

# Slot defect in three-dimensional photonic crystals

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We have designed and simulated with the finite difference time domain method, an all-dielectric slot defect within a three-dimensional photonic band-gap crystal that produces a sharp defect state within the band gap showing a quality of factor exceeding 600 and field enhancement exceeding 25. At the slot defect the field at the resonance is localized in a volume smaller than  $0.15(\lambda)^3$ , far smaller than that achieved with previous defect modes in three-dimensional crystals.

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## I. INTRODUCTION

Optical cavities have been studied extensively because they can localize light in small volumes. They can have a wide range of applications such as sources, modulators, and filters. Also, the strong confinement of light is expected to have a great impact on quantum electrodynamics and enhanced nonlinear effects.<sup>1</sup>

The Purcell factor is a measure of the spontaneous emission rate enhancement of an emitter in a resonant cavity. It has been shown<sup>2</sup> that for an emitter placed at the peak of the electric field inside the cavity and the resonant frequency of the cavity equal to the peak emission frequency, the ratio of spontaneous emission rate in the cavity compared to bulk is

$$\frac{\Gamma}{\Gamma_0} = \frac{6Q}{\pi^2 V_{\text{eff}}}, \quad (1)$$

where  $Q$  is the quality factor of the cavity and it is proportional to the confinement time in units of the optical period.  $V_{\text{eff}}$  is the dimensionless effective mode volume given by

$$V_{\text{eff}} = \frac{\int \epsilon(\vec{r}) |\vec{E}(\vec{r})|^2 d^3r}{\epsilon(\vec{r}_{\text{max}}) \max[|\vec{E}(\vec{r})|^2]} \left[ \frac{2n(\vec{r}_{\text{max}})}{\lambda} \right]^3, \quad (2)$$

where  $r_{\text{max}}$  is the location of the maximum squared field,  $\mathbf{E}$  is the electric field,  $\epsilon$  is the dielectric constant, and  $n$  is the refractive index. It is apparent that increasing the quality factor  $Q$  and decreasing the mode volume  $V_{\text{eff}}$  are important for increasing the spontaneous emission rate. Cavities that can achieve both features are most favorable for micrometer size laser sources. Equations (1) and (2) are valid in the regime where the cavity mode linewidth is greater than the emission linewidth of the active element,<sup>2</sup> and the field does not vary significantly over the size of the emitter—a condition easily satisfied for atom or ion-based emitters.<sup>2</sup> The alternate regime, where the material emission linewidth is greater than the cavity resonance,<sup>3</sup> has the material emission linewidth  $Q_m$  appearing in the enhancement factor rather than the cavity  $Q$ .

Most of the effort on increasing the spontaneous emission rates has been in obtaining high  $Q$  values while their mode volumes are of the order of  $\lambda^3$  (Ref. 1). Very little attention

has been given in decreasing  $V_{\text{eff}}$ . For cavities with resonances at the near infrared, two dimensional slab photonic crystals have been used because it is much easier to fabricate them.<sup>4,5</sup> Such 2D slab photonic crystal (PhC) cavities<sup>6</sup> can achieve quality factors as high as  $10^7$  with measured quality factors of 800000 (Ref. 7).

Recently,<sup>2</sup> a study of a slot waveguide embedded in a photonic band-gap crystal have shown that very small effective mode volumes can be achieved in dielectric optical cavities. In particular they used dielectric discontinuities with subwavelength dimensions as a way of localizing the field. They calculated effective mode volumes ( $V_{\text{eff}}$ ) on the order of  $10^{-2}(\lambda/2n)^{-3}$  in such slot cavities. That corresponds to an increase in the Purcell factor by 2 orders of magnitude relative to the previous photonic crystal cavities without the slots.

More recent calculations have shown that the electric field in the air gap between two Si microdisks can be enhanced by several hundred times relative to the incident electric field.<sup>8</sup> They also showed that there is an increase in the field enhancement as the distance between the microdisks decreases. These are strong indications that the effective mode volume is very small in such double microdisks systems. The new feature in both these systems<sup>2,8</sup> is that all-dielectric materials are used rather than the commonly used metallic components for field enhancement in restricted geometries.

