-24(b)]. On the other hand, if the gap size is sufficiently small, the quality factor exponentially increases without any sign of saturation as the unit cells number $N$ increases. This is evidence of optical confinement owing to the complete photonic band gap. For both the $g = 0$ (black squares) and $g = 0.05a_{2D}$ (red circles) cases, the quality factor can exceed $10^5$ such that, the hybrid microcavity is robust in terms of the gap size in the analyzed range. The hybrid microcavity also preserves the small mode volume: $3.0 (\lambda_0/2n)^3$ for both $g = 0$ and $g = 0.05a_{2D}$; see Figure 3-24(c). Thus, a high quality factor with a similar mode volume is demonstrated. Even a large gap example ($g = a_{2D}$) exhibits the $Q$ improvement.

In order to examine the origin of the $Q$ improvement, we calculate the Fourier-transformed $H_z$ component near the surface of the slab for both $g = \infty$ and $g = 0.05a_{2D}$ in Figure 3-25(a) and (b), respectively. The scattering is slightly enhanced, but the overall pictures are similar to one another, and there are no significant differences in the sum of the Fourier-components inside the escaping light cone. Therefore, we understand that the quality factor is enhanced by the complete photonic band gap and not by removing components from the inner region of the escaping light cone.
Figure 3-24: The characteristics of the hybrid \((g < \infty)\) and L1 \((g = \infty)\) microcavities. (a) The y-dipole mode frequency for different gap and structure sizes. The frequency is reduced by 3.7% for \(g = 0\) in comparison to \(g = \infty\). (b) The quality factor. (c) The mode volume. The structure size is \(N = N_{x,2D} = N_{y,2D} = N_{z,wp}\).

Figure 3-25: The Fourier-transformed \(H_z\) component near the surface of the slab. (a) The L1 cavity. (b) The hybrid cavity with \(g = 0.05a_{2D}\). The black circle indicates the light cone.
The radiation loss due to failure of the total internal reflection in the slab can be suppressed via the sandwiching of the 2D slab with 3D photonic crystals. By cladding woodpile photonic crystals on the top and bottom sides of the L1 cavity, we can increase the quality factor from 205 to more than $10^5$ without complicated redesigning, thanks to the complete photonic band gap. This method is applicable to other lossy 2D slab photonic crystal microcavity and waveguide designs to improve optical confinement while maintaining mode properties such as mode symmetry and mode volume.

3.6 Summary

We demonstrate the uniqueness of the complete bandgap in 3D photonic crystals in terms of omni-directional light confinement. Ultra-high-$Q$ resonant modes are confirmed both in woodpile photonic crystal microcavities and in a hybrid woodpile-2D slab-woodpile microcavity. The latter provides a simple means to improve light confinement in 2D photonic crystal slab devices.

The microcavities formed by unit cell length modulation have several advantages. First, the mode is inside the complete photonic bandgap such that an ultra-high-$Q$ and a small volume can be simultaneously obtained. Second, the microcavity geometries are unique in that they consist of only straight rods. This ensures that the designed microcavities can potentially be implemented using directional etching fabrication methods. We could also fabricate the designed microcavities with various crystal orientations and planes. Third, the direct placement of metal electrodes on the microcavities does not degrade the quality factor, indicating the possibility of current injection 3D photonic crystal microlasers.
Chapter 4
Design of 3D Photonic Crystal Waveguides

Three-dimensional photonic crystal waveguides potentially have two major advantages in comparison to other types of photonic crystal waveguides. First, the propagation loss is expected to be reduced thanks to the complete photonic bandgap in 3D photonic crystals. Second, the 3D geometries make inter-level guiding possible and efficiently use a 3D space. This could reduce the footprint and increase the connections, thus, enhancing the functionalities of 3D integrated optics. We utilize two schemes to guide light in woodpile photonic crystals: self-collimation and photonic bandgap effect.

4.1 Self-collimation in a Double-hetero-junction Woodpile Structure

Self-collimation is a collimated light propagation effect without lens optics, which results from the unique dispersion characteristics of photonic crystals. The group velocity is defined by \( v_g = \frac{\partial \omega}{\partial k} \). The direction of energy flow is vertical to the equi-frequency contour, which is a mapping of angular frequencies \( \omega \) in momentum space. Therefore, when the equi-frequency contour is straight in some frequency and \( k \)-vector ranges, light propagates toward one direction without divergence, i.e. the light beam is self-collimated without a lens. Witzens et al. [66] reported self-collimation in square lattice planar photonic crystals, and self-collimation is also studied in 3D photonic crystal based on simple-cubic and woodpile geometries [67-69]. For example, the equi-frequency contours of the third band in the \( k_yk_z \) plane and the second band in the \( k_xk_y \) plane are shown in Figure 4-1. Some portions of the contours are straight such that light could propagate without divergence in the directions indicated by the arrows.
Figure 4-1: The equi-frequency contour of a woodpile photonic crystal. (a) The contour of the 3\textsuperscript{rd} band in the $k_x,k_y$ plane. (b) The contour of the 2\textsuperscript{nd} band in the $k_x,k_z$ plane.

