Photonic crystal defect tuning for optimized light-matter interaction

Christopher Kang a,b * and Sharon M. Weiss a,b

aInterdisciplinary Graduate Program in Materials Science, Vanderbilt University, Station B 350106, Nashville, Tennessee 37235;
bDepartment of Electrical Engineering and Computer Science, Vanderbilt University, Station B 351824, Nashville, Tennessee 37235

ABSTRACT

Photonic crystal microcavities with multi-hole defects were simulated using finite difference time domain (FDTD) analysis. Subwavelength, multi-hole defects (MHD) offer a significant increase in defect surface area without compromising the quality factor of the photonic crystal. Calculations of the increase in surface area compared to a traditional, single hole defect are performed for MHD structures with varying subwavelength defect hole size, subwavelength defect hole spacing, and effective defect radius. For active photonic crystal applications, the resonance wavelength and quality factor of several different MHD photonic crystal structures was calculated as a function of the dielectric constant of the defect. MHD photonic crystals can be designed to enable large changes in resonance wavelength for small changes in defect dielectric constant. These structures would be advantageous for applications in biosensing and optical switching.

Keywords: photonic crystals, defect structures, finite-difference time-domain, multi-hole defects

1. INTRODUCTION

The discovery of the optical analog of semiconductor electronic bandgaps, the photonic bandgap, has inspired many innovative devices by enabling control of the propagation of light. Photonic devices have utilized photonic bandgaps for advanced waveguiding and interconnects [1-5], optical modulation and switching [6-9], light emission [10-11], and sensor [12-14] applications. Photonic crystal point or line defect structures in particular have proven to be useful in these applications, as they allow for the creation of regions of high intensity field in small mode volumes. While in many lasing and quantum electrodynamics applications it is advantageous for the defect region to be a missing air hole (i.e., solid defect) [15], other applications, such as sensing, require the defect to be an air hole of size sufficiently different than the surrounding photonic crystal holes [14].

In order to maximize light-matter interaction in photonic crystals with air hole defects, we propose a multi-hole defect (MHD), which increases the surface area in the defect region while maintaining a high cavity quality factor. By using 2-D finite-difference time-domain simulations, the fields and resonance wavelength of various MHD cavities are explored. In all experiments, we considered realistic fabrication limits and material properties.

1.1 Multi-hole defect design

A schematic illustrating one example of a MHD photonic crystal is given in Figure 1. The defect region consists of several, subwavelength holes that are substantially smaller than the periodic holes of the photonic crystal. In mixed dielectric media with small features sizes compared to the wavelength of light, an effective medium approximation can be used to determine an effective refractive index of the material [16-17]. This effective refractive index is a weighted average of the refractive index of each of the constituent materials. An effective medium approximation is therefore appropriate for the MHD photonic crystal since we consider individual defect hole radii that are approximately two orders of magnitude smaller than the wavelength of light incident on the photonic crystal.

*Contact: chris.kang@vanderbilt.edu
We define the following terms for clarity:
- **Defect region (MHD region)** = area in which symmetry of surrounding photonic crystal is broken
- **Defect hole** = one of many small holes inside the defect region
- **Defect hole radius** = radius of a defect hole
- **Defect (region) effective radius** = radius of entire defect region that contains multiple defect holes
- **Photonic crystal holes** = periodic holes of photonic crystal with center-to-center spacing $a$

Figures 2 (a) and (b) illustrate MHD photonic crystals with the same defect hole radius and different defect effective radii. Figure 2 (c) has the same defect effective radius as (b) but different defect hole radii.

Fig. 1. Example of a MHD photonic crystal with an effective defect radius of $0.2a$. The defect region consists of 43 defect holes of size $0.02a$. The inset shows a magnified version of the defect region.

Fig. 2. Examples of different MHD photonic crystal configurations: (a) defect hole radius of $0.02a$ and defect effective radius of $0.2a$; (b) defect hole radius of $0.02a$ and defect effective radius of $0.3a$; (c) defect hole radius of $0.04a$ and defect effective radius of $0.3a$. The defect hole spacing for (a) and (b) is $0.06a$ while the defect hole spacing for (c) is $0.12a$, to maintain the same effective refractive index for the defect region.
As shown in Figures 1 and 2, the defect holes are arranged in a hexagonal close-packed lattice, much like the surrounding photonic crystal. This orientation of holes is used in order to maximize the packing of holes within the defect region. The defect holes are generated by a simple program that finds all possible defect hole locations for a hexagonal close-packed lattice within a given defect region, beginning with a defect hole placed in the center of the defect region. Partial holes are not considered.

