Vol 14 No 11, November 2005
1009-1963/2005/14(11)/2241-05

Chinese Physics

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Characteristics of local photonic state density in an infinite two-dimensional photonic crystal*

Zhou Yun-Song(周云松)[a], Wang Xue-Hua(王雪华)[b]†,
Gu Ben-Yuan(顾本源)[b], and Wang Fu-He(王福合)[a]

[a] *Department of Physics, Capital Normal University, Beijing* 100037, *China*

[b] *Institute of Physics, Chinese Academy of Sciences, Beijing* 100080, *China*

(Received 10 March 2005; revised manuscript received 26 May 2005)

The local density of photonic states (LDPS) of an infinite two-dimensional (2D) photonic crystal (PC) composed of rotated square-pillars in a 2D square lattice is calculated in terms of the plane-wave expansion method in a combination with the point group theory. The calculation results show that the LDPS strongly depends on the spatial positions. The variations of the LDPS as functions of the radial coordinate and frequency exhibit "mountain chain" structures with sharp peaks. The LDPS with large value spans a finite area and falls abruptly down to small value at the position corresponding to the interfaces between two different refractive index materials. The larger/lower LDPS occurs inward the lower/larger dielectric-constant medium. This feature can be well interpreted by the continuity of electric-displacement vector at the interface. In the frequency range of the pseudo-PBG (photonic band gap), the LDPS keeps very low value over the whole Wiger–Seitz cell. It indicates that the spontaneous emission in 2D PCs cannot be prohibited completely, but it can be inhibited intensively when the resonate frequency falls into the pseudo-PBG.

Keywords: local density of photonic states, two-dimensional photonic crystal, spontaneous emission
PACC: 4270Q, 7820P, 4250

The properties of atomic spontaneous emissions (ASE) strongly depend on the environment surrounding the excited atom,[1−5] and have been intensively investigated theoretically and experimentally.[6−10] The absolute photonic band gap (PBG), in which the ASE is prohibited completely, may be generated in the three dimensional (3D) photonic crystals (PCs). The features of the ASE in the 3D PCs have received deservedly wide interests and intensive investigations.[11−18]

Two-dimensional (2D) and one-dimensional (1D) PCs also have prospective applications, for instance, they may serve as the reflective mirrors, the mode selective circuits,[19,20] and the wave guides.[21−23] The properties of the ASE in the 1D and 2D PCs also attracted great interests. Local density of photonic state (LDPS) in the PCs plays a dominant role in the understanding of the properties of the ASE in the PCs. The merits of LDPS in the finite 2D PCs have been reported.[24−26] Asatryan *et al* calculated the LDPS in the finite 2D PCs consisting of the circular pillars in a square lattice[24] and triangle lattices[25] with the use of Green's function approach. They showed that the absolute PBG still may be produced in a finite 2D PC, on the contrary, the absolute PBG may be closed for an infinitely extensive 2D PC. In this case, the ASE can not be prohibited completely. Recently, McPhedran *et al* presented the connection between the mutual density of states, local density of states (LDS), spectral density of states, and the conventional density of states (DOS) in the finite PC based on Green's function.[27] The characteristics of the ASE should be significantly modified in different atomic position of the unit cell of PCs because the field distribution inside the PCs is strongly inhomogeneous, so do the LDPS and the interaction between the field and atom. In this paper, we explore the features of the distribution of the LDPS in the 2D infinite extensive PCs with the use of the plane-wave expansion method.

The typical 2D PC considered is composed of a periodic array of the rotated square pillars (with a dielectric constant $\varepsilon_{\rm a}$) of a side-length of l, setting in a 2D square lattice with the lattice constant a, as sketched in Fig.1. The dielectric pillars are embedded

*Project supported by National Key Basic Research Special Fund of China and by Natural Science Foundation of Beijing, China.
†E-mail: wangxh@aphy.iphy.ac.cn

in the background medium with a dielectric constant ε_b. Assume that the 2D PC lies on the xy plane and the axis of pillar is chosen as the z-axis, existing the z-direction translation invariance in structure. The rotating angle θ of the square pillar on the xy plane is measured with respect to the x-axis. Here, the calculation will be limited in a Wigner–Seitz cell (WSC) of this structure which is encircled by the dashed lines in Fig.1. As this WSC possesses C_4 symmetry, therefore, all the calculations of the relevant LDPS are restricted only to the first quadrant marked by the shadow area in the xy coordinate system. For convenience of discussions, we mark out several special points in the first quadrant region: O, X, M, and Y are at (0,0), (1/2, 0)a, (1/2, 1/2)a, and (0, 1/2)a, respectively. The points of p_1, p_2, p_3, and p_4 denote the intersections between the pillar edges and the lines OX, OM, and YM respectively.