Figure 4-2: A one-dimensionally modulated woodpile structure and the associated dispersion relation. (a) A woodpile structure modulated in the $y$ direction. The supercell size is $1 \times 9 \times 1$. (b) The dispersion relation. The shaded region indicates the edge of the complete band gap. (c) The equi-frequency contour of the lowest band in panel b in the ($k_y, k_z$) plane. The arrows indicate the direction of the collimated beam. (d) The equi-frequency contour of the second lowest band in panel b in the ($k_y, k_z$) plane.
We find self-collimation waveguide modes in a double-hetero-junction woodpile photonic crystal. To our best knowledge, self-collimation has only been investigated in photonic crystals without disorders. The dispersion of the photonic crystal determines the self-collimation properties such as the correlation between the allowed incident direction range and the propagation direction. We study self-collimation in a one-dimensionally modulated woodpile photonic crystal, which is the slab-like structure depicted in Figure 4-2(a). This combines photonic bandgap with self-collimation so as to provide the 2D confinement of light propagation.

The slab-like woodpile structure provides a 1D waveguide, which is formed by modulating the central unit cell in the x axis to have a lattice constant of \( a' \) and rod width of \( w' \). The central modulated unit cell is called the core region, whereas the other unit cells form cladding regions. The dispersion relation with the parameters of \( a' = 1.5a \) and \( w_x' = 0.45a \) is displayed in Figure 4-2(b), wherein the k-vectors \((k_x, k_y, k_z)\) in units of \( 2\pi/a \) are along the \((0,0,0.5)\) to \((0,0,0)\) to \((0,0.5,0)\) directions. This band diagram depicts the guided modes inside of the complete photonic bandgap of the cladding region. The modes propagate inside the core region along the yz plane and exponentially decay in the cladding regions toward the x direction. Therefore, this planar waveguide provides 1D confinement for all of the modes that are induced inside of the bandgap. The equi-frequency contours are then mapped in \( k_y k_z \) space for these guiding bands. Figure 4-2(c) depicts the equi-frequency contour for the lowest band [the black solid line in Figure 4-2(b)]. The contour becomes flat in a wide region that ranges from \((k_y, k_z) = (\pm0.25, -0.5)\) to \((\pm0.25, 0.5)\), which is indicated as an arrow, and the self-collimated light propagates in the y direction.

**4.2 Waveguide Modes by 2D Unit Cell Modulation**

The reported photonic crystal waveguides are built via the introduction of line defects, which bring photonic modes into the bandgap. Based on 2D photonic crystal slab geometry, straight and bended waveguides [70, 14] have been demonstrated. Due to the
imperfection of total internal reflection, the radiation loss cannot be efficiently suppressed in the direction that is perpendicular to the slab. Another challenge is to guide light into a different layer, i.e. only the planar direction could be utilized; thus, it is difficult to increase the optical component density using 2D photonic crystal slab waveguides. Three-dimensional photonic crystals may resolve these challenges because of the possibility of multi-level optical signal routing and efficient light confinement by the complete photonic bandgap effect. A few groups, including the Noda Group, have reported single-mode 3D photonic crystal waveguiding in a complete photonic bandgap. These single-mode waveguides are designed by the removal [71, 72] or addition [57] of a single rod or segments of rods in the woodpile structure [18]. L-shaped woodpile photonic crystal waveguides were designed by combining line defects in two orthogonal directions. They include 90° bends from the xy plane to the stacking direction (z axis) [71, 73]. Previous research on 3D photonic crystal waveguides has been focused on the investigation of guided modes. Some important characteristics of the designed waveguides, such as group velocity, and group velocity dispersion, have not been considered.

Single-mode 3D waveguides are designed by a method of two-dimensionally modulating the unit cells in the woodpile photonic crystals toward the horizontal or vertical directions. For each waveguide, we calculate the dispersion relation, group velocity, and group velocity dispersion, and we visualize the field distributions. The waveguide dispersion relations are computed via the 3D plane-wave expansion (PWE) method, wherein Bloch boundary conditions are applied to all of the walls of a supercell. In the non-propagation direction, five unit cells are used in this study to ensure that the guided modes sufficiently decay near the boundary in the non-guided directions and that the mode coupling at boundaries is suppressed. The supercell has $1 \times 5 \times 5$ unit cells for a lateral waveguide along the x direction, and $5 \times 5 \times 1$ for a vertical waveguide along the z direction. The resolution is set to 30 points per lattice constant, which corresponds to approximately 75 points per wavelength. The woodpile unit cell has the same parameters as that discussed in Chapter 2, i.e. $w = 0.3a$, $h = 0.3a$, and $n = 3.4$. From the numerically
obtained dispersion relation, the group velocity \(v_g\) and group velocity dispersion \(D_w\) are calculated. The group velocity dispersion defined by

\[
D_w = -\frac{2\pi c}{\lambda^2} \frac{d^2}{d\omega^2} = \frac{2\pi c}{v_g^2 \lambda^2} \frac{d^2 v_g}{d\omega^2}
\]  

(4.1)

measures the pulse spreading \((\Delta t)\) per unit bandwidth \((\Delta \lambda)\) per unit distance travelled. The units of ps/nm/km are typically used for optical fibers. Low group velocities and small dispersions are desired characteristics for applications that require slow light and large bandwidth, for example, an optical delay line and memory.

