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

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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 wave-guiding theory under the consideration of translational symmetry, the omnidirectional PDOS corresponding to both the radiative and evanescent waves can be calculated 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 three-dimensional BS calculations.

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## I. INTRODUCTION

In the past three decades, photonic crystals (PCs) have attracted much attention [1,2]. PCs, according to the dimension of the periodicity, are divided into three categories: one- (1D), two- (2D), 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 Fermi's 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. In comparison, 2D PCs are easier to fabricate while providing the possibility to control the propagation of light.

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 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 have shown 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 $k_0 = \omega/c$ [19,20]. 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 [21–26].

In order to obtain the total PDOS, the off-plane band structure has to be calculated. In addition, a higher cutoff in $k_z$, i.e., $\max(k_z) = (\omega/c)\max(\sqrt{\varepsilon_r}) > k_0$, is needed [21]. According to Snell's law, a total internal reflection can occur when an EM wave is incident from a region with a higher dielectric constant to that with a lower one. In this case, we have an evanescent wave with a corresponding imaginary in-plane wave vector in the latter region. A quantitative analysis of PDOS for 1D PCs with omnidirectional light propagation had been done using the transfer matrix method [12]. It was found that the PDOS contributed from an evanescent wave is larger than that from a radiative one, and this is consistent with the result in Ref. [10], which shows that when a dielectric layer is in the near-field region of an atom, the emission rate is greatly enhanced by the evanescent wave. The total PDOS of 2D PCs were first calculated by Busch and John [21] using the plane wave expansion method (PWEM).

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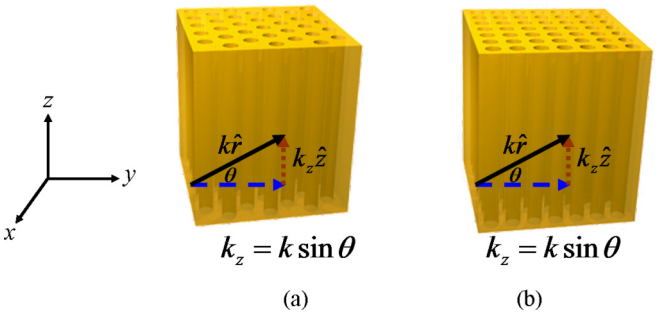


FIG. 1. Schematics of omnidirectional light propagation in 2D PCs for (a) a triangular lattice and (b) a square lattice with $k_z = k \cdot \sin\theta$ (black solid line) and the in-plane light propagation with $k_z = 0$ (blue dashed line), where $\theta$ is the off-plane incident angle.

However, the 3D dispersion relation computed by solving the full vector wave equation was very time consuming. The PWEM was further simplified and used by Li and Xia [19] and Haas *et al.* [20] to discover the "omnidirectional PGBs" considering only radiative waves. Qiu and He [27] developed an efficient finite-difference time-domain (FDTD) algorithm for computing off-plane band structure in 2D PCs as the 3D problem can be reduced to a 2D one when considering the translational symmetry and that the FDTD method is of order $N$. In spite of this, the time-stepping limit depending on $k_z$ would introduce some difficulty, either suffering a numerical instability or enforcing a tiny time step for large angle cases. Nevertheless, in these cases, one still has to solve the time-consuming eigenvalue systems or 2D FDTD updates with a fast Fourier transform (FFT) for each individual angles. Therefore, a complete band structure with all angles is difficult to obtain and an efficient method to calculate the total PDOS is still not available yet.

In this work, by adopting a wave-guiding 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 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 validate 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.

## II. FORMULATION

The propagation of light in a PC can be studied by solving Maxwell's equations. Figure 1 shows the schematics of omnidirectional light propagation in 2D PCs for (a) a triangular lattice and (b) a square lattice with $k_z = k \cdot \sin\theta$ (brown dotted line), and the in-plane light propagation with $k_z = 0$ (blue dashed line), where $\theta$ is the off-plane incident angle. For time-harmonic fields, it is convenient to use phasor notation. Maxwell's equations lead to the wave equations, or the master equations:

$$\nabla \times \left[\frac{1}{\mu(r)}\nabla \times \vec{E}(r)\right] - \omega^2\varepsilon(r)\vec{E}(r) = 0, \tag{1}$$

