# Analysis of Microcavities on Two-Dimensional Photonic Crystals

Dan Zhang, <sup>#</sup>Kiyotoshi Yasumoto, Hongting Jia Department of Computer Science and Communication Engineering, Kyushu University 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan zhang@green.csce.kyushu-u.ac.jp, yasumoto@csce.kyushu-u.ac.jp, jia@csce.kyushu-u.ac.jp

## **1. Introduction**

Photonic crystals are periodic dielectric or metallic structures in which the periodicity is of the order of the wavelength of light. When a point defect is introduced into a photonic crystal, a microcavity is formed and the energy of light is trapped into a small area around the defect. By making use of the coupling of the point defects to line defects forming photonic crystal waveguides, a variety of passive optical devices can be comprised and integrated in a small volume. During the past decay, the mode resonance or mode guidance in photonic crystals with point or line defects have been extensively investigated using various analytical or numerical approaches. In this paper, we shall analyze the resonant modes of microcavities formed by a point defect on a twodimensional photonic crystal, using a Fourier series expansion method [1] combined with perfectly matched layers (PMLs). The numerical examples are compared with those [2] computed by the FDTD method based on a supercell approximation. It is shown that the present method provides stable and convergent solutions to the resonance frequency and quality factor Q of the cavity. Although only the TE mode is discussed here, the TM mode case can be treated in a similar way.

### 2. Formulation

We consider a two-dimensional dielectric waveguide which is uniform in the x and z directions as shown in Fig. 1(a). The waveguide is characterized by a function n(y) of the refractive index. To use the Fourier series expansion, the waveguide is bounded by the PMLs with a thickness w at a proper distance away from the guiding region, and an array of waveguides which repeat the same configuration with a period  $\Lambda$  in the y direction is assumed. The original waveguide is approximated by a unit cell of the waveguide array located in  $0 \le y \le \Lambda$ . Assuming the propagation of a two-dimensional TE wave, the Maxwell equations are written as follows:

$$v(y)\frac{\partial}{\partial y}E_z = ik_0\tilde{H}_x, \quad \frac{\partial}{\partial x}E_z = -ik_0\tilde{H}_y, \quad \frac{\partial}{\partial x}\tilde{H}_y - v(y)\frac{\partial}{\partial y}\tilde{H}_x = -ik_0n^2(y)E_z \tag{1}$$

where  $\tilde{H}_{x(y)} = \sqrt{\mu_0 / \varepsilon_0} H_{x(y)}$ , and  $v(y) = [1 + i\sigma(y)]^{-1}$  denotes the stretched coordinate variable [1]





characterizing the assumed PMLs. Under the fictitious periodicity of the system, the electric and magnetic fields are approximated by the truncated Fourier series as follows:

$$E_{z} = \sum_{m=-M}^{M} e_{z,m}(x) e^{i\alpha_{m}y}, \quad \tilde{H}_{y} = \sum_{m=-M}^{M} \tilde{h}_{y,m}(x) e^{i\alpha_{m}y}, \quad \tilde{H}_{x} = \sum_{m=-M}^{M} \tilde{h}_{x,m}(x) e^{i\alpha_{m}y}$$
(2)

where  $\alpha_m = 2m\pi / \Lambda$ . Substituting (2) into (1) and using the orthogonallity of the Fourier bases, a set of linear equations for the Fourier coefficients  $\{e_{z,m}(x)\}$  and  $\{\tilde{h}_{y,m}(x)\}$  are derived as follows:

$$\frac{\partial^2}{\partial x^2} \mathbf{e}_z(x) = -k_0^2 \mathbf{C} \cdot \mathbf{e}_z(x), \quad \tilde{\mathbf{h}}_y(x) = i \frac{1}{k_0} \frac{\partial}{\partial x} \mathbf{e}_z(x)$$
(3)

with

$$\mathbf{e}_{z}(x) = \begin{bmatrix} e_{z,-M} & \cdots & e_{z,0} & \cdots & e_{z,M} \end{bmatrix}^{T}, \quad \tilde{\mathbf{h}}_{y}(x) = \begin{bmatrix} \tilde{h}_{y,-M} & \cdots & \tilde{h}_{y,0} & \cdots & \tilde{h}_{y,M} \end{bmatrix}^{T}$$
(4)

