Nondegenerate monopole mode of single defect two-dimensional triangular photonic band-gap cavity

Joon Huh a)
Agency for Defense Development, Taejon 305-600, Korea
Jeong-Ki Hwang, Han-Youl Ryu, and Yong-Hee Lee
Department of Physics, Korea Advanced Institute of Science and Technology, Taejon 305-710, Korea
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The two-dimensional monopole mode is investigated as a candidate for a nondegenerate photonic band-gap (PBG) cavity mode. This monopole mode formed in a single defect triangular PBG cavity is truly nondegenerate and remains nondegenerate in the sense that the introduction of asymmetry does not result in splitting of the mode. Several methods to tune the resonant frequency of the mode are studied. The radii, positions, and shapes of the nearest-neighbor air holes are varied in this analysis using the three-dimensional finite-difference time-domain calculation. The quality factor of the monopole mode formed in a slab waveguide structure is found to be larger than that of the dipole mode when the shape of the nearest-neighbor holes is elliptical. © 2002 American Institute of Physics. [DOI: 10.1063/1.1481965]

I. INTRODUCTION

In 1946, Purcell predicted that the spontaneous emission rate could be altered by the modification of the density of states of electromagnetic modes. 1 Since then the modification of the spontaneous emission has been studied by numerous groups. 2–5 Recently, a simple numerical method to obtain the spontaneous emission rate of a dipole placed in a general microcavity was reported. 4,5 One method to control the spontaneous emission is to create a wavelength-size cavity in a photonic crystal. When a defect is introduced in a photonic crystal, resonant modes are formed inside the photonic band gap (PBG). 2,4–8 Many optoelectronic devices based on photonic crystals such as low-threshold microcavity lasers, 9–11 high-efficiency light emitting diodes, 12–14 and low-loss waveguides 15 have been demonstrated recently.

One of the most attractive applications of the photonic crystal is a zero-threshold laser 16–18 in which the boundary between spontaneous and stimulated emissions becomes ambiguous. Since the use of a single defect PBG cavity offers the possibility of nearly thresholdless laser operations, the development of this ultimate nanolaser has drawn strong attention from many research groups. Recently, the Caltech group demonstrated a single defect laser fabricated in a half-wavelength-thick two-dimensional (2D) PBG slab. 9,18 The single defect microcavity confines photons by the 2D photonic band gap in the horizontal plane and by the total internal reflection in the vertical direction. They observed pulsed lasing from a dipole defect mode.

In this article, we theoretically study the nondegenerate 2D monopole mode as a candidate for the zero-threshold laser. In Sec. II, we briefly mention the finite-difference time-domain (FDTD) method and the perfectly matched layer (PML) boundary conditions used for the analysis of defect modes of 2D cavities. In Sec. III, we show that the monopole mode is truly nondegenerate and remains nondegenerate even for asymmetric cavities made of infinitely long 2D photonic crystals. Then the resonant mode profile of the nondegenerate monopole mode is studied. In Sec. IV, using the practical 2D slab cavity, methods to tune the resonant frequency of the monopole mode from 3D FDTD calculations are described. At the same time, quality (Q) factors for the dipole and the monopole modes are calculated and compared.

II. COMPUTATIONAL METHOD

Time-dependent Maxwell’s equations in a material with electric conductivity σ in a source-free region can be written as follows:

\[ \mu \frac{\partial \vec{H}}{\partial t} = -\nabla \times \vec{E}, \]  

(1)

\[ \varepsilon \frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{H} - \sigma \vec{E}. \]  

(2)

Here, \( \varepsilon \) and \( \mu \) are the position-dependent permittivity and permeability of the material, respectively. In an ideal 2D photonic crystal consisting of a periodic array of air holes in the \( xy \) plane, electromagnetic fields can be decoupled into two distinct polarization modes, the transverse electric (TE) mode and the transverse magnetic mode. 8 In the case of the TE mode, the 2D FDTD space and time discretizations of Eqs. (1) and (2) by the Yee algorithm 19 yield the following field components:

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a) Electronic mail: huhjoon@kaist.ac.kr
where $n$ is the number of time steps and $i$ and $j$ are the discretized grid points in the $xy$ plane, respectively. $\Delta t$ is a time step, and $\Delta x$ and $\Delta y$ are the space steps along the $x$ and $y$ directions, respectively.