and

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

where $\varepsilon(r)$ and $\mu(r)$ are the permittivity and permeability functions of the PCs, respectively, and $\omega$ is the angular eigenfrequency. In a 2D periodic system, the dielectric function is a periodic function of $x$ and $y$. We assume that the materials are linear, homogeneous, isotropic, lossless, and nonmagnetic. We have

$$\varepsilon_r(x, y) = \begin{cases} \varepsilon_a, & x, y \in \text{air region} \\ \varepsilon_d, & x, y \in \text{dielectric region} \end{cases}, \tag{3}$$

where $\varepsilon_r(x, y)$ is the dielectric function profile, and $\varepsilon_a$ and $\varepsilon_d$ are the dielectric constants of the air and dielectric regions, respectively. The two master equations are reduced to two homogeneous Helmholtz's equations for the air (dielectric) region:

$$\nabla^2\begin{Bmatrix}\vec{E}(r)\\ \vec{H}(r)\end{Bmatrix} + \frac{\omega^2}{c^2}\varepsilon_{a(d)}\begin{Bmatrix}\vec{E}(r)\\ \vec{H}(r)\end{Bmatrix} = 0. \tag{4}$$

A 2D PC is periodic in two directions $(x, y)$ and homogeneous in the third one $z$. For light propagating in the system retaining translational symmetry, we can separate the modes into two independent polarizations, TM and TE modes, and consider the band structures and photon density of states accordingly. Based on the theory of wave guiding, the propagation properties of TM and TE modes can be characterized by the field components parallel to the rods or along the $z$ direction, $E_z(x, y, z)$ and $H_z(x, y, z)$, respectively. The corresponding Helmholtz's equations, the $z$ components of Eq. (4), for the air (dielectric) region can be rearranged as

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + \frac{\omega^2}{c^2}\varepsilon_{a(d)}\right]\begin{Bmatrix}E_z(x, y, z)\\ H_z(x, y, z)\end{Bmatrix} = 0. \tag{5}$$

As the system has translational symmetry along the $z$ axis, we can assume the longitudinal wave functions to be a plane wave, $\exp(-ik_z z)$. By using separation of variables, Eq. (5) can be split into transverse and longitudinal parts, and the problem can be simplified as solving Helmholtz's equations in the $xy$ plane. We obtain

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \left(\frac{\omega^2}{c^2}\varepsilon_{a(d)} - k_z^2\right)\right]\begin{Bmatrix}E_z(x, y, z)\\ H_z(x, y, z)\end{Bmatrix} = 0. \tag{6}$$

The in-plane propagation ($k_z = 0$) can be considered as a limiting case or a cutoff condition of the omnidirectional propagation ($k_z \geqslant 0$), as shown in Fig. 1. Therefore, we can solve the following 2D Helmholtz's equations for the cutoff eigenvalues:

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \left(\frac{\omega_c^2}{c^2}\varepsilon_r\right)\right]\begin{Bmatrix}E_z(x, y)\\ H_z(x, y)\end{Bmatrix} = 0, \tag{7}$$

where $\omega_c$ is the cutoff angular eigenfrequency for the omnidirectional propagating waves. Then the corresponding dispersion relations for the omnidirectional light propagation in the

2D PCs can be determined by [12]

$$k_z^2 = \frac{\omega^2 - \omega_c^2}{c^2}\varepsilon_r. \tag{8}$$

To perform the 3D PDOS calculations, we construct two equifrequency regions $\omega(k_x, k_y, k_z) = \omega$ and $\omega(k_x, k_y, k_z) = \omega + d\omega$, where $\omega$ is an arbitrary value of the angular frequency and $d\omega$ is an infinitesimal increment [12,13]. The differential volume element in $\mathbf{k}$ space is $dV_k = dk_x dk_y dk_z$ Finally, according to the definition, the expression for the total PDOS is $dN(\omega) \equiv D(\omega)d\omega$:

$$D(\omega) = \frac{V\sqrt{\mu_r\varepsilon_r}}{8\pi^3 c}\int_{\omega_k}\frac{\omega}{\sqrt{\omega^2 - \omega_c^2}}\,dk_x\,dk_y, \tag{9}$$

where $V$ is the volume of the system in real space and $\mu_r = 1$ for nonmagnetic material. One should note that Eq. (9) includes all the propagating modes if $\omega > \omega_c$. Here we can further differentiate radiative and evanescent modes by using Snell's law for a total internal reflection at the interface between the dielectric and air,

$$\begin{cases} \theta \leqslant \theta_c, & D(\omega) \in \text{radiative wave} \\ \theta > \theta_c, & D(\omega) \in \text{evanescent wave}, \end{cases} \tag{10}$$

where $\theta$ is $\cos^{-1}(\omega_c/\omega)$ and $\theta_c$ is $\sin^{-1}(\sqrt{\varepsilon_a}/\sqrt{\varepsilon_d})$.

