Efficient and accurate analysis of photon density of states for two-dimensional photonic crystals with omnidirectional light propagation

Ruei-Fu Jao\(^1\) and Ming-Chieh Lin\(^2\)

\(^1\)School of Information Technology, Guangdong Industry Polytechnic, Guangzhou, Guangdong 510500, P. R. China
\(^2\)Multidisciplinary Computational Laboratory, Department of Electrical and Biomedical Engineering, Hanyang University, Seoul 04763, Korea

(Dated: April 3, 2018)

Omnidirectional light propagation in two-dimensional (2D) photonic crystals (PCs) has been investigated by extending the formerly developed 2D finite element analysis (FEA) of in-plane light propagation in which the corresponding band structure (BS) and photon density of states (PDOS) of 2D PCs with complex geometry configurations had been calculated more accurately by using an adaptive FEA in real space for both the transverse electric (TE) and transverse magnetic (TM) modes. In this work, by adopting a waveguiding theory under the consideration of translational symmetry, the omnidirectional PDOS corresponding to both the radiative and evanescent waves can be calculated accurately and efficiently based on the in-plane dispersion relations of both TE and TM modes within the irreducible Brillouin zone. We demonstrate that the complete band gaps shown by previous work considering only the radiative modes will be closed by including the contributions of the evanescent modes. These results are of general importance and relevance to the spontaneous emission by an atom or to dipole radiation in 2D periodic structures. In addition, it may serve as an efficient approach to identifying the existence of a complete photonic band gap in a 2D PC instead of using time-consuming 3D BS calculations.

I. INTRODUCTION

In the past three decades, photonic crystals (PCs) have attracted much attention\(^1\),\(^2\). Photonic crystals, according to the dimension of the periodicity, are divided into three categories, namely one-, two-, and three-dimensional (3D) crystals. Periodic dielectric materials are characterized by photonic band gaps (PBGs). A PBG can prohibit the propagation of electromagnetic (EM) waves whose frequencies fall within the band gap region. These materials are expected to have many applications in optoelectronics and optical communications. Controlling the optical properties of materials has become a key issue in material engineering. It was proposed that the emission of EM radiation can be modified by the environment\(^3\),\(^4\). Several environments such as metallic cavities\(^5\), dielectric cavities\(^6\), and superlattices\(^7\)–\(^12\) have been studied. The environmental effects have been described by the photon density of states (PDOS) which is related to the transition rate of the Fermi golden rule. In principle, a complete PBG along all dimensions in space can be best realized in a 3D system. However, the difficulty in fabricating such 3D crystals with PBGs in the optical regime prohibits the progression of many applications. Many studies in 2D PCs have been mainly focused on the in-plane propagation of EM waves\(^13\)–\(^18\). In our previous work\(^13\), we analyzed the in-plane light propagation in 2D PCs and demonstrated that the corresponding band structure (BS) and PDOS of 2D PCs can be calculated more accurately by using an adaptive finite element analysis (FEA) in real space for both the transverse electric (TE) and transverse magnetic (TM) modes, with even more complex geometry configurations. Various types of period structures exhibit PBGs. However, for some applications, the investigation of an omnidirectional light propagation is crucial. Previous studies showed the possibility of having omnidirectional absolute band gaps in some 2D crystal structures by adopting the off-plane wave vector \(k_z = k_0 \sin \theta\), where \(k_0 = \omega/c\)\(^3\),\(^13\),\(^20\). Theoretically, there are no band gaps for propagation in the \(z\) direction. As \(k_z\) increases, the modes decouple and the bandwidth shrinks to zero\(^19\),\(^20\).

In this work, by adopting a waveguiding theory under the consideration of translational symmetry and extending the in-plane model\(^13\), the omnidirectional PDOS corresponding to both the radiative and evanescent waves can be calculated accurately and efficiently based on the in-plane dispersion relations within the irreducible Brillouin zone\(^13\). In the following, we first provide the detailed formulations in our simulation model in which the contributions of the total PDOS from both the radiative and evanescent waves for different polarization characteristics including both the TE and TM modes can be distinguished, then the validation of our approach, and finally demonstrate that the complete band gaps shown by previous work considering only the radiative modes will be closed by including the contributions of the evanescent modes.