One of the key issues in the FDTD calculation is how to apply the absorbing boundary conditions that approximate the open space. The PML boundary conditions introduced by Berenger are to create nonphysical absorbing materials adjacent to the outer FDTD mesh boundary. There is no reflection for any frequency, polarization, and angle of incidence at the interfaces between the PMLs and the FDTD computation regions. In the 2D TE case, the approach of such PML is based on the splitting of the magnetic component $H_x$ in the PLM region into two subcomponents $H_{x1}$ and $H_{x2}$. If the PML material is impedance matched with the computational region, it allows all the electromagnetic waves to be completely absorbed without reflection.

Since the 2D triangular lattice of air holes has a large photonic band gap for TE modes, this lattice is widely accepted by experimentalists. The single defect cavity shown in Fig. 1 will be used as a basic structure for our article. Generally, the optical properties of a 2D photonic crystal depend on parameters such as the lattice constant $a$, the ratio of air-hole radius to lattice constant $r/a$, and the refractive index of the material $n$.

The resonant frequencies and field distributions of defect modes are calculated by the FDTD method using the PML boundary conditions. Actually, to analyze defect modes, the space and time steps have to be determined first. In our calculation, 20 space steps ($20\Delta d$) are equal to one lattice constant ($a$) and the time step $\Delta t = \Delta d/2c$, where $\Delta d$ is either $\Delta x$ or $\Delta y$. This choice of the steps guarantees good computational stability. The FDTD method calculates field distributions in the time domain. Therefore, it is possible to obtain quantities of interest such as $Q$ factors, transmittance, resonant frequencies, and field distributions. However, the 3D FDTD method should be employed to analyze the 2D slab structures. As will be shown in Sec. III, mode profiles are symmetric about the $x$ and $y$ directions and have a mirror symmetry along the $z$ axis. Hence, only one eighth of the computational space is sufficient for the calculation. Also, the number of computational space steps is set to 15 intervals per lattice constant in the 3D FDTD calculation in order to reduce the computation time.

The time evolution of electromagnetic fields is generated by exciting several pulse sources with a Gaussian frequency profile in the vicinity of the defect. The frequency bandwidths of these pulse sources are broad enough to cover the entire photonic band-gap region. The resonant frequencies are calculated by the Fourier transform of the time varying fields in several arbitrary points near the defect.

### III. Nondegenerate Monopole Mode in a Modified Single Defect Cavity

The single defect 2D triangular cavity structure used in our article has the air-hole radius of 0.35 $a$ and the refractive index of 2.65. Both radii and positions of the six nearest-neighbor holes around the defect are varied. The degeneracy of modes is to be analyzed using the infinitely long 2D photonic crystal, since the symmetry of this 2D structure should be the same as the 2D slab structure to be investigated in the coming sections.

#### A. Resonant Defect Modes

By introducing a single defect in the 2D triangular photonic crystal, several resonant modes are usually generated inside the photonic band gap. The band diagram for the TE
mode is obtained by the plane-wave expansion method as shown in Fig. 2. The vertical axis of the band diagram is the normalized frequency \( v_{\text{a}}/2c \), where \( c \) is the speed of light in vacuum. The TE band gap is centered near a normalized frequency of 0.34 and formed between the lowest point of the second band \(~0.389\) and the highest point of the first band \(~0.286\).

Resonant frequencies of the single defect cavity are plotted in Fig. 3(a). Here, the radius \( r' \) of holes adjacent to the defect is gradually reduced, while the host radius \( r \) is kept constant. Let us begin with the normal single defect cavity where \( r' = 0.35 \) \( a \) and \( r = 0.35 \) \( a \). When the radius \( r' \) is equal to 0.35\( a \), the dipole mode exists solely within the photonic band gap. However, as one decreases \( r' \), several resonant modes begin to show up from the second band edge. When \( r' = 0.25 \) \( a \), four modes are found inside the photonic band gap. These four modes are names as the monopole, the quadrupole, the hexapole, and the dipole modes, respectively, from the top. The resonant frequencies of the defect modes sweep downward across the gap as the radius \( r' \) decreases, since the reduction of air-hole size increases the filling ratio of the dielectric material. Accordingly, the resonant frequencies of the single defect mode can be tuned by adjusting the radius of the six nearest-neighbor air holes around the defect. The electric-field distributions of the four resonant modes are shown in Fig. 4, where \( r' = 0.2 \) \( a \).