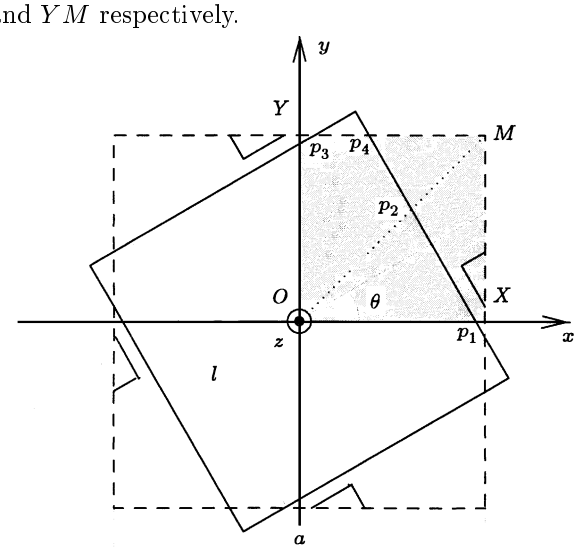


Fig.1. Sketch of Wigner–Seitz cell of the photonic crystal composed of square pillars in a square lattice. The solid lines denote the edges of pillars and dashed lines denote the boundary of Wigner–Seitz cell. Here a is the lattice constant and θ the rotating angle. The points p_1, p_2, p_3 and p_4 denote the intersections between the edges of pillar and the lines OX, OM and OY respectively. The terminal coordinates of these lines OX, OM and OY are O=(0, 0), X=(1, 0), M=(1, 1) and Y=(0, 1) in the unit of $a/2$ respectively.

The LDPS and DOS are given by[6,7]

$$\mathrm{DOS}(\omega) = \frac{1}{(2\pi)^3} \sum_n \int_{\mathrm{FBZ}} \mathrm{d}\boldsymbol{k} \delta(\omega - \omega_{n\,\boldsymbol{k}}) \quad (1)$$

and

$$\mathrm{LDPS}(\omega, \boldsymbol{r}) = \frac{1}{(2\pi)^3} \sum_n \int_{\mathrm{FBZ}} \mathrm{d}\boldsymbol{k} \, |E_n(\boldsymbol{k}, \boldsymbol{r})|^2 \times \delta(\omega - \omega_{n\,\boldsymbol{k}}), \quad (2)$$

where $\mathrm{d}\boldsymbol{k} = \mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z$ and the integral over k_x and k_y is restricted only to the first Brillouin zone (FBZ) while the special integral over k_z is limited in a range of $[-k_{z0}, k_{z0}]$, where k_{z0} corresponds to the z-direction wave number associated with a special upper limit of frequency $\omega_0(k_{z0})$. The LDPS$(\omega, \boldsymbol{r})$ will be calculated over a frequency range of $[0, \omega_0]$, where $\omega_0(k_{z0}) = \min\{\omega(k_x, k_y, k_{z0}), k_x, k_y \in \mathrm{FBZ}\}$. The eigen modes of the electric fields, $\boldsymbol{E}_n(\boldsymbol{k}, \boldsymbol{r})$, are calculated with the use of the plane-wave expansion method in a combination with the point group theory[14,15] and $\boldsymbol{k}$ runs over an irreducible Brillouin zone.

It is noted that even though the pseudo-BPG may be generated in the $k_x k_y$ domain when fixing $k_z = 0$ for a 2D PC, when considering the case of nonzero k_z, i.e., the light waves propagate out off the xy plane, the width of the existing pseudo-PBGs may be gradually decreased, and finally goes to zero, i.e., the pseudo-PBGs are completely closed. Wang *et al* have reported that the largest pseudo-PBG of $\Delta\omega = 0.063(2\pi\, c/a)$ appears at a midgap frequency of $\omega_g = 0.425(2\pi\, c/a)$ for a 2D PC composed of square air pillars (with $\varepsilon_a = 1$) in a square lattice.[28] They adopted the following parameters: the dielectric constant of the background is $\varepsilon = 12.96$, the filling fraction $f = 0.680$, the side-length of square pillars $l = \sqrt{f}a$, and the rotating angle $\theta = 30°$. Here, we employ these parameters and the PW expansion method (the number of the PWs is $N = 31 \times 31 = 961$) to calculate the pseudo-PBGs and then the LDPS. To confirm the convergence of the eigen solution, we reduce N to 441, the relative deviation is 1.99% for $\Delta\omega$ and 0.139% for ω_g. In the following calculations, the number of the PWs will be fixed as $N = 961$.