Here, we computationally study three-dimensional (3D) PhC having slot type defects. The aim of this study is to find such defects that can localize light in very small areas with ultrasmall effective mode volumes. That can be achieved by creating sub-wavelength-sized slots with dielectric constant discontinuities and ensuring that the defect modes have an electric-field distribution perpendicular to those discontinuities. In contrast to the quasi-one-dimensional photonic crystals studied before,<sup>2</sup> the present photonic crystals can have almost unlimited theoretical  $Q$  values because in 3D photonic crystals,  $Q$  increases exponentially as the size of the crystal increases. It should be pointed out though that 3D PhC require many fabrication steps and that it increases the effort and costs as one compares them with the two-dimensional (2D) slab PhC. For those reasons, the maximum thickness of 3D PhC fabricated in the near infrared (IR) region is just a few unit cells.<sup>9</sup>

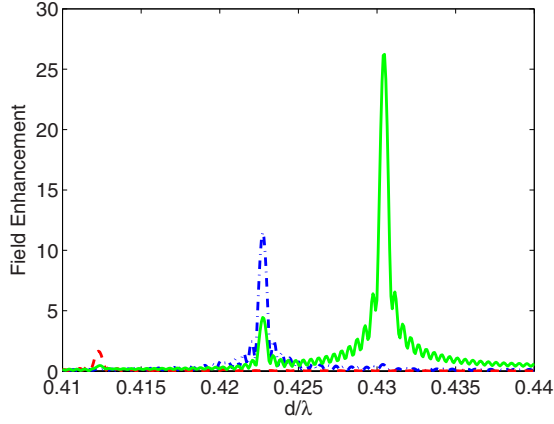


FIG. 1. (Color online) The  $x$ ,  $y$ , and  $z$  components (blue/dark gray, red/gray, and green/light gray lines, respectively) of the electric field in the middle of the slot defect are shown as a function of  $d/\lambda$ .  $d$  is the separation of the rods within the plane and  $\lambda$  is the wavelength in air.

## II. RESULTS AND DISCUSSIONS

The finite difference time domain (FDTD) method has been used. The 3D photonic crystal has a layer-by-layer structure<sup>10,11</sup> made up of alumina rods (refractive index of 3). In each layer the separation between the rods is  $d$ . The rods have a square cross section with width of  $0.3d$  and a filling ratio of 30%. The present photonic crystal has a full band gap from  $d/\lambda=0.392$  to  $0.464$  (Ref. 12).

The following results can be scaled appropriately to any dimensions including the near infrared region where most of the optoelectronic devices operate. Also, materials such as silicon and GaAs, commonly used in optoelectronics, are expected to have similar behavior as the alumina studied here because their refractive indices have similar values. In the FDTD calculations, the grid size used was  $dx=dy=0.05d$  for the in-plane axes ( $x$  and  $y$ ) and  $dz=0.025d$  along the stacking direction ( $z$  axis). The 3D photonic crystal used in the calculations consisted of 10 unit cells in the  $x$  and  $y$  direction and 5 unit cells (20 layers) in the  $z$  direction. A plane-wave incident from the  $z$  axis with  $x$  and  $y$  polarization has been used to excite the resonances.

The slot defect is made in two steps. First a material is added in the middle of the photonic crystal having a width,  $w_d$ , length,  $l_d$ , and thickness,  $t_d$ , along the  $x$ ,  $y$ , and  $z$  directions, respectively. Then, a slot is created in the middle of the added material of thickness  $t_s$  along the  $z$  direction and of the same width and length as the added material defect.

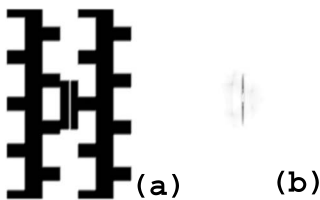


FIG. 2. (a) The dielectric constant and (b) the electric-field intensity in the  $yz$  cross section of the PC. Horizontal and vertical axes are the  $z$  and  $y$  directions, respectively.