## 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 wave-guiding 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 $[\cos^{-1}(\omega_c/\omega) \leqslant \sin^{-1}(\varepsilon_a/\varepsilon_d)^{1/2}]$ 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 [12]. 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, since the calculation of total 3D PDOS for a 2D PC is based on the adaptive FEM and numerical integration, the evaluation of the 3D PDOS in our extended model is justified. Furthermore, we should emphasize that the calculation of the in-plane dispersion relations is a one-time evaluation process, and therefore the total PDOS determination using this approach is very efficient. For all cases demonstrated here, the eigenfrequencies for 861 k-points uniformly distributed in the irreducible Brillouin zone have been calculated via the FEM approach. Due to the symmetry consideration, we effectively discretize the first Brillouin zone into 6241 and 9852 grid points for the square array and the triangular array, respectively, ensuring the fractional errors of all eigenvalues are smaller than $10^{-3}$ [13].

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

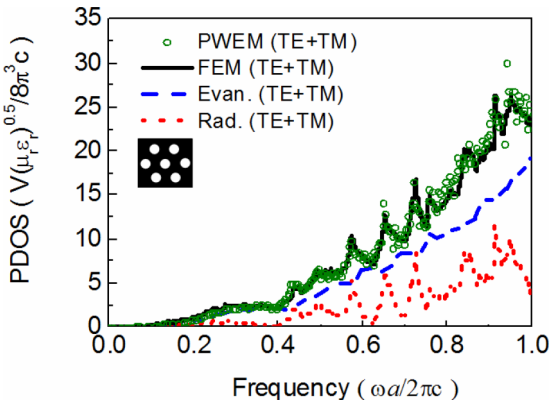


FIG. 2. Comparisons of 3D total PDOS calculated by the FEM (black solid line) and the PWEM (green open circles) for a 2D PC with a triangular lattice of air cylinders etched into silicon ($\varepsilon_d = 11.90$) at a filling ratio of 67% as used in Ref. [21]. The total PDOS is contributed from both the radiative (red dotted line) and evanescent (blue dashed line) modes. The PBG calculated by the FEM for the off-plane 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].

($\varepsilon_d = 11.90$) at a filling ratio of 67% air as calculated by the PWEM in Ref. [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, and the results showing no complete 3D PBG are in good agreement with those calculated by the PWEM. The PWEM is based on the Bloch-Floquet theorem, which states that eigensolutions of differential equations with periodic coefficients can be expressed as a product of plane waves and lattice-periodic functions. Consequently, all periodic functions are expanded into appropriate Fourier series. Inserting these expansions into the differential equation results in an infinite matrix-eigenvalue problem, which, suitably truncated, provides the eigenfrequencies and expansion coefficients for the eigenfunctions. In the framework of PWEM, the 3D total PDOS calculation is based on fully 3D PBG computations, and the Fourier coefficients are determined by integrating over the 3D Wigner-Seitz cell. Therefore, there is no decoupling of the two transverse polarizations, and the full 3D vector problem has to be solved [21]. A Fourier-based method is not only time-consuming but also suffers from several problems. For instance, the dielectric function is discontinuous, so Fourier-type expansions converge slowly. Furthermore, it was found that the discontinuous nature of the dielectric function severely limits the accuracy of the PWEM [28].

On the other hand, the FEM can be easily adapted to solve problems of great complexity and unusual geometry. The eigenvalues can be 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