Both horizontal and vertical waveguides consist of only straight and connected rods; therefore, they could be fabricated using the directional etching methods discussed in Chapter 2.

### 4.2.1 Lateral Waveguide

In the lateral waveguide, the modulation is applied to the unit cells in both the x and z directions; see Figure 4-3(a) for the supercell, which repeats in the y direction. The middle unit cells in the y direction are widened such that \(a' = 1.2a\) and \(w_x' = 0.4a\), whereas the rod height in the central unit cells in the z direction are increased so as to achieve \(h' = 0.367a\). The dispersion relation of this structure is shown in Figure 4-4(a). This way, the bands are pulled down into the complete bandgap of the surrounding unit cells. Note that the lowest band is a single mode in the normalized frequency ranging from 0.3951 to 0.4060. The mode profile of the lowest band is drawn in Figure 4-3(b), and the field is confined inside the central unit cell in the xz plane. With the modulation size fixed in the x direction, we vary the rod height in the z direction and analyze the frequency ranges of single mode operation [Figure 4-4(b)]. The group velocity and the group velocity dispersion of the single mode are shown in Figure 4-5(a) and (b) for the waveguide with \(h' = 0.367a\). Small group velocities are achieved in the designed waveguide such that it might be used for enhancing light-matter interaction.
Figure 4-3: Lateral waveguide structure and mode profile. (a) The geometry of the lateral waveguide that is formed by modulating the unit cells in the x and z directions. The parameters of the central unit cell are $a' = 1.2a$ and $w_y = 0.4a$ in the x direction and $h' = 0.367a$ in the z direction. The propagation is along the y direction. (b) The $E_z$ component of the lowest band at central the xz plane.

Figure 4-4: The band structure of the lateral waveguide. (a) The dispersion relation of the lateral waveguide with $a' = 1.2a$, $w_y = 0.4a$, and $h' = 0.367a$. The shaded region indicates the edge of the complete band gap. Note the lowest band has a single mode region. (b) The single mode ranges as a function of $h'/a$, wherein $a' = 1.2a$, $w_y = 0.4a$. 
Figure 4-5: The group velocity and the group velocity dispersion of the lowest guiding band in the lateral waveguide. (a) The group velocity. (b) The group velocity dispersion.

Figure 4-6: The dispersion relation of the vertical waveguide. The shaded region indicates the edge of the complete band gap. The single mode is in the range (0.3849, 0.3876).
4.2.2 Vertical Waveguide

A waveguide propagating in $z$ direction is formed by modulating the unit cells along the $x$ and $y$ directions in a woodpile photonic crystal. The parameters in the central unit cells are $a' = 0.8a$, and $w' = 0.167a$ in both the $x$ and $y$ directions. When the unit cells are decreased, the bands are pushed up into the complete bandgap of the cladding unit cells. The dispersion of this waveguide is displayed in Figure 4-6. The single mode region is narrow in frequency. We find that the bands positions are sensitive to the rods width in the core region. By changing the rods width, we believe that the single-mode range can be widened.

4.3 Summary

Two types of three-dimensional photonic crystal waveguides are designed: self-collimation in a modulated woodpile photonic crystal and waveguides formed by unit cell size modulation in two dimensions. Both the lateral and vertical propagation directions are demonstrated. Low-loss and small $D_n$ optical interconnect devices may be realized on the developed waveguiding system.
Chapter 5
Conclusions and Future Prospects

5.1 Conclusions

We examined subwavelength-scale light localization via the complete photonic bandgap in 3D woodpile photonic crystals with a combination of multi-directional etching method and mode gap design approach.

We fabricated woodpile photonic crystals of different crystal orientations with multi-directional etching methods. We demonstrated that multi-directional etching is a simple two-patterning and two-etching procedure to make woodpile photonic crystal with high precision because the only one pattern alignment is required with high-resolution EBL overlay process. By changing the dry etching directions, we could vary the crystal orientations of the fabricated photonic crystal. GaAs woodpiles with (110) surface planes, and both silicon and GaAs woodpiles with (100) and (010) planes were fabricated. The GaAs woodpiles with (110) planes show high reflectance at 1.2–1.55 µm wavelengths in measurement, indicating the existence of a photonic bandgap.