1.2 FDTD simulation details

The defect hole locations are imported into a finite difference time domain (FDTD) software program utilizing subpixel averaging for increased accuracy. All units in the simulation are relative to a scale factor denoted \( a \), which is the lattice spacing between the photonic crystal air holes around the defect region. The photonic bandgap of the surrounding crystal was computed using a fully-vectorial eigenmode solver of Maxwell’s equations with periodic boundary conditions. A perfectly matched layer (PML) of one scale unit thickness \( a \) was used on the border of the simulation area, in order to prevent reflections and absorb any fields leaving the simulation area. Reflections interfering with the field in the defect region would cause inaccurate measurements of the cavity quality (Q) factor and resonance frequency. The entire simulation area is shown in Figure 1.

In this paper, we limit our analysis to two-dimensional calculations since the simulations were computationally intensive, requiring high resolution (150 grid points per scale factor \( a \)) to resolve the small defect holes within the MHD region. Mirror symmetries were implemented to effectively reduce the simulation area. The exact numbers reported in the following sections likely will not perfectly map to experiments until a complete three-dimensional analysis is completed; however, the trends will be relevant and should provide insight for future experiments and calculations. For this work, we chose to center the bandgap at the technologically relevant wavelength of 1550 nm. Given the two-dimensional analysis, the value of \( a \) was calculated to be 504.52 nm, in order to equate the central bandgap wavelength to 1550 nm.

The resonance frequency and cavity quality factor of various MHD structures were recorded by introducing a Gaussian pulse of frequency width equal to the bandgap and centered at the mid-gap frequency. For each simulation, the source was positioned in the middle of the defect region and gradually turned on in order to minimize high frequency components. The source was then shut off after 200 periods in frequency to allow the field to resonate in the cavity. The entire simulation area is shown in Figure 1.

Harmonic inversion code based on the filter diagonalization method was used to extract the frequency and quality factor of the fields remaining in defect region after the source was turned off.

1.3 Surface area

The primary advantage of the MHD photonic crystal is the increased surface area that results from the multiple holes utilized in the defect region. For example, biosensing applications require biomolecules to be immobilized on a surface. Hence, available surface area is the limiting factor for the number of molecules that can be attached. Larger numbers of immobilized biomolecules, often referred to as probe molecules, increase the likelihood of capturing and detecting the complementary biomolecules of interest, often called target molecules. Optical switching applications that rely on the attachment of an electro-optic polymer may also benefit from the increased surface area of MHD photonic crystals.

In order to quantitatively demonstrate the surface area enhancement achieved by MHD photonic crystals compared to traditional, single-hole defect (SHD) photonic crystals, the surface area for various MHD structures and SHD structures was calculated. The defect holes were generated as described at the end of section 1.1 and a photonic crystal slab thickness of 0.7\( a \) was assumed in the calculations. We evaluated MHD photonic crystals with various defect hole spacings and various defect hole radii over a range of defect region effective radii. The surface area of photonic crystals with different SHD sizes was also computed.

Figure 3 summarizes the results of the surface area calculations. The available surface area increases for increased defect effective radius and decreased defect hole spacing. For large defect effective radii, the available surface area for a MHD approaches nearly 25 times that of the single hole. Figure 4 provides schematics for many of the MHD configurations considered in Figure 3 with a defect effective radius of 0.3\( a \).
Fig. 3. Surface area in units of $a^2$ assuming device slab thickness of $0.7a$, for (a) defect radius held constant at $0.02a$ and variable defect hole spacing, and (b) relative spacing kept constant at $a_{defect\ hole} = 3r_{defect\ hole}$ with variable defect hole radius. A plot of the SHD surface area is also shown for comparison.

Fig 4. View of defect regions for generated MHDs corresponding to some of the configurations analyzed in Figure 3: defect holes with (a) radius 0.02a, spacing 0.06a, (b) radius 0.02a, spacing 0.08a, (c) radius 0.04a, spacing 0.12a, and (d) radius 0.06a, spacing 0.18a. All defects have a specified effective MHD radius of 0.3a.

2. SIMULATION RESULTS

Simulations were performed for photonic crystals with a range of defect hole dielectric constants, representing additional material added inside the defect holes for active photonic crystal applications. The defect hole radius was varied as $0.02a$, $0.04a$, and $0.06a$, with respective defect hole spacings of $0.06a$, $0.12a$, and $0.18a$. The ratio between defect hole radius and spacing was kept constant in order to keep the same effective refractive index for each defect region. Because
the effective index approximation takes into account the fraction of high and low index materials in the overall region, scaling the dimensions (defect hole size and defect hole spacing) by the same factor ensures the effective refractive index is kept constant. For these three defect hole sizes, the defect effective radius was varied as 0.2\(a\) and 0.3\(a\). In the case of defect hole spacing 0.18\(a\), only the 0.3\(a\) effective radius MHD was simulated, as a smaller defect effective radius resulted in only one defect hole by our hole generation method.