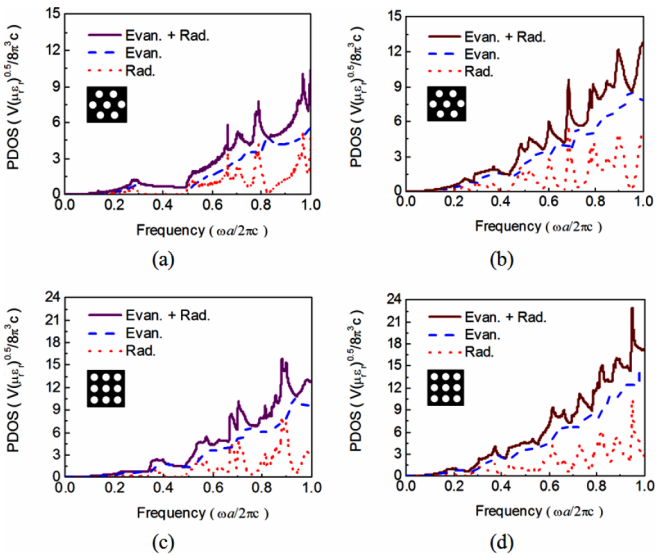


FIG. 3. 3D PDOS for (a) TE modes and (b) TM modes of a triangular array with air cylinders etched into a dielectric ($\varepsilon_d = 12.96$) at a filling ratio of 75% [19] and for (c) TE modes and (d) TM modes of a square array with air cylinders etched into a dielectric ($\varepsilon_d = 16.00$) at a filling ratio of 72.38% [20]. 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($2\pi c/a$).

can be calculated more efficiently by extending our previous model with the wave-guiding 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($2\pi c/a$) [13]. 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 ($\varepsilon_d = 12.96$) at a filling ratio of 75% [19] and a square array with air cylinders etched into a dielectric ($\varepsilon_d = 16.00$) at a filling ratio of 72.38% [20]. Both these two specific cases were previously studied and demonstrated to exhibit large omnidirectioinal 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 dotted lines correspond to the PDOS of evanescent and radiative waves. The corresponding PBGs for the radiative waves are determined as (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

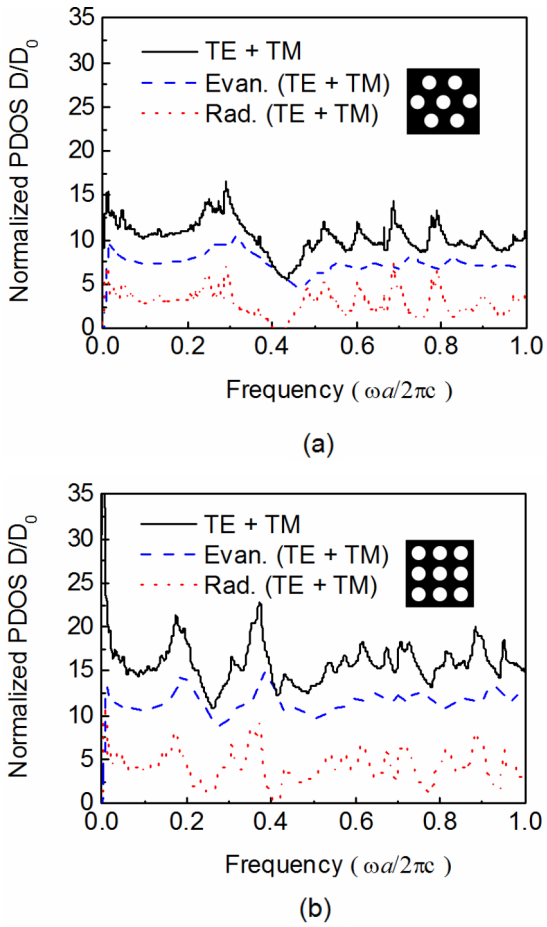


FIG. 4. 3D total PDOS (black solid lines) of (a) a triangular array and (b) a square array normalized to that of the vacuum. The blue dashed (red dotted) lines correspond to the normalized PDOS of evanescent (radiative) waves. The PBGs calculated by the FEM for the radiative waves in (a) and (b) range from 0.403($2\pi c/a$) to 0.434($2\pi c/a$) and from 0.410($2\pi c/a$) to 0.416($2\pi c/a$), respectively. In comparison, those calculated by the PWEM in Refs. [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($2\pi c/a$)

the radiative and evanescent parts are quite different. To better understand the spontaneous emission or dipole radiation in a 2D PC, 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 of both the TE and TM modes. The PBGs calculated by the FEM for the radiative waves in (a) and (b) range from 0.403($2\pi c/a$) to 0.434($2\pi c/a$) and from 0.410($2\pi c/a$) to 0.416($2\pi c/a$), respectively. In comparison, those calculated by the PWEM in Refs. [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 PCs 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 comparing the results with 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 efficiently. 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 PBG in a 2D PC instead of using time-consuming 3D BS calculations.

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