The 3D plot of the variation of the LDPS as functions of frequency and the reduced radial coordinate r (measured with the lattice constant a) along the line OX in the 3D plot is displayed in Fig.2. For clarity of observing the variation of the LDPS, we demonstrate two plots in the figure from two different view angles. The profile exhibits "mountain chain" structures with sharp peaks. It is worth pointing out that this "mountain chain" only occupies a finite area of r, for instance, beyond $p_1(r/a = 0.476)$, as marked in Fig.1, the calculated LDPS rapidly drops down to a small value. This quenching phenomenon of the LDPS always appears at the edges of the pillar. Inside the pillar, the LDPS varies smoothly.

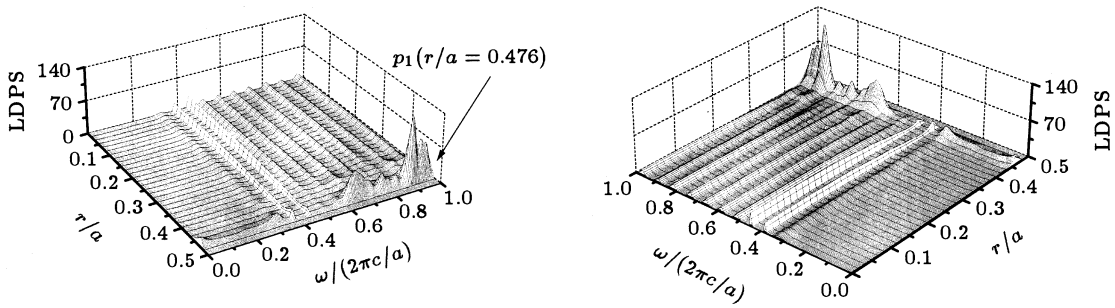


Fig.2. 3D plot of the LDPS as functions of frequency ω and the reduced radial position r along the OX line. The relevant parameters are chosen as: $\theta = 30°$, $f = 0.680$, $\varepsilon_a = 1$, and $\varepsilon_b = 12.96$.

To confirm this conclusion, we now change the azimuth angle of the radial vector and examine the LDPS distribution as functions of frequency and the reduced radial r. The calculated LDPS is displayed in Fig.3 for the case of (a) the radial vector is aimed to be parallel to line OM and (b) the end of the radial vector is moved along the line YM. It is evident that the LDPS distribution always exhibits "mountain chain" structures with a single sharp peak in each "mountain chain" of Fig.3(a) and two sharp peaks in each "mountain chain" of Fig.3(b). Two adjacent "mountain chain" are separated by a deep valley. The "mountain chain" always occupies a finite region of r, for instance, $r \in [0, p_2]$ in Fig.3(a) and $r \in [p_3, p_4]$ in Fig.3(b).

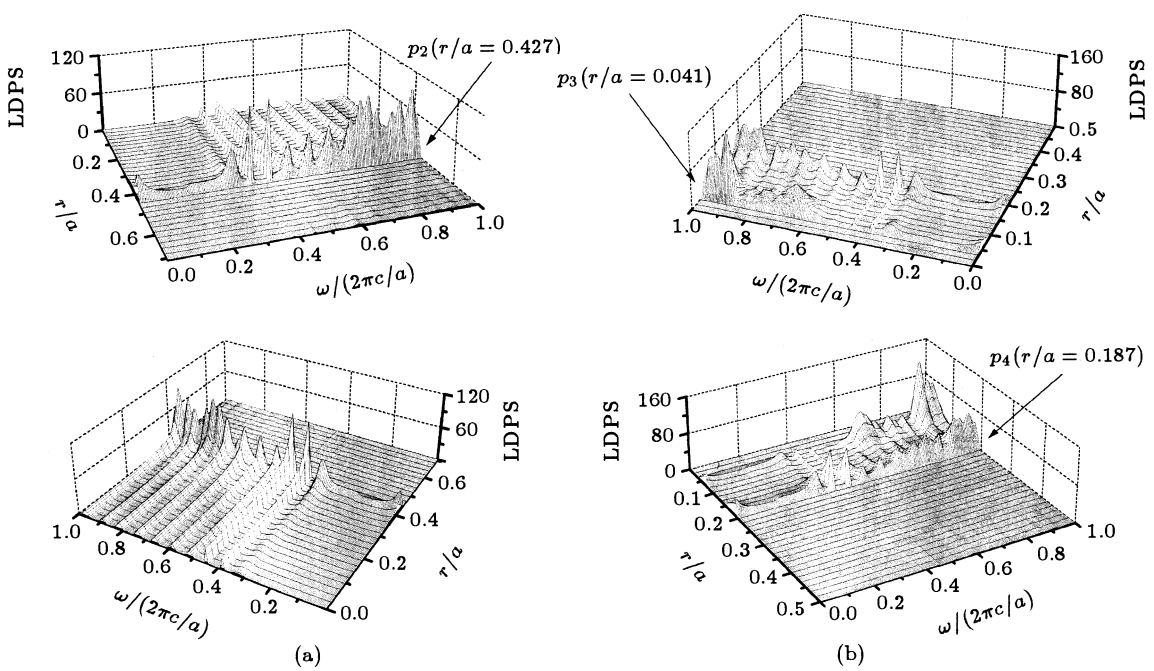


Fig.3. Same as Fig.2 except for (a) r along the OM line, (b) r along the YM line.