For the monopole mode and the dipole mode, the directions of electric fields are shown and compared in Fig. 5. The monopole mode oscillates with respect to the center of the defect as drawn in Fig. 5(a). On the other hand, the degenerate dipole mode have two types of mode profiles: The one oscillates along the \( \Gamma\text{-}K \) direction (left) and the other along the \( \Gamma\text{-}M \) direction (right).
The structure used for the computation of $\sim x$ in the try along the field directions. One of them is characterized by the symmetry along the horizontal direction is varied from $a - \Delta a$ to $a + \Delta a$. (b) Schematic diagram of the structure used for the computation of (a).

contrary, the doubly degenerate dipole modes have different field directions. One of them is characterized by the symmetry along the $\Gamma$-$K$ direction and the other by symmetry along the $\Gamma$-$M$ direction. Since the dipole mode is doubly degenerate, the probability of photon coupling into a given resonant mode should be small as compared to that of the nondegenerate monopole mode. Accordingly, one can argue that the monopole mode is advantageous for near zero-threshold laser operations since the nondegeneracy will result in a large spontaneous emission factor.

**B. Nondegenerate monopole mode**

When the symmetry with respect to the center of a defect cavity is broken, the degenerate mode should split into two different modes. Here, we will confirm the nondegeneracy of the monopole mode by introducing an intentional asymmetry into the photonic cavity structure. Any deviation from the sixfold symmetry of the triangular lattice is denoted as the asymmetry in our analysis. Introduction of the asymmetry modifies the field profile of the monopole mode only slightly.

To check the degeneracy of the mode, the lattice spacing along the horizontal $x$ axis is varied up to $\pm 4\%$ as shown in Fig. 6(b), while the lattice size along the vertical axis is fixed. Calculated resonant frequencies are given in Fig. 6(a). The degenerate modes, dipole and quadrupole, tend to split and the size of the splitting increases with the degree of the asymmetry. However, the monopole and the hexapole modes do not split into two modes. These modes are nondegenerate. The resonant frequencies decrease as the lattice spacing along the horizontal direction is gradually increased. Other forms of the asymmetry are also tested by varying the radii or positions of air holes. The nondegeneracy of the monopole mode is again confirmed under this kind of perturbation.

**IV. TAILORING OF MONOPOLE MODES IN 2D PBG SLAB: 3D CALCULATIONS**

So far, the properties of the monopole mode have been analyzed for ideal infinite 2D photonic crystal cavities. However, experimentally 2D slab photonic crystal cavities are more widely fabricated and tested.9,10,13 To analyze this 2D slab photonic crystal of air holes, full 3D calculations should be performed. In the 2D slab structure, photons are confined by the photonic band gap in the in-plane direction and by total internal reflection in the vertical direction. Here, the photons can be more tightly confined horizontally by adding more air holes. However, the radiation into the vertical direction cannot be prevented. This radiation loss tends to decrease with the size of the air holes, while the band-gap size shrinks because of the reduced index contrast. In fact, the six nearest holes around the defect have dominant influence on the vertical coupling. Therefore, we try to investigate the effect of these nearest-neighbor holes more closely by varying the position, size, and shape. In general, the monopole mode of sixfold symmetry extends farther away from the center of a cavity compared to the dipole mode of two-fold symmetry. The extended monopole mode usually shows higher $Q$ factors than the dipole mode.

To find a high-$Q$ resonant mode, it is usually helpful to tune the resonant frequency to the middle of the photonic band gap. In addition, if one wants to use this high-$Q$ cavity as a laser, good spatial overlap between the optical gain and the mode profiles is also required. To find a single defect 2D slab triangular PBG cavity with a high-$Q$ value that meets these requirements, we reduce the size of the six nearest-neighbor holes around the central defect and investigate two types of holes, circular holes and elliptical holes, as shown in Figs. 7(b) and 8(b). In the case of the elliptical air holes, we denote the length of the semimajor axis of the holes by $r''$ and the length of the semiminor axis by $r'$, respectively. Here, the radius $r$ of the host holes is 0.35 $a$ and the length $r''$ of the elliptical holes is kept at 0.35 $a$, while $r'$ varies from 0.35 $a$ to 0.15 $a$. The thickness of the slab is set to 0.4 $a$ which is slightly less than a half wavelength to make it a single mode waveguide. When we change $r'$, we displace the six nearest-neighbor holes outward simultaneously by the same distance $d$ as shown in Figs. 7(b) and 8(b).

Plots of the resonant mode frequencies versus $r'$ for the elliptical and circular holes are shown in Figs. 7(a) and 8(a), respectively. Several defect modes (denoted by the symbols, $\times$ and $+$) begin to show up as one decreases the size of air holes. The electric-field distributions of these modes are mostly concentrated near the air-hole surface and these modes would undergo relatively large optical and carrier losses. Therefore, we will not continue our investigation into these modes. As $r'$ is reduced, the resonant frequencies are decreased for both the elliptical and the circular holes. When one adjusts $r'$ around 0.2 $a$, the resonant frequency of the monopole mode can be tuned to the middle of the photonic band gap. Remember that the $Q$ factor of the cavity is ex-
the resonant frequencies of the hexapole and the quadrupole modes differ more than 100 nm which corresponds to a normalized frequency difference of 0.02.