The mode gap design is unique to obtain resonant modes inside the complete photonic bandgap without the introduction of local disorders. We fabricated the designed dipole mode microcavity with (110) surface in GaAs with two-top etching method. The complete photonic bandgap provides omni-directional light confinement, resulting in exponential development of the quality factors without saturation when we increase the number of unit cells used for confinement. Small modal volumes were accomplished in the designed microcavities—0.36 $(\lambda_0/2)^3$ and 2.88 $(\lambda_0/2n)^3$ for the electric fields maximum in air and dielectric, respectively. Therefore, we achieved ultra-high quality factors and small modal volumes simultaneously. With this method, we engineered the mode locations (in air or dielectrics) and varied the symmetry of the modes.
The complete photonic bandgap is used to reduce the radiation loss in low-$Q$ 2D photonic crystal slab microcavities. We designed hybrid woodpile-2D slab-woodpile microcavities and improved the quality factor of the single defect 2D slab microcavities without increasing the modal volume.

We achieved high-$Q$ metal clad 3D photonic crystal microcavities thanks to the confinement by Bragg reflection in all directions. Our analysis shows that the quality factors are not significantly influenced by the absorptive metallic materials; therefore, common metallic materials can be selected as electrodes.

Single-mode waveguides in lateral and vertical directions are designed in woodpile photonic crystals by 2D unit cell modulation. We also found the existence of the self-collimation mode in a double-hetero-junction woodpile photonic crystal.

5.2 Future Prospects

The unique features of 3D photonic crystals, such as the complete photonic bandgap and dispersion characteristics, are useful for building compact and high quality optical devices. Some potential application devices are listed below.

(i) Low-threshold woodpile photonic crystal nanolasers

Microcavities with ultra-high quality factor and small modal volume are designed. This could greatly enhance the spontaneous emission rate of the lasing mode by Purcell effect and increase spontaneous emission coupling coefficient. This helps the reduction of laser threshold, or even the realization of thresholdless lasers.

(ii) Current injection woodpile photonic crystal nanolasers

As we have confirmed in numerical analysis, metal electrodes in direct contact with the designed woodpile microcavities do not significantly deteriorate the quality factor. This is promising for realization of electrically-pumped photonic crystal nanolasers.

(iii) Surface or interface modes with woodpile photonic crystals
Within the complete photonic bandgap, the field is expected to evanescently decay into the woodpile structures without absorption loss. We expect to observe low-loss surface mode at the interface of two different woodpile photonic crystals, e.g. different orientation or lattice constants. Moreover, with the capability of building woodpile photonic crystals with various crystal planes, we anticipate more degree of freedom in the surface mode design.

(iv) Low-loss and high-density 3D integrated optics

With the designed lateral and vertical waveguides, we expect to construct low-loss bended waveguides to change light propagation direction on the same level and into a different level as well. This could help to increase the number of connects in each optical devices, and place these devices three-dimensionally to reduce the footprint and increase the integration density.
Appendix A. ITO Clad 2D Photonic Crystal Microcavity

High quality factor photonic crystal microcavities are the first step towards electrically pumped photonic crystal lasers. However, the widely used metallic materials, such as gold and silver, are highly absorptive at optical wavelengths. In order to reduce the overlapping between metals and optical fields, thus to reduce the absorption, researchers utilize a complex configuration with indirect metal contacts to realize current-injection photonic crystal lasers [10]. This results in low thermal conductance, large electrical resistance and large leak current. Moreover, the fabrication is complicated.

To solve this challenge, we use low-absorptive indium tin oxide (ITO), which is an optically transparent and electrically conducting material with a small imaginary part \(k\) in the complex refractive index \((k < 1.0\) for \(\lambda_0 < 1.5\ \mu\text{m})\). Numerical analysis confirms that a reasonable quality factor can be obtained for 2D photonic crystal slab microcavities with ITO directly placed on both the bottom and the top of the slab (see Section 3.4). For example, the \(Q\) factor is about 800 for ITO clad L3 microcavity comparing to only 60 for gold clad the same L3 cavity. This provides us with a simple microcavity configuration that might be applied to current-injection photonic crystal nanolasers.

We demonstrate the fabrication of L3 microcavity with full ITO contacts on bottom and top of the slab. In order to place ITO contacts on both sides of the slab, we deposit ITO on a substrate, and utilize an epitaxial lift-off and van der Waals bonding technique to bond a thin GaAs membrane on top of ITO. The GaAs membrane is patterned and etched so that 2D photonic crystal microcavities are formed; see Figure A-1(a). To isolate the top ITO electrode from the one on the bottom, we coat a silica layer on the top of the patterned membrane. The second electron beam lithography step is conducted to open the areas with 2D photonic crystal microcavities. At the open areas, the silica layer is etched through so that the top ITO electrode would directly contact the GaAs membrane as displayed in Figure A-1(b). Next, the top ITO is deposited. Many
optical microcavities are fabricated on a single chip, so each device needs to be electrically isolated. The third EBL step is performed, and the top ITO is wet etched for isolation; see Figure A-1(c). Figure A-2 sketches the cross-section view of the fabricated microcavities.