The quenching phenomenon of the LDPS usually occurs at the boundaries between the square pillar and the background material, for instance, at the critical points p_2, p_3 and p_4, as marked in the figures for clarity. We also choose other parameters of θ, f, ε_a, ε_b, and different directions of the radial vector to calculate the LDPS, the similar characteristics in the LDPS can be observed except for different detailed patterns.

The above result can be well interpreted from the simple physical argument: the electric displacement component normal to the interface on the xy plane must be continuous when it crosses the interface, i.e., $\varepsilon_a E_a = \varepsilon_b E_b$ at the interface, therefore, when $\varepsilon_a < \varepsilon_b$, we have $E_a > E_b$. It manifests that the larger electric field should be concentrated on the air-pillars, on the contrary, the smaller electric field appears in the di-

electric background region. Consequently the remarkable discontinuity of the electric field should take place at the interfaces. Meanwhile it is clearly known from the definition of the LDPS in Eq.(2) that the LDPS is tightly related to the modulus of the electric field distributions within a unit cell of PC. So the discontinuity of the LDPS should also take place at the interface.

The 3D LDPS discussed above is essential when investigating ASE in 3D or 2D PCs because the light would radiate in all directions. But in many cases, for 2D PCs, it is enough to calculate the partial band structures for light transmitting in xy plane. Here we would like to compare the 3D LDPS with the partial in-plane LDPS to see what difference would occur. The partial in-plane LDPS as function of ω and r along line OM is plotted in Fig.4, which is calculated with the same parameters as used in Fig.3 (a) but keeps $k_z = 0$. To compare with Fig.3(a), the similar spatial characteristic that the abrupt change presents at $r/a = 0.427$ is observed. Besides that, a frequency gap occurs in the range of about $[0.39, 0.45](2\pi\, c/a)$. This result coincides with the pseudo-PBG position reported in Ref.[28]. We may see from Fig.3(b) that, in the pseudo-PBG range of $[0.39, 0.45](2\pi\, c/a)$, the gap has disappeared though, but the LDPS keeps a very lower value which looks like a strip over all range of r. In fact, the 'strip' may be also observed from Fig.2, and Fig.3(b) in the same frequency range,which spans from inside to outside of the scatterer. This result implies that, in the pseudo-PBG range, the whole WSC will be covered by very low LDPS without 'mountain chain' or peaks again. Therefore we may believe that, the spontaneous emission in 2D PCs can not be prohibited completely, as opposed to the case in 3D PCs, but it can be inhibited intensively when the resonated frequency falls into the pseudo-PBG range.

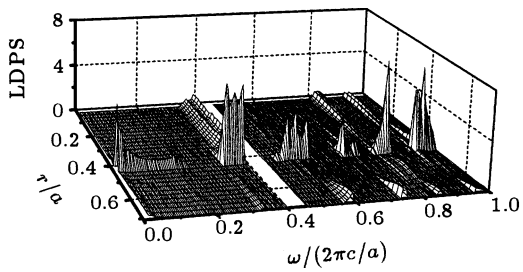


Fig.4. 3D plot of the partial in-plane LDPS as functions of frequency ω and the reduced radial position r along the OM line. which is calculated with the same parameters as used in Fig.2 but $k_z = 0$.

In summary, we have calculated the LDPS of the infinite 2D PC composed of square pillars in a square lattice with the use of PW expansion method in a combination with the point-group theory. The results show that the large LDPS always takes place near the boundary between the pillar ($\varepsilon_{\rm a}$) and background medium ($\varepsilon_{\rm b}$) and inward side of pillar when $\varepsilon_{\rm a} < \varepsilon_{\rm b}$. This feature of the spatial distribution of LDPS is closely related to the distribution of electric field of the eigen modes in the PC. The larger electric field is always condensed on the region with smaller dielectric constant and the electric field distribution varies abruptly at the boundary between the pillar and the background medium. So does the LDPS. In the frequency range of the pseudo-PBG, the LDPS with very low value spreads over all the area of WSC. It indicates that the spontaneous emission in 2D PCs can not be prohibited completely, but it can be inhibited intensively when the resonate frequency falls into the pseudo-PBG range.

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