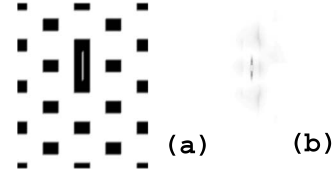


FIG. 3. (a) The dielectric constant and (b) the electric-field intensity in the  $xz$  cross section of the PC. Horizontal and vertical axes are the  $z$  and  $x$  directions, respectively.

Figure 1 shows the electric field in the middle of the slot defect with  $w_d=0.7d$ ,  $l_d=d$ ,  $t_d=0.7d$ , and  $t_s=0.025d$ . There are three resonances inside the band gap at  $d/\lambda=0.412$ ,  $0.4232$ , and  $0.4305$ . The resonance at  $d/\lambda=0.4305$  has the electric field predominantly along the  $z$  axis. That means that the electric field inside the slot is predominantly polarized vertically to the walls of the slot. This is similar with the quasi-one-dimensional photonic crystal case studied before.<sup>2</sup> The  $Q$  factor is higher than 600, with a field enhancement exceeding 25.

The intensity of the electric field at  $d/\lambda=0.4305$  resonance is shown in Figs. 2–4. Both the  $xz$  and  $yz$  cross sections show that the electric field is mostly concentrated inside the slot (see Figs. 2 and 3). The  $xy$  cross section (Fig. 4) shows the field inside the slot. The field is mostly localized in the center of the defect [not shown in Fig. 4(a) since the dielectric constant inside the slot is one] between the two regular rods.

The resonant frequency increases when the slot thickness is increased. In particular for  $t_s/d=0.025$ ,  $0.05$ ,  $0.075$ , and  $0.1$  (and holding the other dimensions constant at the values above) the resonant frequency is  $d/\lambda=0.4305$ ,  $0.4382$ ,  $0.4441$ , and  $0.4494$ , respectively. Calculations also show that decreasing  $l_d$ , the resonance moves to higher frequencies. For  $l_d/d=1.4$ ,  $1$ , and  $0.6$  mm, the resonance frequency is  $d/\lambda=0.4257$ ,  $0.4305$ , and  $0.4469$ , respectively. Also, decreasing  $w_d$ , the resonance frequency increases. For  $w_d/d=0.7$ ,  $0.5$ ,  $0.3$ , and  $0.1$ , the resonance frequency is  $d/\lambda=0.4305$ ,  $0.4348$ ,  $0.4426$ , and  $0.4617$ , respectively.

A parameter that shows the high localization of the electric field inside the slot is the mode volume  $V_{\text{eff}}$ . It is shown that the dimensionless mode volume (Fig. 5) decreases almost linearly as the thickness of the slot decreases reaching a value of 0.115 at  $t_s/d=0.025$ . It is expected that the effective mode volume will become even smaller as  $t_s$  decreases further.

The slot defects discussed here are slightly more difficult to fabricate compared to the other type of defects. In particular, the fabrication of the layer, where the slot is located, can be done in three steps instead of one.

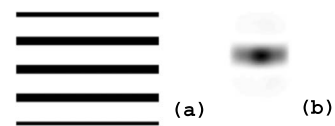


FIG. 4. (a) The dielectric constant and (b) the electric-field intensity in the  $xy$  cross section of the PC. Horizontal and vertical axes are the  $y$  and  $x$  directions, respectively.

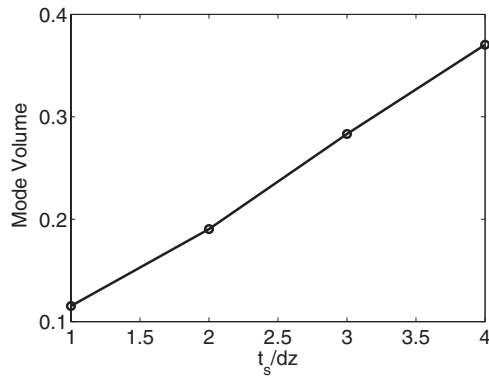


FIG. 5. The dimensionless mode volume [integral in Eq. (1)] is shown as a function of the slot thickness,  $t_s$ . The grid size along the  $z$  axis,  $dz/d=0.025$ .