\* mclin@hanyang.ac.kr Also at the Institute for Pulsed Power and Microwave Technology, Karlsruhe Institute of Technology, Germany as a visiting scholar.
and the air (dielectric) region:

\[ \nabla \times \left[ \frac{1}{\mu(r)} \nabla \times \hat{E}(r) \right] - \omega^2 \varepsilon(z) \hat{E}(r) = 0 \quad (1) \]

and

\[ \nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times \hat{H}(r) \right] - \omega^2 \mu(r) \hat{H}(r) = 0, \quad (2) \]

where \( \varepsilon(r) \) and \( \mu(r) \) are the permittivity and permeability functions of the PCs, respectively, and \( \omega \) is the angular eigen-frequency. In a 2D periodic system, the dielectric function is a periodic function of the variables, Eq. (5) can be split into transverse and longitudinal parts and the problem can be simplified as solving Helmholtz’s equations in the \( xz \)-plane. We obtain

\[ \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\omega^2}{c^2} \varepsilon_a(d) - k_z^2 \right] \left\{ \begin{array}{c} \hat{E}(r) \\ \hat{H}(r) \end{array} \right\} = 0. \quad (5) \]

As the system has translational symmetry along the \( z \)-axis, we can assume the longitudinal wave functions to be a plane wave, \( exp(-i k_z z) \). By using separation of variables, Eq. (5) can be solved as:

\[ \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \left( \frac{\omega^2}{c^2} \varepsilon_a(d) - k_z^2 \right) \right] \left\{ \begin{array}{c} \hat{E}(r) \\ \hat{H}(r) \end{array} \right\} = 0, \quad (6) \]

where \( \omega_c \) is the cut-off angular eigen-frequency for the omnidirectional propagating waves. Then the corresponding dispersion relations for the omnidirectional light propagation in the 2D PCs can be determined by

\[ k_z^2 = \frac{\omega^2 - \omega_c^2}{c^2} \varepsilon_r. \quad (8) \]

To perform the 3D PDOS calculations, we construct two equifrequency regions \( \omega(k_x, k_y, k_z) = \omega \) and \( \omega(k_x, k_y, k_z) = \omega + dw \), where \( \omega \) is an arbitrary value of the angular frequency and \( dw \) is an infinitesimal increment. The differential volume element in \( k \) space is \( dV_k = dk_x dk_y dk_z \). Finally, according to the definition, the expression for the total PDOS is

\[ D(\omega) = \frac{V \mu_t \varepsilon_r}{8 \pi^2 c} \int_{\omega_c}^{\omega} \frac{\omega}{\sqrt{\omega^2 - \omega_c^2}} dk_x dk_y, \quad (9) \]

where \( V \) is the volume of the system in real space and \( \mu_t = 1 \) for nonmagnetic material.
III. RESULTS AND DISCUSSION

The omnidirectional PDOS can be obtained by employing Eq. (9) in which we perform a numerical integration of the 2D in-plane dispersion relations, Eq. (7). According to the waveguiding theory, the contributions to the total PDOS from both the TE and TM modes can be considered and calculated independently, so that the polarization characteristics of PDOS can be distinguished. In addition, using the formulation of the critical angle from Snell’s law, the PDOS of the radiative \( \cos^{-1}(\omega_c/\omega) \leq \sin^{-1}(\varepsilon_a/\varepsilon_d)^{1/2} \) and evanescent \( \cos^{-1}(\omega_c/\omega) > \sin^{-1}(\varepsilon_a/\varepsilon_d)^{1/2} \) modes can be calculated separately while performing the numerical integration. One should note that the in-plane dispersion relations, Eq. (7), are calculated using the adaptive finite element method (FEM) in real space which had been demonstrated to be very accurate [13]. Therefore, as the calculation of total 3D PDOS for a two-dimensional photonic crystal is based on the adaptive FEM and numerical integration, the accurate evaluation of the 3D PDOS in our extended model is justified.

In order to validate the extended model, we consider the omnidirectional light propagation in an inhomogeneous, linear, and nonmagnetic medium and employ a 2D PC model with a triangular lattice of air cylinders etched into silicon \((\varepsilon_r = 11.90)\) at a filling ratio of 67% as used in Ref. [20]. Both these calculations are carried out using the plane wave expansion method (PWEM) in real space [21], similar to the schematic shown in Fig. 1(a). Figure 2 shows the comparisons of 3D total PDOS of the 2D PC calculated using the FEM and PWEM, represented by the black solid line and the green open circles, respectively. As one can see, the 3D total PDOS calculated by our method is contributed from both the radiative (red dotted line) and evanescent (blue dashed line) modes. The PBG calculated by the FEM for the off-plane or omnidirectional radiative waves ranges from 0.395(2\(\pi c/a\)) to 0.399(2\(\pi c/a\)) while that for the in-plane case ranges from 0.382(2\(\pi c/a\)) to 0.400(2\(\pi c/a\)) [13].