2.1 Resonance

The resonance wavelengths of each simulated MHD photonic crystal are shown in Figure 5. By using the effective medium approximation, a change in the refractive index of the defect holes results in an overall change in the defect region effective index. From a perturbation standpoint, the changing index contrast between the defect region and the surrounding photonic crystal causes the resonance state to be pushed deeper into the bandgap for increasing defect hole refractive index\(^{[22]}\). The slope of the curves shown in Figure 5, which can be taken as the sensitivity of the MHD to changes in defect hole refractive index, is found to be higher for larger defects. This is due to the fact that there is reduced surface area in smaller defects due to the presence of a smaller number of defect holes, which results in a slower change in the overall effective index of the MHD region. However, as will be shown in the next section, the higher sensitivity of the larger effective defect radius comes with the trade-off of reduced cavity quality factor.

A few aspects of the graphs in Figure 5 should be noted. First, the resonance wavelength in all cases converges to the same value at the limiting case of \(\varepsilon = 12\), which is the dielectric constant of silicon. When the dielectric constant of the defect holes is 12, then the defect holes are in fact completely filled in and become a solid defect (i.e., missing hole); in this case, the dimensions of the MHD are irrelevant. Also notable is the slight difference in resonance wavelength for MHDs with the same effective defect radius but differing defect hole size and spacing. Since the ratio of defect hole size and spacing is equivalent, and thus the effective index within the defect regions are equal, the anticipated behavior of the MHD photonic crystals should be the same. However, Figure 5 shows that the wavelength of the resonance state increases as the defect hole spacing is increased. For defect hole dielectric constant equal to that of air (\(\varepsilon = 1\)) and MHD effective radius of 0.3\(a\), the resonant state increases as 1253.00 nm, 1264.65 nm, and 1281.81 nm for 0.02\(a\), 0.04\(a\), and 0.06\(a\) defect hole radii, respectively. We account for the unexpected, slight change in defect resonance wavelength due to the method in which the defect hole positions are generated. Since defect hole positions are found only for complete holes within a specified defect effective radius, it is possible a small change in the specified effective radius will not increase the number of holes generated within the MHD region. Thus, it is possible that there is some contribution to the effective index from additional high dielectric region around the defect holes, but still within the defect effective radius. Consequently, it is possible to compensate for the slight change in defect resonance position by slightly adjusting the effective radius of the defect region in our simulations.

Fig. 5. Resonance wavelength of the MHD sensor for varied dielectric constant and defect hole radius/spacing: (a) radius 0.02\(a\), spacing 0.06\(a\), (b) radius 0.04\(a\), spacing 0.12\(a\), (c) radius 0.06\(a\), spacing 0.18\(a\).
2.2 Quality factor

While the photonic crystals with larger MHD effective radii are more sensitive to small changes in refractive index of the defect holes, it is found that the quality factor is much higher for a smaller MHD radius photonic crystal, as shown in Figure 6. The smaller number of defect holes within the smaller MHD effective radius results in a greater overall effective index within the photonic crystal defect region. Thus, the perturbation in the dielectric constant is less than that of a large MHD defect, resulting in a more tightly confined mode. While the change in quality factor due to defect hole index change is more linear in the $0.2a$ radius case, for an effective radius of $0.3a$, the quality factor increases far more rapidly at higher dielectric constants. This is due to the overall faster change in effective defect dielectric constant, as there are fewer holes for $0.2a$ and the change is more gradual. As explained at the end of section 2.1, the differences in the quality factor of MHD photonic crystals with different defect hole sizes and spacing but the same defect effective radius and effective refractive index can be accounted for by the method of generating the defect hole positions within the defect effective radius.

Based on the analysis of resonance wavelength and quality factor, a trade-off is present for the design of MHD photonic crystals. The sensitivity or quality factor of the MHD photonic crystal, or a combination of the two parameters, can be chosen as the figure of merit depending on the intended application. The defect hole radius and spacing, along with the defect region effective radius, can be adjusted to tune the desired characteristics of the photonic crystal. While high sensitivity may be advantageous for applications such as sensing, for other applications such as low threshold light emission, it may be more useful to have a cavity with higher quality factor.

![Fig. 6. Quality factor of the MHD sensor for varied dielectric constant and defect hole radius/spacing: (a) radius 0.02a, spacing 0.06a, (b) radius 0.04a, spacing 0.12a, (c) radius 0.06a, spacing 0.18a.](image)

3. CONCLUSION

We have presented a multi-hole defect, consisting of several small defect holes, that provides increased surface area within a photonic crystal point defect region compared to a single hole defect. The property of increased surface area is especially advantageous in applications such as sensing, for which the number of molecules attached in the defect region directly impacts the performance of the device. In general, the MHD can be tuned to the application at hand by changing the defect hole radius and spacing, as well as the MHD effective radius, in order to focus on a particular figure of merit such as the surface area, sensitivity, or quality factor of the device.

REFERENCES