The fabrication procedures for this photonic crystal microcavity with metal contacts are much easier than the previous reported designs [10]. Indium tin oxide may be a promising candidate for electrodes in current-injection optical devices.

Figure A-1: Optical microscope images of ITO clad 2D photonic crystal slab microcavity. (a) Microcavities with ITO on the bottom of the slab. (b) After coating an insulting layer and open the microcavities. (c) After isolating the top ITO for each microcavity.

Figure A-2: A sketch of the cross-section view of the fabricated ITO clad L3 microcavities.

This project is collaborated with Ms. Pantana Tor-ngern. She is charge of ITO sputtering, epitaxial lift-off and van der Waals bonding. The other microfabrication procedures are completed by me.
Appendix B. Single-mode Waveguide Optical Isolator

B.1 Introduction

An optical isolator is a component that transmits light efficiently in one direction but prevents backward propagation. The optical isolator is used, for example, to prevent optical feedback into lasers. Integration of optical isolators with other optical devices is desired because they can improve on-chip optical systems and reduce device size and cost. On-chip optical interconnect technology requires a high data rate with a large signal-to-noise ratio, so unwanted backward propagation should be minimized.

Research on optical isolators has been extensive in the past decade, leading to a wide range of isolator designs. The most traditional design consists of a Faraday rotator and two polarizers [74, 75]. The need of polarizers makes these devices complicated for on-chip integration. To avoid this drawback, in the past few years a new generation of isolators have been developed that operate on the magneto-optical phenomenon of a nonreciprocal phase shift, rather than polarization conversion as for Faraday rotation based isolators [76-78]. A nonreciprocal phase shift is used to achieve isolation in asymmetric Mach-Zehnder interferometers (MZI), where one branch is nonreciprocal; some of these devices use 2D photonic crystals as the waveguide branches [79]. Although they have fewer components than rotators, a major obstacle is that phase shift isolators require precise wave interference from two long waveguides. Other designs include 1D or 2D photonic crystal, single waveguide isolators where isolation is displayed in nonreciprocal band diagrams, i.e. $\omega(k) \neq \omega(-k)$. To generate such nonreciprocal dispersion, time reversal $T$ and spatial inversion $S$ symmetries need to be broken—magnetic material is capable of breaking $T$, and an asymmetric distribution of this material can break $S$ [80]. One model of this phenomenon is that isolation occurs at Dirac points: frequencies where only backward propagating waves have a zero group velocity [81]. Another model of isolation using band diagrams shows that modes of backward
waves are eliminated by waveguide cutoff frequencies [82, 83]. A similar design includes coupling between 2D photonic crystal waveguide modes and plasmon modes for a metal/dielectric waveguide subject to a magnetic field [84]. More recently, 2D photonic crystal waveguides have shown isolation using metal/dielectric interfaces where unidirectional modes exist that are analogous to Chiral states of the quantum Hall effect [85].

The promising features of the designs listed above include: analysis using nonreciprocal band diagrams where isolation is produced by cutoff of backward propagating modes; and the simplicity of single waveguide isolator design, rather than a rotator or MZI. This type of band diagram analysis is useful for finding unidirectional single mode operation—all other modes are unguided. The single waveguide designs given above can be further simplified by confining modes using a dielectric waveguide. Amemiya et al. have simulated and fabricated isolators using this approach, where $T$ and $S$ are broken by asymmetrically distributing magnetic material in the rib waveguide’s cross section [86]. However, they do not achieve isolation by modal cutoff, but by increased absorption loss for backward modes: they rely on an active guiding region to balance gain and loss [87].
Figure B-1: Dispersion curves of the proposed optical waveguide isolator. Solid lines are the lowest and second lowest modes. Dashed lines indicate forward and backward propagating modes for $\Delta \varepsilon \neq 0$. Only one forward wave is guided within the isolation range $\Delta w$.

Figure B-2: Optical isolator structures: (a,b) right-left configuration, (c,d) up-down configuration, (e) rib waveguide, and (f) trapezoidal configuration. C is a low-index material, A is a reciprocal material, and B is non-reciprocal material; B+ and B- have anti-parallel magnetizations.

Figure B-3: (a) Dispersion curves of the optical isolator in Figure B-2(b), where $w/a = 0.4$ and $h/a = 0.3$. The value $a$ is the scaling length. The permittivity tensors are $\varepsilon_0 [12.25 \ 0 \ 0; 0 \ 12.25 + i \ 0 \ i \ 12.25]$ for B+ and B-. The substrate C is isotropic ($\varepsilon = 2.13 \varepsilon_0$). The value $\varepsilon_0$ is the permittivity of vacuum. We have selected relatively large off-diagonal values so that optical isolation is clearly shown. (b) Electric field component profiles of the lowest TE and TM modes at $|\beta|a/2\pi = 0.8$. “A on C” represents a reciprocal waveguide ($\Delta \varepsilon = 0$).
B.2 Proposed optical isolator designs