V. DISCUSSION

The $Q$ factor of a defect mode is defined as the ratio of the stored energy $E$ and the radiated power $P$ as follows,

$$Q = \frac{\omega_0 E}{P},$$

where $\omega_0$ is the eigenfrequency of the mode. Here, $P = -\frac{dE}{dt}$ is the ratio at which energy is dissipated in the cavity. At first, the field is initialized by a single Gaussian pulse that excites only one resonant mode. Then, we measure energy of the mode as a function of time. From the slope of this logarithm energy-time relation, the $Q$ factor is calculated. The $Q$ factor of a given mode can be divided into two components, the in-plane $Q$ factor which represents the propagation loss of the guide mode into the dielectric slab and the vertical $Q$ factor which represents the radiation out of the slab waveguide. The in-plane $Q$ factor increases continuously as one adds air holes, while the vertical $Q$ factor improves only asymptotically. In other words, the total optical loss of a 2D photonic crystal slab cavity is mainly determined by the vertical loss. Therefore, the control of the vertical loss is critical for a high-$Q$ cavity. Unlike the dipole mode, the fact that the monopole mode has a node of electric field at the defect center of the resonant cavity is advantageous in terms of the vertical loss, because the radiation along the normal direction will interfere destructively.

In addition, the monopole mode profile overlaps favorably with the region of the material gain. Since the electric field is negligible around the center, the introduction of a small post would not increase losses significantly. This post acts as a current injection path for the electrically pumped operation. This expectation is confirmed by the FDTD simulation for the circular holes as shown in Fig. 11. Little change of vertical $Q$ factors is observed until the radius $r_p$ of the central post reaches 0.2 $a$.

Recently, we experimentally observed the nondegenerate lasing action from the monopole mode cavity with threshold pump power of 0.3 mW.

VI. CONCLUSION

The characteristics of the 2D monopole mode found from single defect triangular photonic crystals are studied. The monopole mode is nondegenerate in the sense that the mode does not split even under asymmetric deformations.
This inherent nondegeneracy of the monopole mode should be advantageous to achieve a large spontaneous emission factor. In addition, from 3D FDTD calculations of 2D slab photonic crystal structures, several ways to tune the resonant frequency to the middle of the TE band gap are suggested and characterized. It is found that the $Q$ factor of the monopole mode is larger than that of the dipole mode in the case of the elliptical nearest holes around the defect. Moreover, the in-plane $Q$ factor of the monopole mode should be much larger than that of the dipole mode.

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The geometry of the calculation domain for the single defect 2D triangular photonic crystal slab cavity. (a) In the top view, there are five layers of air holes around the defect and the structure is surrounded by PML boundaries. (b) In the side view, the PML boundaries above and below slab are placed approximately at $\lambda/2$ from the surface of the slab, where $\lambda$ is the light wavelength in air.

This in-plane $Q$ factor of the monopole mode is much larger than that of the dipole mode.

Introduction of a small central post does not increase optical losses significant. Therefore, the electrical pump through the central post is physically feasible.

FIG. 9. Geometry of the calculation domain for the single defect 2D triangular photonic crystal slab cavity. (a) In the top view, there are five layers of air holes around the defect and the structure is surrounded by PML boundaries. (b) In the side view, the PML boundaries above and below slab are placed approximately at $\lambda/2$ from the surface of the slab, where $\lambda$ is the light wavelength in air.

FIG. 10. Quality factors of the monopole and the dipole modes versus $r'$ of air holes in the case of Figs. 7(b) and 8(b). (a) Vertical $Q$ factors. The maximum vertical $Q$ factor of the monopole mode appears at a normalized resonant frequency of 0.36 slightly above the center of the photonic band gap. The maximum vertical $Q$ factor of the dipole mode appears at 0.304 just above the first band edge. See Figs. 7(a) and 8(a). (b) In-plane $Q$ factors. The in-plane $Q$ factor of the monopole mode is much larger than that of the dipole mode.

FIG. 11. Vertical $Q$ factors of the monopole mode versus the radius $r_p$ of the central post when $r'=0.25\, a$. The inset shows the position of the post placed underneath the photonic crystal slab cavity. The refractive index of the post is the same as that of the slab material.