$$\mathbf{C} = \mathbf{N} - (\mathbf{V}\mathbf{A})^2, \quad [\mathbf{N}]_{mm'} = \frac{1}{\Lambda} \int_0^{\Lambda} n^2(y) e^{-i(\alpha_m - \alpha_{m'})y} dy$$
(5)

$$[\mathbf{V}]_{mm'} = \frac{1}{\Lambda} \int_0^{\Lambda} v(y) e^{-i(\alpha_m - \alpha_{m'})y} dy, \quad [\mathbf{A}]_{mm'} = \frac{\alpha_m}{k_0} \delta_{mm'}$$
(6)

where  $\delta_{nm'}$  is the Kronecker's delta. The eigenvalues  $\kappa_n$   $(n = 1, 2, \dots 2M + 1)$  of matrix **C** and the eigenvectors  $\mathbf{p}_n$  determine the propagation constant  $\beta_n = \sqrt{\kappa_n}$  and the field distributions for guided and radiation modes in the assumed waveguide. The solutions to (3) are expressed as follows:

$$\begin{bmatrix} \mathbf{e}_{z}(x) \\ \tilde{\mathbf{h}}_{y}(x) \end{bmatrix} = \mathbf{F}\mathbf{U}(x-x') \cdot \mathbf{a}(x'), \quad \mathbf{F} = \begin{bmatrix} \mathbf{P} & \mathbf{P} \\ -\mathbf{P}\mathbf{B} & \mathbf{P}\mathbf{B} \end{bmatrix}, \quad \mathbf{U}(x) = \begin{bmatrix} \mathbf{U}^{+}(x) & \mathbf{0} \\ \mathbf{0} & \mathbf{U}^{-}(x) \end{bmatrix}$$
(7)

with

$$\mathbf{P} = [\mathbf{p}_1 \ \mathbf{p}_2 \cdots \mathbf{p}_{2M} \ \mathbf{p}_{2M+1}], \quad \mathbf{U}^{\pm}(x) = [\mathbf{e}^{\pm i k_0 \beta_n x} \ \delta_{nn'}], \quad \mathbf{B} = [\beta_n \delta_{nn'}]$$
(8)

$$\mathbf{a}(x) = [\mathbf{a}^{+}(x) \ \mathbf{a}^{-}(x)]^{T}, \quad \mathbf{a}^{\pm}(x) = [a_{1}^{\pm}(x) \ a_{2}^{\pm}(x) \ \cdots \ a_{2M}^{\pm}(x) \ a_{2M+1}^{\pm}(x)]$$
(9)

where  $Im\{\beta_n\} \ge 0$ ,  $\{a_n^{\pm}(x)\}$  denote the amplitudes of the forward and backward propagating *n*-th modes. The eigenmode field representation based on the Fourier series is efficiently applied to various problems in dielectric waveguides. Figure 1(b) shows a two step discontinuities where waveguides *j*-1, *j*, and *j*+1 are connected at  $x = x_j$  and  $x = x_{j+1}$ . In each waveguide section, the solutions to (1)-(3) are given by (7)-(9). The boundary conditions for  $E_z$  and  $H_y$  at each step-discontinuity can be fulfilled by equating the Fourier coefficients  $\{e_{z,m}(x)\}$  and  $\{\tilde{h}_{y,m}(x)\}$  in both sides of the step. This procedure leads to the scattering matrix  $\mathbf{S}_j$  defined at the interface  $x = x_j$  as

$$\begin{bmatrix} \mathbf{a}_{j-1}^-(x_j-0)\\ \mathbf{a}_j^+(x_j+0) \end{bmatrix} = \mathbf{S}_j \cdot \begin{bmatrix} \mathbf{a}_{j-1}^+(x_j-0)\\ \mathbf{a}_j^-(x_j+0) \end{bmatrix}$$
(10)

where

$$\mathbf{S}_{j} = \begin{bmatrix} \mathbf{R}_{j}^{-} & \mathbf{T}_{j} \\ \mathbf{T}_{j} & \mathbf{R}_{j}^{+} \end{bmatrix} = \begin{bmatrix} \mathbf{P}_{j-1} & -\mathbf{P}_{j} \\ \mathbf{P}_{j-1}\mathbf{B}_{j-1} & \mathbf{P}_{j}\mathbf{B}_{j} \end{bmatrix}^{-1} \begin{bmatrix} -\mathbf{P}_{j-1} & \mathbf{P}_{j} \\ \mathbf{P}_{j-1}\mathbf{B}_{j-1} & \mathbf{P}_{j}\mathbf{B}_{j} \end{bmatrix}.$$
 (11)