We propose a novel isolator design that both: (1) operates via backward propagating mode cutoff, and (2) employs a simple dielectric waveguide design. Furthermore, we achieve single mode, unidirectional propagation in simulation. Non-reciprocal material is included to break time-reversal symmetry, but the spatial inversion symmetry needs to be broken as well. This is accomplished by distributing magnetic material non-uniformly in the waveguide’s cross-section. In our isolator designs, we choose appropriate modes and an inhomogeneous distribution of non-reciprocal materials so that only the forward propagating mode(s) is guided. Figure B-1 shows dispersion curves for the first and second lowest modes (solid lines labeled by $\Delta \varepsilon = 0$) and their forward and backward modes (dashed lines labeled by $\Delta \varepsilon \neq 0$ indicating the incorporation of non-reciprocal material). Single mode optical isolation is realized between the cut-off frequencies of the lowest forward and backward propagating modes; the isolation bandwidth is shown in the figure.

In order to confirm this concept, we simulate multiple waveguide designs; see Figure B-2. The two-dimensional plane wave expansion (PWE) method [54] is used to calculate the waveguide dispersion. In our design, the waveguide is a nanowire on a low-index substrate. We take the z axis as the propagation direction and the permittivity is a function of x and y and independent of z. Non-reciprocal materials have the permittivity tensor:

$$
\tilde{\varepsilon} = \begin{pmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz}
\end{pmatrix}
$$

(B.1)

which has nonzero off-diagonal components. We explore different waveguide shapes that include: a rectangle, a trapezoid, and a rib waveguide. A rectangle nanowire with a width $w$ and a height $h$ is the first design simulated. The left half of the nanowire is reciprocal material A, and the right half non-reciprocal material B—a material distribution that we call the “right-left” configuration; see Figure B-2(a). Variations on the configuration
include: changing the reciprocal material on the left to non-reciprocal material, but with magnetization anti-parallel to the material on the right, as in Figure B-2(b); and stacking the materials vertically—the “up-down” design, as in Figure B-2(c, d).

Figure B-3(a) gives the dispersion relation for the right-left structure with the B+ and B- anti-parallel magnetizations. The dispersion diagram indicates single-mode optical isolation. The effect of off-diagonal components on the electric field is negligible, as shown in Figure B-3(b). The modeling results are summarized in Table B-1. The distribution of the non-reciprocal materials is an important factor that determines the isolation bandwidth. The isolator with anti-parallel magnetization gives a larger bandwidth than an isolator with reciprocal material in one half. However, these “right-left” designs may not be simple in terms of fabrication; this could be avoided in the “up-down” configuration. Figure B-3(c) and (d) show the “up-down” configuration, where TM mode isolation can be achieved in a waveguide with \( w < h \). The simulation results show inversion symmetry in the dispersion relation, i.e., no isolation if we use non-reciprocal materials with the same permittivity tensors as those in the “right-left” configuration. Instead, in this “up-down” configuration different off-diagonal components are needed to break the inversion symmetry—changing the off-diagonal components is effectively changing the direction of the magnetization. We also analyze the structures that account for imperfections in fabrication, such as rib [Figure B-2(e)] and trapezoid waveguides [Figure B-2(g)]. The trapezoidal structure shows a slightly smaller bandwidth than the rectangular structure.
Table B-1: Isolation bandwidth of some analyzed isolators. Bandwidth is obtained from 2D PWE modeling. $\varepsilon_{B}=\varepsilon_{0} \begin{bmatrix} 6.25 & 0.06i & 0 \\ 6.25 & 0 & 0 \\ 0 & 6.25 & 0 \end{bmatrix}$, $\varepsilon_{C} = 2.13\varepsilon_{0}$. This models BIG waveguides on silica. The value $I_{xy}+I_{xz}+I_{yz}$ is evaluated at a guiding dispersion point $\beta = 0.6$.

<table>
<thead>
<tr>
<th>Lowest mode</th>
<th>Design</th>
<th>Parameters</th>
<th>Bandwidth</th>
<th>$I_{xy}+I_{xz}+I_{yz}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TE</td>
<td>right-left B+/A (a)</td>
<td>0.8 0.6 -</td>
<td>0.53%</td>
<td>0.00836</td>
</tr>
<tr>
<td></td>
<td>B+/B- (b)</td>
<td>0.8 0.6 -</td>
<td>1.07%</td>
<td>0.01672</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.2 0.6 -</td>
<td>0.94%</td>
<td>0.02080</td>
</tr>
<tr>
<td>TM</td>
<td>B+/A (c)</td>
<td>0.8 0.6 $\hat{h}=0.56a$</td>
<td>0.39%</td>
<td>0.00722</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.8 0.6 $\theta_{1}=\pi/3 \quad \theta_{2}=\pi/3$</td>
<td>0.48%</td>
<td>0.01036</td>
</tr>
<tr>
<td></td>
<td>B+/B- (d)</td>
<td>0.6 0.8 -</td>
<td>0.54%</td>
<td>0.00920</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.6 1.2 -</td>
<td>0.90%</td>
<td>0.02064</td>
</tr>
</tbody>
</table>