On the other hand, the FEM can be easily adapted to solve problems of great complexity and unusual geometry. The eigenvalues can be accurately and efficiently calculated no matter how complex the geometric structures are, as demonstrated in our previous work [13]. Based on the finite-element analysis of the in-plane dispersion relations of the 2D PCs in the irreducible Brillouin zone, the 3D total PDOS of a 2D PC can be calculated more accurately and efficiently by extending our previous model with the waveguiding theory to consider omnidirectional or off-plane light propagation. In Fig. 2, the PBG calculated by the FEM for the off-plane or omnidirectional radiative waves ranges from 0.395(2\(\pi c/a\)) to 0.399(2\(\pi c/a\)) while that for the in-plane case ranges from 0.382(2\(\pi c/a\)) to 0.400(2\(\pi c/a\)) [12]. The PBG diminishes when one considers off-plane or omnidirectional propagation of the radiative modes. However, there is no complete PBG when one also includes the evanescent waves. For demonstration, we further consider two more cases, as illustrated in Figs. 1(a) and 1(b), respectively, including a triangular array with air cylinders etched into a dielectric \((\varepsilon_r = 12.96)\) at a filling ratio of 75% [10] and a square array with air cylinders etched into a dielectric \((\varepsilon_r = 12.96)\) at a filling ratio of 72.38% [20]. Both these two specific cases were previously studied and demonstrated to exhibit large omnidirectional PBGs. Figures 3(a) and 3(b) show our calculated 3D PDOS for the TE (purple solid lines) and TM (brown solid lines) modes of the triangular array, respectively. Figures 3(c) and 3(d) show those of the square array. The blue dashed and red
FIG. 3. 3D PDOS for (a) TE modes and (b) TM modes of a triangular array with air cylinders etched into a dielectric ($\varepsilon_r = 12.96$) at a filling ratio of 75% and for (c) TE modes and (d) TM modes of a square array with air cylinders etched into a dielectric ($\varepsilon_r = 16.00$) at a filling ratio of 72.38%. The blue dashed (red dotted) lines correspond to the PDOS of evanescent (radiative) waves. The PBGs calculated by the FEM for the radiative waves are (a) $0.310 - 0.495(2\pi c/a)$ and $0.827 - 0.834(2\pi c/a)$, (b) $0.403 - 0.434(2\pi c/a)$, (c) $0.410 - 0.487(2\pi c/a)$, and (d) $0.218 - 0.259(2\pi c/a)$ and $0.389 - 0.416(2\pi c/a)$.

As one can see, the 3D PDOS of the evanescent waves is larger than that of the radiative waves for both the TE and TM modes. Although the 3D PDOS for the TE and TM modes exhibit similar behavior, the corresponding contributions from the radiative and evanescent parts are quite different. For better understanding spontaneous emission or dipole radiation in a two-dimensional photonic crystal, one may differentiate the PDOS contributed from not only different polarizations, i.e., TE and TM modes, but also different types of waves, i.e., radiative and evanescent waves, by employing our approach.

Figure 4 shows the 3D PDOS normalized to that of the vacuum for the two cases. The blue dashed and red dotted lines correspond to the normalized PDOS of evanescent and radiative waves. The PBGs calculated by the FEM for the radiative waves in (a) and (b) range from $0.430(2\pi c/a)$ to $0.437(2\pi c/a)$ and from $0.410(2\pi c/a)$ to $0.416(2\pi c/a)$, respectively. In comparison, those calculated by the PWEM in [19] and [20] range from $0.423(2\pi c/a)$ to $0.437(2\pi c/a)$ and $0.4045(2\pi c/a)$ to $0.4197(2\pi c/a)$, respectively. Although the 3D PDOS of the radiative waves for both cases exhibit a PBG, the "complete band gaps" predicted by previous work have been closed by including the contribution of the evanescent modes. Therefore, there is no complete PBG for omnidirectional light propagation in a 2D PC if one considers both radiative and evanescent waves.