Slot defects in PhCs can be used as lasers with special design. As we mentioned earlier, the slot defects are based on the discontinuity of the normal component of the electric field along the surface of the slot. In order to have that type of defects, the refractive index of the material inside the slot has to be lower than the surrounding material. In the present design we used air inside the slot and  $\epsilon=9$  for the surrounding material. A possible laser structure could have a  $\text{SiO}_2$  or  $\text{Al}_2\text{O}_3$  inside the slot and Si or GaAs as a surrounding material. In that case, the material within the slot has to be

doped with an active material (e.g., Er) in order to be able to lase.

### III. CONCLUSIONS

In conclusion, we have designed and simulated an all-dielectric slot defect within a three-dimensional photonic band-gap crystal. The fields are remarkably enhanced within the air cavity of the slot by a factor exceeding 25. We show that light can be localized in volumes smaller than  $0.15(\lambda)^3$  far smaller than the wavelength. These mode volumes are considerably smaller than those typically found for defects in 3D photonic crystals. These results can be scaled down to smaller dimensions associated with infrared and optical wavelength photonic crystals. In general, the requirements for making defects with such small effective mode volumes are: first, to create sub-wavelength-size dielectric constant discontinuities and, second, to find such defects with their electric-field distribution perpendicular to those discontinuities.

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<sup>1</sup>J. Vahala, *Nature (London)* **424**, 839 (2003).

<sup>2</sup>J. T. Robinson, C. Manolatou, L. Chen, and M. Lipson, *Phys. Rev. Lett.* **95**, 143901 (2005).

<sup>3</sup>R. Coccioli, M. Boroditsky, K. W. Kim, Y. Rahmat-Samii, and E. Yablonovitch, *IEEE Proc.: Optoelectron.* **145**, 391 (1998).

<sup>4</sup>Y. Akahane, T. Asano, B. S. Song, and S. Noda, *Nature (London)* **425**, 944 (2003).

<sup>5</sup>T. Yoshie, J. Vuckovic, A. Scherer, H. Chen, and D. Deppe, *Appl. Phys. Lett.* **79**, 4289 (2001).

<sup>6</sup>B. S. Song, S. Noda, T. Asano, and Y. Akahane, *Nat. Mater.* **4**, 207 (2005).

<sup>7</sup>E. Kuramochi, M. Notomi, S. Mitsugi, and T. Watanabe, *Appl.*

*Phys. Lett.* **88**, 041112 (2006).

<sup>8</sup>M. M. Sigalas, D. A. Fattal, R. S. Williams, S. Y. Wang, and R. G. Beausoleil, *Opt. Express* **15**, 14711 (2007).

<sup>9</sup>S. Y. Lin, J. Fleming, R. Biswas, M. M. Sigalas, K. M. Ho, B. K. Smith, D. L. Hetherington, W. Zubrzycki, S. R. Kurtz, and Jim Bur, *Nature (London)* **394**, 251 (1998).

<sup>10</sup>K. M. Ho, C. T. Chan, C. M. Soukoulis, R. Biswas, and M. Sigalas, *Solid State Commun.* **89**, 413 (1994).

<sup>11</sup>E. Ozbay, G. Tuttle, J. S. McCalmont, M. Sigalas, R. Biswas, C. M. Soukoulis, and K. M. Ho, *Appl. Phys. Lett.* **67**, 1969 (1995).

<sup>12</sup>P. Kohli, C. Christensen, J. Muehlmeier, R. Biswas, G. Tuttle, and K.-M. Ho, *Appl. Phys. Lett.* **89**, 231103 (2006).