B.3 Discussions

We use non-degenerate perturbation theory to understand the correlation between the inhomogeneity of nonreciprocal materials and phase shifts. This knowledge will help us optimize the isolation bandwidth. The modal electric field is written by $E_{n}=E_{n0}\exp[i(\omega t-\beta z)] |n\rangle$ where the amplitude $E_{n0}$ is determined by normalizing $|n\rangle$. Assuming $\text{div}E \approx 0$ and $\beta \approx \beta_{0}$, the unperturbed eigenvalue equation with eigenvalue $\beta^{2}$ and eigenmode $|n\rangle = (E_{x}, E_{y}, E_{z})^{T}$ is:

$$\hat{H}_{0}|n\rangle \approx \beta^{2}|n\rangle \tag{B.2}$$

where

$$\hat{H}_{0} = \begin{pmatrix}
\nabla_{i}^{2} + \omega^{2}\mu_{0}\varepsilon_{i} & 0 & i\beta_{0}\partial / \partial x \\
0 & \nabla_{i}^{2} + \omega^{2}\mu_{0}\varepsilon_{i} & i\beta_{0}\partial / \partial y \\
0 & 0 & \nabla_{i}^{2} + \omega^{2}\mu_{0}\varepsilon_{i} + \beta_{0}^{2}
\end{pmatrix} \tag{B.3}$$

and the transverse Laplacian is $\nabla_{i}^{2} = \partial^{2} / \partial x^{2} + \partial^{2} / \partial y^{2}$. Here, we add a small perturbation to the operator $\omega^{2}\mu_{0}\hat{A}_{z}$ by changing the permittivity tensor given by
\[
\hat{\Delta}_e = \varepsilon_0 \begin{pmatrix}
0 & iu_{xy} & -iu_{xz} \\
-iu_{xy} & 0 & iu_{yz} \\
iu_{xz} & -iu_{yz} & 0
\end{pmatrix}
\]  

(B.4)

where \( u_{ij} \) is real. This tensor can represent magnetization parallel to one of the Cartesian axes \((x,y,z)\). In our modeling results, the bandwidth is small relative to the operation frequency, so \( \beta \approx \beta_0 \) is justified. A square of the propagation constant is corrected to the first order:

\[
\beta^2 \equiv \beta_0^2 + \omega^2 \mu_0 \langle n | \hat{\Delta}_e | n \rangle = \beta_0^2 \left\{ 1 + 2 \left( \frac{\omega}{c \beta_0} \right)^2 (I_{yx} + I_{xz} + I_{yz}) \right\}
\]  

(B.5)

or

\[
\beta \equiv \beta_0 + \frac{\omega^2 \mu_0}{2 \beta_0} \langle n | \hat{\Delta}_e | n \rangle = \beta_0 \left\{ 1 + \left( \frac{\omega}{c \beta_0} \right)^2 (I_{yx} + I_{xz} + I_{yz}) \right\}
\]  

(B.6)

where

\[
I_{ij} = \iint u_{ij}(x,y) \text{Im}[E_i^*(x,y)E_j(x,y)]dxdy.
\]  

(B.7)

The isolation bandwidth obtained from practical materials is so small that the bandwidth \( \Delta \omega \) is approximated to be proportional to the shift \( \Delta \beta \) between forward and backward waves:

\[
\Delta \beta = 2\omega^2 (I_{yx} + I_{xz} + I_{yz})/(c^2 \beta_0) \propto \Delta \omega.
\]  

(B.8)
Figure B-4: Profiles of Im[$E_y^*E_z$] and Im[$E_x^*E_z$]. Im[$E_y^*E_x$] is negligible. (a) TE mode, $h/a = 0.6$ and $w/a = 0.8$. (b) TE mode, $h/a = 0.6$ and $w/a = 1.2$. (c) TM mode, $h/a = 0.8$, $w/a = 0.6$. (d) TM mode, $h/a = 1.2$, $w/a = 0.6$.

Figure B-5: (a) Dispersion curves obtained from perturbation theory and 2D PWE modeling for the structure Figure B-2(b). $\varepsilon_{B\pm}=\varepsilon_0 [6.25 \ 0 \ 0; 0 \ 6.25 \mp 0.06i; 0 \pm0.06i \ 6.25]$, $\varepsilon_C=2.13\varepsilon_0$, $w = 0.8a$ and $h = 0.6a$. Materials B± represent BIG. (b) Bandwidth obtained from PWE vs. $I_{yx}+I_{zy}+I_{yx}$. Data from various designs shown in this paper are plotted. There are errors in finding the bandwidth as well as ones caused by neglecting the gradient of permittivity.