IV. CONCLUSIONS

In summary, omnidirectional light propagation in 2D photonic crystals has been investigated. The polarization characteristics including both the TE and TM modes was considered in our simulation model by extending the
formerly developed 2D finite element analysis. The contributions to the 3D total PDOS from the radiative and evanescent waves of different polarizations can be determined separately. We have carefully validated our extended model by benchmarking the results against those calculated by the well-known PWEM, resulting in good agreement. It has been demonstrated that the complete PBGs shown by previous work considering only the radiative modes will be closed by including the contributions of the evanescent modes. Therefore, a complete PBG does not exhibit in 2D PCs retaining translational symmetry in the longitudinal direction, if one considers both radiative and evanescent modes. With our approach, an omnidirectional PDOS of 2D PCs can be determined accurately and efficiently. These results are of general importance and relevance to the spontaneous emission by an atom or to dipole radiation in two-dimensional periodic structures. In addition, it may serve as an efficient approach to identifying the existence of a complete PBG in a 2D PC instead of using time-consuming 3D BS calculations.

ACKNOWLEDGMENTS

The authors would like to thank the late Prof. B. Y. Gu at the Institute of Physics, CAS and Prof. C. T. Chan at the Department of Physics, HKUST for the helpful comments, discussions, and encouragement. This work was partially supported by Guangdong Industry Polytechnic, P. R. China, under Grant No. RC201402, the research fund of Hanyang University (HY-20150000002559), and the Alexander von Humboldt Foundation of Germany.

[1] J. D. Joannopoulos, S. G. Johnson, J. N. Winn, and R. D. Meade, Photonic Crystals: Molding the Flow of Light (Princeton University Press, 2008).
[2] J. D. Joannopoulos, P. R. Villeneuve, and S. Fan, Nature (London) 386, 143 (1997).
[3] E. M. Purcell, Phys. Rev. 69, 681 (1946).
[4] D. Kleppner, Phys. Rev. Lett. 47, 233 (1981).
[5] A. O. Barut and J. P. Dowling, Phys. Rev. A 36, 649 (1987).
[6] H. Rigneault and S. Monneret, Phys. Rev. A 54, 2356 (1996).
[7] J. P. Dowling and C. M. Bowden, Phys. Rev. A 46, 612 (1992).
[8] T. Suzuki and P. K. L. Yu, Opt. Soc. Am. B 12, 570 (1995).
[9] A. Kamli, M. Babiker, A. Al-Hajry, and N. Enfati, Phys. Rev. A 55, 1454 (1997).
[10] A. S. Sánchez and P. Halevi, Phys. Rev. E 72, 056609 (2005).
[11] P. Halevi and A. S. Sánchez, Opt. Commun. 251, 109 (2005).
[12] M. C. Lin and R. F. Jao, Phys. Rev. E 74, 046613 (2006).
[13] M. C. Lin and R. F. Jao, Opt. Express 15, 207 (2007).
[14] I. A. Sukhoivanov, I. V. Guryev, J. A. Andrade Lucio, E. Alvarado Mendez, M. Trejo-Duran, M. Torres-Cisneros, Microelectronics Journal 39, 685 (2008).
[15] Y. C. Tsai, C. F. Lin, and J. W. Chang, Optical Review. 16, 347 (2009).
[16] Q. Wang, S. Stobbe, and P. Lodahl, Phys. Rev. Lett. 107, 167404 (2011).
[17] S. R. Huisman, G. Cistis, S. Stobbe, A. P. Mosk, J. L. Herek, A. Lagendijk, P. Lodahl, W. L. Vos, and P. W. H. Pinkse, Phys. Rev. B 86, 155154 (2012).
[18] E. Yeganegi, A. Lagendijk, A. P. Mosk, and W. L. Vos, Phys. Rev. B 89, 045123 (2014).
[19] Z. Y. Li and Y. Xia, Phys. Rev. B 64, 153108 (2001).
[20] T. Haas and A. Hesse, T. Doll, Phys. Rev. B 73, 045130 (2006).
[21] K. Busch and S. John, Phys. Rev. E 583896 (1998).
[22] D. P. Fussell, R. C. McPhedran, C. Martijn de Sterke, and A. A. Asatryan, Phys. Rev. E 67, 045601(R) (2003).
[23] M. M. Sigalas, R. Biswas, K. M. Ho, and C. M. Soukoulis, Phys. Rev. B 58, 6791 (1998).
[24] S. Foteinopoulou, A. Rosenberg, M. M. Sigalas, and C. M. Soukoulis, J. Appl. Phys. 89, 824 (2001).
[25] A. Rosenberg, R. J. Tonucci, and E. L. Shirley, J. Appl. Phys. 82, 6354 (1997).
[26] R. D. Meade, K. D. Brommer, A. M. Rappe, and J. D. Joannopoulos, Appl. Phys. Lett. 61, 495 (1992).
[27] H. S. Sözüer, J. W. Haus and R. Inguba, Phys. Rev. B 45, 13962 (1992).