Using the scattering matrix  $\mathbf{S}_{j+1}$  at the interface  $x = x_{j+1}$  defined in the same way and taking into account the modes propagation over the distance  $x_{j+1} - x_j$ , the generalized scattering matrix  $\overline{\mathbf{S}}_{j+1}$  which relates  $[\mathbf{a}_{j-1}(x_j-0) \ \mathbf{a}_{j+1}(x_{j+1}+0)]^T$  and  $[\mathbf{a}_{j-1}(x_j-0) \ \mathbf{a}_{j+1}(x_{j+1}+0)]^T$  can be obtained. If the waveguide changes continuously in the *z* direction, the transition section is approximated by a series of large number of step-discontinuities and this process of calculation [3] is repeatedly used.

#### **3.** Analysis of Microcavity

The cross sectional view of a microcavity on a two-dimensional photonic crystal and the coordinate system are shown in Fig. 2(a). The crystal consists of an  $(2L_x + 1) \times (2L_y + 1)$  array of circular dielectric rods located on a square lattice of length *h* in free space. The radius and relative permittivity of the rods are *r* and  $\varepsilon_r$ , respectively. A point defect is introduced into the crystal by modifying the radius  $r_0$  and the relative permittivity  $\varepsilon_{r,0}$  of a single rod located at the centre of the crystal. The crystal is bounded in the *y* direction by the PMLs discussed in the preceding section. To apply the proposed method, each circular rod is divided into an enough number of thin parallel

rectangular rods and the unit cell of the crystal in the *x* direction is replaced by a cascade connection of  $2L_y + 1$  layered parallel planar waveguides. Taking into account the periodicity and symmetry, the whole system is divided into three sections as shown in Fig. 2(b). Let **R** and **T** be the reflection and transmission matrices of the section *II* located in  $|x| \le h/2$  which are viewed from the plane  $x = \pm h/2 \pm 0$ ,  $\overline{\mathbf{R}}_{L_x}$  be the generalized reflection matrix [3] of the  $L_x$  layered arrays *I* and *III* viewed from the same reference planes, and  $\mathbf{a}^{\pm}(\pm h/2)$  be the amplitude vectors of the forward and backward propagating modes at  $x = \pm h/2$ . Then the boundary conditions lead to the relations:

$$\mathbf{a}^{+}(h/2) = \mathbf{T} \cdot \mathbf{a}^{+}(-h/2) + \mathbf{R} \cdot \mathbf{a}^{-}(h/2), \quad \mathbf{a}^{-}(-h/2) = \mathbf{R} \cdot \mathbf{a}^{+}(-h/2) + \mathbf{T} \cdot \mathbf{a}^{-}(h/2)$$
(12)

$$\mathbf{a}^{-}(h/2) = \overline{\mathbf{R}}_{L_{x}} \cdot \mathbf{a}^{+}(h/2), \quad \mathbf{a}^{+}(-h/2) = \overline{\mathbf{R}}_{L_{x}} \cdot \mathbf{a}^{-}(-h/2).$$
(13)

From (12) and (13) the characteristic equations for the resonant modes are obtained as follows:

$$\det[\mathbf{R}_{L_x}(\mathbf{R} + \mathbf{F}) - \mathbf{I}] = 0 \quad \text{for even modes with } \mathbf{a}^+(h/2) = \mathbf{a}^-(-h/2) \tag{14}$$

$$\det[\overline{\mathbf{R}}_{L_x}(\mathbf{R}-\mathbf{F})+\mathbf{I}] = 0 \quad \text{for odd modes with } \mathbf{a}^+(h/2) = -\mathbf{a}^-(-h/2). \tag{15}$$

Since **R**, **T**, and  $\overline{\mathbf{R}}_{L_x}$  are systematically obtained as functions of the frequency  $\omega$  using the method discussed in the preceding section, the resonant frequency  $\omega = \omega_0 + i\sigma$  and the quality factor  $Q = \omega_0 / 2\sigma$  of the microcavity can be calculated from (14) and (15).

Equation (14) was used to compute the resonant frequency and Q of the fundamental cavity mode which is even in x and y. The lattice parameters were chosen as r = 0.2h,  $\varepsilon_r = 11.56$ ,  $r_0 = 0$ , and  $L_x = L_y$  where a single rod located at the centre of  $(2L_x+1) \times (2L_y+1)$  sized crystal is removed. The PML parameters in  $\sigma(y)$  [1] are assumed to be w = h,  $\sigma_M = 8.0$ , and q = 2.1. Figure 3 shows the resonance frequency  $\omega_0$  of the fundamental cavity mode as functions of the fictitious period  $\Lambda/h$  for three different crystal sizes  $(2L_x+1)\times(2L_y+1)$ . For comparison, the results obtained without using PMLs are plotted by dotted lines. The resonance frequency calculated using the PMLs is stable for the change of the fictitious period, whereas the result obtained without using PMLs exhibits a strongly oscillatory behaviour as the fictitious period increases. This feature in the case without PMLs is due to the undesirable reflection of leakage fields from the assumed periodic boundary. The resonance frequency moves downward as the size of the crystal increases. The values of Q are shown in Fig. 4 for (a) five different crystal sizes with a fixed fictitious period  $\Lambda/h = 20$  and for two different crystal sizes (b) and (c) as functions of the fictitious period. In Fig. 4(a), for comparison, the results [2] computed by the FDTD method with a supercell approximation are plotted by the crosses. We can see from Fig.4(a) that there are noticeable differences between both Q values. It should be noted that the supercell approximation assumes a periodic boundary condition similar to the Fourier series expansion method without PMLs. Figures 4(b) and 4(c) show a stable and convergent behaviour of Q values calculated by the present method using PMLs.



Figure 2: (a) Microcavity formed by a point defect in a two-dimensional photonic crystal of  $(2L_x + 1) \times (2L_y + 1)$  square lattice and (b) Decomposition of  $2L_x + 1$  layered lattice into three subsections I, II, and III.

## Acknowledgments

This work was supported in part by the 2006 Special Coordination Funds for Promoting Science and Technology granted by the Ministry of Education, Culture, Sports, Science and Technology, Japan

## References

- [1] D. Zhang and H. Jia, "Numerical analysis of leaky modes in two-dimensional photonic crystal waveguides using Fourier series expansion method with perfectly matched layer," IEICE Trans. Electron., vol. E90-C, no. 3, March 2007 (to appear).
- [2] P. R. Villeneuve, S. Fan, and J. D. Joannopoulos, "Microcavities in photonic crystals: Mode symmetry, tenability, and coupling efficiency," Phys. Rev. B., vol. 34, no.11, pp. 7837-7842, Sept. 1996.
- [3] K. Yasumoto and H. Jia, "Modeling of Photonic Crystals by Layered Periodic Arrays of Cylinders," in *Electromagnetic Theory and Applications for Photonic Crystals*, Ed. K. Yasumoto, CRC Press, Taylor & Francis, London-New York, pp.123-190, 2005.



Figure 3: Resonance frequency  $\omega_0$  of the fundamental cavity mode as functions of the fictitious period  $\Lambda/h$  for three different crystal sizes  $(2L_x+1)\times(2L_y+1)$  where r = 0.2h,  $\varepsilon_r = 11.56$ ,  $r_0 = 0$ , and a single rod located at the centre of the crystal is removed. The results obtained without using PMLs are shown by dotted lines. *M* is the truncation number of Fourier series.



Figure 4: Quality factor Q of the fundamental cavity mode for (a) five different crystal sizes  $(2L_x+1)\times(2L_y+1)$  with a fixed fictitious period  $\Lambda/h = 20$  and for two different crystal sizes (b) and (c) as functions of the fictitious period  $\Lambda/h$ , where r = 0.2h,  $\varepsilon_r = 11.56$ ,  $r_0 = 0$ . The crosses plotted in (a) indicate the results [2] obtained by FDTD method.