Figure B-6: Profiles of Im[$E_y^*E_z$] and Im[$E_x^*E_z$] for the lowest TE and TM mode. Im[$E_y^*E_x$] is negligible. (a) TE mode, $h = 0.6a$, (total $w$) = 1.2$a$, $w_{n=2.5} = 0.8a$, $w_{n=1.46} = 0.2a$. (b) TM mode, $w = 0.6a$, (total $h$) = $a$, $h_{n=2.5} = 0.8a$, $h_{n=1.46} = 0.2a$. 

Using equation (B.6) and the electric field of an unperturbed mode, we can calculate dispersion curves of forward and backward waves. Thus, we do not need to model different distributions of non-reciprocal materials in order to evaluate the bandwidth. We can visualize the contribution of non-reciprocal material to the propagation constant shift and conduct a direct comparison between different material distributions for the same unperturbed mode. Figure 4 shows two functions $\text{Im}[E_z^*E_y]$ and $\text{Im}[E_x^*E_z]$ calculated from the lowest TE and TM mode profiles. For the TE mode (figure 4 a,b), the largest component $\text{Im}[E_z^*E_y]$ is odd about $y=0$, but is almost even about a waveguide mid-plane parallel to the substrate. Therefore, it is desired that the function $u_{yz}$ is odd about $y=0$, i.e. the “right-left” anti-parallel magnetization is appropriate, and the “right-left” configuration produces a larger isolation for the lowest TE mode than for the lowest TM mode; see Figure B-3(a). Two components $\text{Im}[E_i^*E_j]$ of the lowest TM mode are shown in Figure B-4(c) and (d). The largest component $\text{Im}[E_x^*E_z]$ is almost odd about waveguide mid-plane, but is even about $y=0$. Therefore, it is desired that the function $u_{zx}$ is odd about the waveguide mid-plane, i.e. the “up-down” anti-parallel magnetization is appropriate. Table B-1 also shows the value $I_{yx}+I_{xz}+I_{zy}$, which is approximately proportional to the bandwidth obtained from rigorous 2D PWE modeling.

Figure B-5(a) shows both the dispersion curves obtained from perturbation theory and those from 2D PWE modeling. For the different isolator configurations, the deviation of our perturbation theory results from 2D PWE modeling is approximately 20% (Figure B-5(b)) and independent of the perturbation strength. The second order correction $\sum_{\Delta,\epsilon} |(\epsilon|\omega^2\mu_0\Delta_z|\epsilon)\rangle^2 (\beta_\epsilon^2 - \beta_\epsilon^2) / (\beta_\epsilon^2 - \beta_\epsilon^2)$ is small (the TE-TM mode conversion is small as well) and does not effectively contribute to the isolation bandwidth, because dispersion curves of forward and backward waves shift by the same amount to the same direction. Epsilon averaging is not used in our PWE modeling. We obtain the eigenvalue equation (B.2) by assuming that the gradient of the permittivity is negligible everywhere. High index contrast waveguides give a larger error than low contrast waveguides—a result of the
assumption \( \text{div} E \approx 0 \). Knowing this limit of the analysis, we can use perturbation theory to optimize optical isolators.

Lastly, we show how to improve the isolator bandwidth via \( \text{Im}[E_i^*E_j] \) analysis. Non-reciprocal materials only exist in a rectangular waveguide region for the analyzed isolators. As seen in Figure B-4, there are large components outside of the waveguide—these components do not contribute to \( \beta \) shift. In order to use these components, we analyze two structures and calculate \( \text{Im}[E_x^*E_y] \) and \( \text{Im}[E_y^*E_z] \) for each case; see Figure B-6. A low-index rectangle (n=1.46) is added to each side of the high-index (n=2.5) waveguide in Figure B-6(a). A low-index rectangle is added on top of the high-index waveguide in Figure B-6(b). The overlap of the components with the waveguide is increased. The off-diagonal component of the permittivity tensor, for the low index material, is \( \pm 0.06i \). As a result, the values \( I_{xx} + I_{xz} + I_{zy} \) are (a) 0.02738 and (b) 0.02154 at \( \bar{\beta} = 0.6 \), and the bandwidth obtained from PWE is increased to (a) 1.81% and (b) 1.17%. It is reconfirmed that the \( \text{Im}[E_i^*E_j] \) analysis is useful for designing the isolation bandwidth. Although some papers discuss perturbation theory, the above method of visualizing the contribution of non-reciprocal materials to the phase shift provides a unique and versatile tool for designing isolators based on \( \beta \) shift.

**B.4 Conclusions**

We propose a waveguide isolator design based on the cut-off frequencies. Our waveguide isolator has the advantage of simplicity in design over traditional structures. Various structures are simulated in order to optimize the isolation bandwidth. A means of optimizing the isolation bandwidth is developed based on perturbation theory. Future research will include: FDTD simulation of transmission properties, and fabricating the isolators.

This project is collaborated with Mr. Samuel M. Drezdzon.
References


Biography

Lingling Tang received BS degree in Electrical Engineering (EE) from Peking University in 2005, and MS degree in EE from Duke University in 2007.

List of Publications:


